

## Ion Mobility Spectrometry for the Detection of Explosives

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**Abstract**—Due to the major societal problems associated with explosives abuse, the detection of illicit explosives is currently an area of major research interest. Several broad categories of detection techniques are important, including imaging methods such as X-ray based technologies, the use of trained canines, and trace chemical detection utilizing various “sniffer” technologies. The last category involves indirect detection of explosives by collecting and analyzing minute quantities of vapor or particle contamination. Several technologies have been developed for this type of application, of which ion mobility spectrometry (IMS) is perhaps the most widely utilized. This technology has a number of advantageous features, including the potential ability to detect almost all explosives of interest, moderate cost, near instantaneous response time, and sensitivity in the sub-parts per billion ranges in some cases. The present paper describes basic principle, instrumentation of Ion Mobility Spectrometry (IMS), advantages, disadvantages, applications and the results.

**Key Words**—Ion Mobility Spectrometry (IMS), Explosives, ionization, drift time, membrane filter.

### I. INTRODUCTION

The ion mobility spectrometer (IMS) was introduced as an analytical instrument in the late 1960s/early 1970s by Cohen and Karasek. The principle of IMS is that a sample is being introduced in the instrument, brought into the vapor phase by flash heating, the vapor is ionised and the resulting ions are introduced into a drift tube (Figure 1). Ion mobilities are determined from ion velocities measured in the drift tube at ambient pressure and are characteristic for the analyte. Therefore, they can be used for the identification of substances. When a gaseous ion at atmospheric pressure is placed in a constant electric field, it accelerates down the field until it collides with a neutral molecule, accelerates again until it has another collision, and so forth. This chaotic sequence of accelerations and collisions at the molecular level translates into a constant ion velocity over macroscopic distances. The ratio of the ion velocity to the magnitude of the electric field is called the ion mobility, and separation of ions on the basis of mobility differences is called ion mobility spectrometry (IMS). Because it can measure ion currents below  $10^{-12}$  A, IMS is highly sensitive as a detection technique [1].

Due to the fact that explosives have only very low vapor pressures efficient sampling techniques are required to successfully detect the compounds of interest. Therefore explosive residues are "collected" either by

wiping the corresponding objects with specially treated filters, paper or even tooth picks. The entrapment of the drug micro-particles is also achieved by the utilization of a specially constructed vacuum cleaner. The particles are directly sucked on a Teflon membrane filter and evaporated at an elevated temperature in a furnace directly into the IMS system.

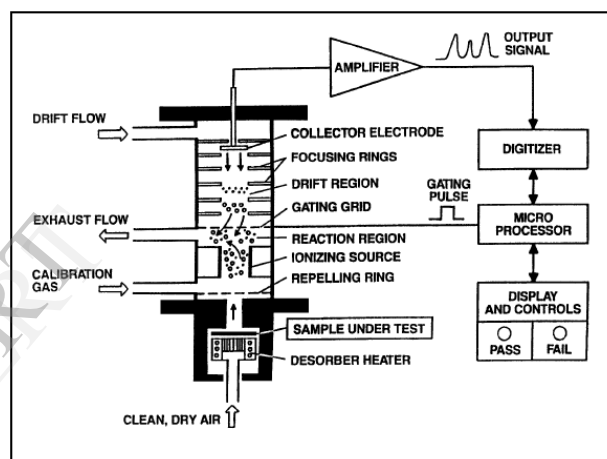


Figure 1. Schematic representation of the IMS Detection System

### II. BASIC PRINCIPLES

#### 2.1 The ion mobility spectrometer

Ion mobility spectrometry refers to the principles, practice and instrumentation for characterizing chemical substances through their gas-phase ion mobility. IMS is an analytical technique that distinguishes ionic species on the basis of the differences in the drift velocity through a gas under an applied electrostatic field. It is a sensitive technique for the detection of trace organics under atmospheric pressure conditions. Figure 1 depicts the schematic representation of the basic IMS detection system. The sample, collected for example on a membrane filter, is heated to vaporization by the desorber heater. The neutral molecules of the vapor are carried in a stream of dried, filtered, ambient air through the heated transfer line into the reaction region. Here, ionization is initiated by high-energy electrons emitted from a  $^{63}\text{Ni}$  beta-ray source. The product ions (positive or negative) are gated with a pulse width of 0.3 ms into the heated drift region for mobility analysis every  $\sim 30$  ms. Under the influence of a controlled electric field and against a counter flow of ambient air drift gas, the ions

