The Science Behind Ion Trap Mobility Spectrometry®

This paper explains and compares the different technologies that may be used to analyze the contamination and residue from explosive and narcotic substances.

Introduction

Advances in trace detection—the discovery and identification of microscopic particles and vapors emitted by explosives and narcotics—have kept pace with the increasingly complex security risks of our time. Innovative technology now makes it possible to detect a wide range of substances with greater accuracy, speed and reliability than ever before.

As a result, trace detection can now be an integral component of a total security solution. Used alone or as a complement to X-ray scanners, metal detectors and canine patrols, it can help close security loopholes by reliably detecting residue from explosives and narcotics on skin, clothing, parcels, bags, cargo, vehicles and other surfaces.

Trace detection technologies differ significantly in sensitivity, specificity, reliability and ease of use. The development of single-sample substance collection and analysis has helped to revolutionize the landscape of threat prevention. Sophisticated, precision sample testing, once possible only in laboratories or clean rooms, can now be routinely performed in the real world, in real time, where real threats exist.

This paper compares the benefits and drawbacks of the most prevalent technologies in use today. It examines the advantages of one technology in particular: Ion Trap Mobility Spectrometer (ITMS®) technology, an enhanced ion mobility spectrometry (IMS) technology patented by GE.

How trace analysis technologies detect and identify explosives and narcotics in security applications

The Technologies of Trace

Trace detection captures and analyzes the microscopic particles and vapors naturally emitted by organic substances. Trace samples are collected by wiping surfaces suspected of contamination or by “sniffing” concentrated vapors trapped within a sealed container.

Three technologies are used most often for trace detection of explosives and narcotics: 1): Combination Gas Chromatography Chemiluminescence (GC-CLD); 2): Ion Mobility Spectrometry (IMS); and, 3): enhanced IMS, or Ion Trap Mobility Spectrometry (ITMS). A fourth combination, gas chromatography and mass spectrometry (GC-MS) is also available, but its use is confined mostly to laboratory environments.

GC-Chemiluminescence measures the optical emission from excited molecules to determine the concentration of a contraband substance. Although GC-CLD technology has good sensitivity and selectivity, it lacks the versatility required for maximum effectiveness against common threats.

With today’s increasing threats from explosive substances, using GC-CLD outside the structured controls of a laboratory becomes impractical. The technology involves expensive maintenance, complex instruments, high consumable gas costs, and the need to prevent and monitor operators’ exposure to potentially harmful materials such as ozone.

Ion Mobility Spectrometry identifies compounds based on the amount of time it takes for ionized molecules to pass through an electrified field in a tube.[1,2] This time, sometimes called “time of flight” or “drift time”, is then compared to a database containing the transit times of known compounds, making it possible to distinguish the target material (explosives or narcotics) from other molecules. This technique is fast and can be adapted to fit a compact, portable device.

As shown in Figure 1, gaseous samples enter an ionization chamber where an ionizing source emits low-energy beta particles, resulting in ion formation in the gaseous phase. The shutter grid—a gating mechanism—allows ions of the correct polarity to pass through and enter the ion drift region where an applied electric field mobilizes them. Less than 1% of the ions created in the ionization chamber actually reach the drift tube, because more than 99% of the ions are discharged on the shutter grid. The rate at which these ions cross the ion drift region is inversely proportional to the size of the ion. This correlation allows for the identification of the target substance.[3]

Ion Trap Mobility Spectrometer® technology significantly improves the performance of traditional IMS. Like IMS, ITMS separates ionized vapors and then measures the mobility of the ions in an electric field. The gaseous samples enter an ionization chamber where an ionizing source emits low-energy beta particles, resulting in ion formation in the gaseous phase.

However, ITMS breaks new ground by eliminating the shutter grid and the associated loss of ions and sensitivity. With ITMS, ionization reaches equilibrium in a field-free region and is then pulsed into the drift tube where an electric field guides the ions to the collector. (Figure 2) Without a shutter grid, a much greater number of ions enters the drift tube.