move to the collector electrode. The drift times required by the ions to reach the collector electrode are proportional to their masses but inversely proportional to their characteristic reduced ion mobility ( $K_0$ ) [2].

### 2.2 The ion mobility spectrum

The output spectrum is generated by first forming ions from the sample and then measuring ion migration in the electric field. The selection of ionization method is important because the ions formed and the ionization efficiency depend on this choice. Once formed, each ion migrates at its own characteristic velocity down the constant electric field in the drift tube. The qualitative information from the experiment is usually reported as the spectrum of ion arrival times at the collector. The y-axis shows the ion current from the collector, and the x-axis records the arrival times of ions.

### 2.3 Ion migration

After formation, ions are accelerated in the direction of the field between collisions with drift gas molecules. The energy gained from the electric field is randomized by these collisions, and the combination of acceleration and collision results in a constant average ion velocity ( $v_d$ ) that is directly proportional to the electric field ( $E$ )[1].

$$v_d = KE \quad (2)$$

The proportionality constant  $K$  is called the ion mobility and is usually computed in units of  $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$

$$K = v_d / E = L^2 / N t_d \quad (3)$$

where  $L$  is the ion drift distance in centimeters,  $V$  is the voltage drop across  $L$ , and  $t_d$  is the time it takes the ion to traverse  $L$ .

In a review of ion mobility theory, Revercomb and Mason have given the fundamental relationship between ion mobility and collision processes at the molecular level:

$$K = (3q/16N) (2\pi/kT)^{1/2} ((m+M)/Mm)^{1/2} (1/\Omega) \quad (4)$$

Where  $q$  is the charge on the ion,  $N$  is the number density of the drift gas,  $k$  is Boltzmann's constant,  $T$  is absolute temperature,  $m$  is the mass of the ion,  $M$  is the mass of the drift gas, and  $\Omega$  is the collision cross section of the ion in the drift gas. When the instrument operating conditions are held constant (constant  $T$  and  $P$ , and thus constant  $N$ ), the mobility depends only on ion charge, reduced mass, and collision cross section:

$$K \propto q / \mu^{1/2} \Omega \quad (5)$$

Where  $\mu = mM/(m + M)$  For ions much more massive than the drift gas molecules,  $\mu$  is nearly equal to the drift gas mass  $M$ , and  $K$  varies only with  $q$  and  $\Omega$  collision cross section is determined by ion size, shape, and polarizability.

## III. INSTRUMENTATION AND OPERATION

The IMS is mainly used for on-site detection of explosives, for example at custom services and airports. The block diagram of IMS is shown in *Figure 2*. The carrier gas and the drift gas are dry, purified air, which is made from ambient air by a filtering unit in the IMS itself.

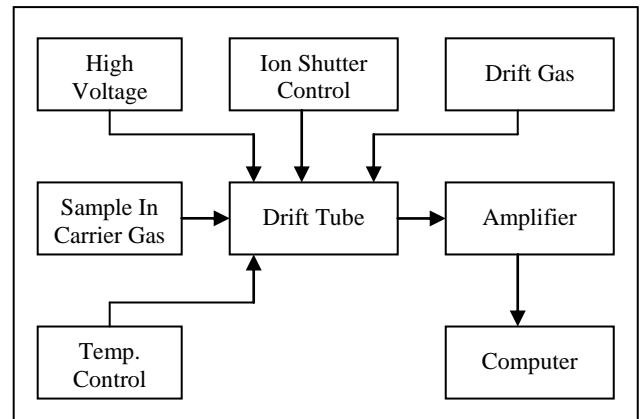


Figure2. Block diagram of Ion Mobility Spectrometry (IMS)

A number of additional components are needed to provide drift field high voltage, control the drift tube temperature and drift gas flow rate, generate timing signals for the gates, isolate gates timing signals from the high voltage of the drift field, amplify the ion signal as it arrives at the collector, and provide signal averaging or other signal processing for the amplifier output.

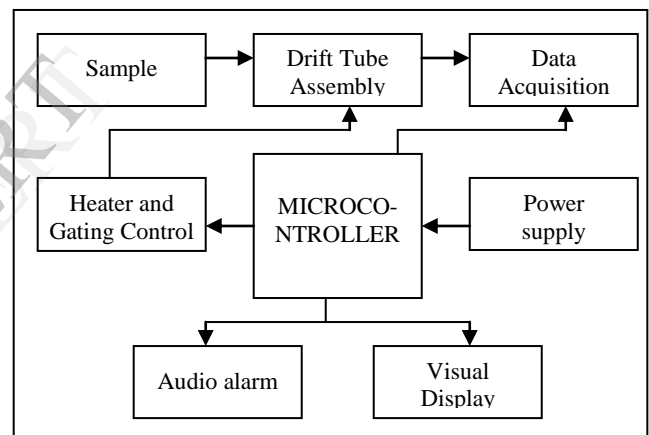


Figure3. Operational diagram

The desorbed material is swept into the detector by the carrier gas. The vapors are then ionised in the reaction region. When the gating grid opens the ions of the correct polarity can enter the drift region. They are focused and accelerated by the electric field along the drift region to arrive at the collector electrode. The collector current, of which the magnitude is proportional to the number of ions detected, is then amplified. A calibrate of known mobility is added to the drift gas to ensure that the IMS is functioning properly and to correct the  $K_0$  values for small changes in circumstances. For substances of interest the time required for the ion to drift down the tube can be programmed into the microcontroller memory [3]. The operational diagram is as in *Figure3*. The microcontroller monitors the signals at those drift times to detect the presence of target ions. When certain pre-programmed criteria are met the software then triggers an alarm. The same software also controls the gas flows and time sequences in the IMS. The operator

interacts with this software through the control panel on the detector module or through an external personal computer.

Electronic components of the spectrometer include an IMS controller, a current amplifier, a data acquisition/control system, and a temperature controller. The IMS controller was a custom-built device containing drift field high-voltage supplies, and a "gate driver". The drift field supply provided negative voltage which was variable up to -5000V. The drift tube field strength was set at 200-300 V/cm. The drift gas was dry air with a flow rate of 800 mL/min. The drift tube temperature was set at 60 or 80 °C.

### 3.1 Drift tube

The heart of the instrument is the drift tube, which provides a region of constant electric field where ions are created and allowed to migrate. In the design shown in Figure 4, the tube is built from a stack of metal guard rings separated by thin insulators; each ring is connected to a node in a string of electrical resistors. The drift tube potential was provided by a single 5000 V high-voltage supply. The current limit of the power supply was 0.5mA. At the total drift tube resistance of about 16 M $\Omega$ , only about 0.31mA was flowing through the resistor chain [4] connecting the guard rings. This arrangement provides a smooth progression of voltages from one ring to the next when a supply voltage is connected across the whole string. A steady flow of ambient pressure drift gas, usually N<sub>2</sub> or air, sweeps through the drift tube and minimizes the buildup of impurities that could otherwise react with ions and distort mobility spectra.

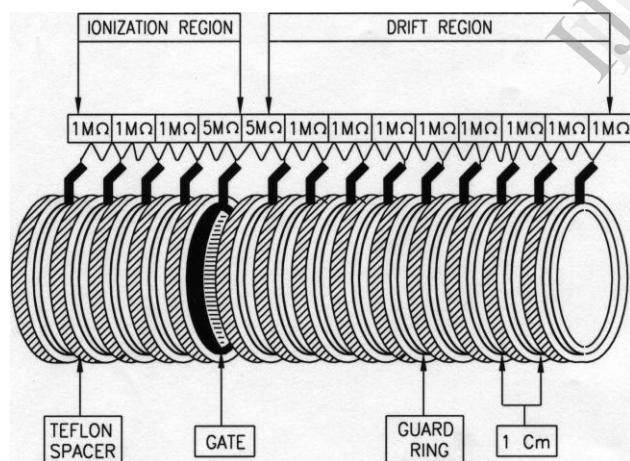


Figure4. Cut-away design of the Drift tube

### 3.2 Ion gates

Gates are used to block or pass ions traveling in the drift field. The most common design is a planar array of thin parallel wires oriented perpendicular to the ion drift. When the gate is closed, voltage on nearest-neighbor wires is  $(V_r - V_c/2)$  and  $(V_r + V_c/2)$ , where  $V_r$  is the voltage of the drift field in the plane of the gate and  $V_c$  is the gate closure voltage. When  $V_c$  is large enough, essentially all the ions are collected on the gate wires. To open the gate, the voltage on all the gate wires is pulsed to  $V_r$ .

An alternative design uses two closely positioned planar arrays. The "downstream" array (closest to the collector) is kept at a constant voltage,  $V_r$ , and the voltage on the upstream array is changed to open and close the gate. For positive ions, a voltage somewhat above  $V_r$  allows ions to pass; if the voltage is below  $V_r$ , ions are collected on the upstream array and the gate is closed.

If  $V_c$  is too small, ions can leak through the gate. On the other hand,  $V_c$  can become so large that the region immediately upstream of the gate becomes significantly depleted of ions, a condition known as the gate depletion effect. A plot of sensitivity versus  $V_c$  has a rather broad maximum where the closure electric field is 1-10 times the drift electric field.

## IV. ADVANTAGES OF IMS

The advantages of IMS are its sensitivity in the sub-pb or pg range, its continuous real time monitoring capability, its reasonable price due to instrumental simplicity and the easy automation. The excellent sensitivity of IMS is mainly due to the negligible loss of ions and neutrals to vacuum pumps, analytical flexibility, Add to this such features as long-term reliability; ruggedness for harsh environments; low maintenance without the need for consumables, paper tape or optics.

## V. DISADVANTAGES OF IMS

Slower response than IR (Infrared Spectrometry), application dependent, limited linear range. It is relatively easy to overload the IMS and, therefore, sample size must be controlled with care. Another weakness is the response variation that occurs with different background gas compositions and with different sample compositions. The reproducibility of IMS has not been studied extensively. Usually standard deviations of 5 to 25% are reported. Under similar conditions reduced mobility can be reproducible to within 1 to 2 %.

## VI. APPLICATIONS

Applications of Ion Mobility Spectrometry are in health care [5], biotechnology [6], and security [7]. IMS is limited to analyses that can be vaporised under reasonable temperature conditions without undergoing too much decomposition. Major industrial and environmental applications of IMS are the monitoring of toxic chemicals, stack gases and chemicals that are considered hazardous to man or to the environment. For the detection of contraband explosives no quantitative measurements are required. IMS is particularly suited for these applications, because of the low detection limits and the fact that it operates at atmospheric pressure. Another advantage is that results can be obtained very quickly. IMS is also used for the detection of chemical warfare agents. Other fields of applications are the semi-conductor industry (detection of surface contaminants), the identification of trees after stripping of the bark, the monitoring of macrobiotics in water, the monitoring of anesthetics in operating rooms and the sensing of petrochemical fuels in soils, as shown in

Table 1. IMS can detect a wide variety of different compounds [8]. In our research we are interested to use IMS in the detection of Explosives such as Trinitrotoluene (TNT), Nitro Esters (PETN, Nitroglycerene, Ethylene glycol Dinitrate), Ammonium Nitrate (AN), Tricyclaacetone Peroxide(TATP),Plastic Explosives-RDX(C4), PENT and HMX and Narcotics such as Cocaine, Heroine, THC, Methamphetamine, MDMA, Amphetamine, MDA, Morphineand others.

Table 1. Gases Detectable by IMS

INORGANIC & ACID GASES	Hydrogen Chloride, Hydrogen Fluoride, Chlorine, Chlorine Dioxide, Iodine, Bromine, Ammonia, Sulfur Dioxide, Sulfur Trioxide, Nitrogen Dioxide, and Hydrogen Cyanide
ORGANIC COMPOUNDS	Acids, Aldehydes, Ketones, Esters, Alcohols, Ethers, Isocyanates, Chemical Warfare Agents, Explosives, Chlorinated Compounds, Brominated Compounds, and Nitrogen, Sulfur & Phosphorous Containing Compounds

## VII. RESULTS

The explosives RDX and TNT are successfully identified using this method and the spectrums are given in Figure 5. The instrument is calibrating using the react ion peak of air. The first spectrum represents the react ion peak, TNT and RDX peaks at 10.425mSec, 15.245mSec and 18.425mSec respectively. The time delays of the peak will be depend on the drift tube length and speed of the ions. The bottom spectrum represents the react ion peak, once the explosive ions disappear, and then the react ion peak will grow up, but in the top spectrum the react ion peak almost negligible due to domination of explosive ions.

## VIII. CONCLUSION

As we look to implement a total solution for security, trace detection technologies become an integral component of that solution. Complementing X-ray scanners and metal detection, trace detection closes security loopholes by detecting microscopic particles that remain on clothing, luggage, ID cards, and more, after explosives are handled. Because it can sniff out vapors that build up in confined spaces, trace detection is especially effective for finding contraband hidden in compartments, suitcases, and lockers. IMS technology offers the advantage of detecting a wider range of targeted substances in a more flexible detector design. Therefore it is ideal for practical applications such as checkpoint security and screening vehicles, personnel, shipside, sea craft, packages, luggage, and cargo.

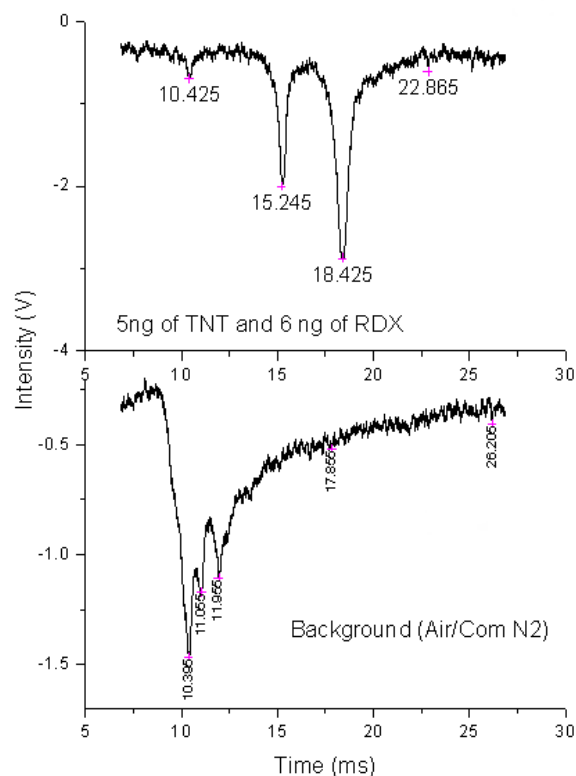


Figure 5. Spectrum of Reactant ion, RDX, and TNT Peaks

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