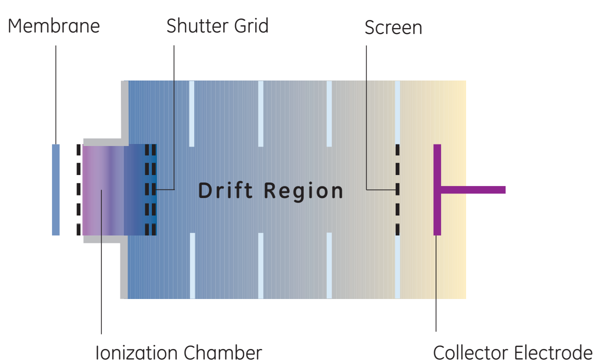


Figure 1:
Schematic of Ion Mobility Spectrometer

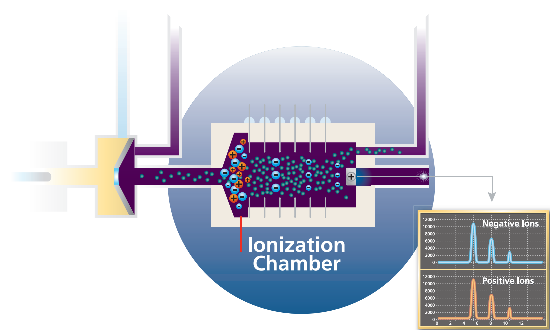


Figure 2:
Ion Trap Mobility Spectrometer (ITMS®)

Performance Requirements of Trace Detection

The best way to compare technologies is to evaluate them based on performance requirements critical to security applications. These include sensitivity, selectivity, range of compounds detected, logistics, and reliability/maintenance.

Sensitivity (detection effectiveness) refers to the instrument's ability to detect low levels of the target explosive or narcotic. The lower the detection level, the better; since often only a single sample is available and threat compounds may be present in very small amounts.

In real-world security applications, there is a practical time limit to performing the test on people, packages, or baggage. If we consider 3-10 seconds a realistic testing time range, GC-CLD technology will have a loss in selectivity, as the GC column will not provide enough separation of the nitro compounds within the time limit.

IMS loses sensitivity because it loses ions to the shutter grid with its non-equilibrium ionization. ITMS detectors increase ionization efficiency, the main factor in determining detection sensitivity. ITMS instruments also feature a semi-permeable membrane that reduces interference from non-target substances and assures reliable operation in dusty, dirty environments.

Selectivity, the ability to distinguish between compounds, is critical to trace testing because of the urgency of correctly identifying specific explosives or narcotics in a sample.

Typically, samples of explosives or narcotics will include other substances. Although significant operational differences exist between technologies, all three can accurately select the target compound if present in quantities above the instrument's sensitivity level. The advanced detection algorithm of ITMS increases selectivity and minimizes false positives.

Range of compounds detected refers to the spectrum of material that the device can detect simultaneously.

IMS can detect *either* negative or positive ions, but not both at the same time. ITMS, on the other hand, can simultaneously detect negative and positive ions, including both nitro and non-nitro target substances. ITMS can detect narcotics and a wide range of explosives at the same time, from the same sample, without sacrificing sensitivity or time.

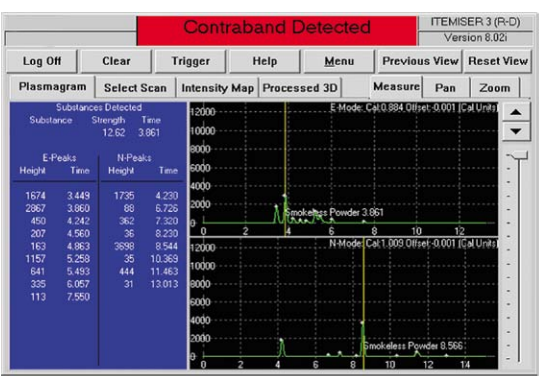
Logistics, or the practicality of using a particular trace detection technology in a specific application, must also be carefully considered. Regulatory issues for ozone, radioactive sources, and bottled gases may impact which technology can be used.

GC-CLD requires handling of sensitive gases such as hydrogen, ozone, or helium. IMS and ITMS contain radioactive sources.

Reliability/Maintenance factors affect the performance of trace detection technologies outside the controlled laboratory environment. To be effective in a real-world security environment, trace technologies must maintain peak performance in high traffic, dusty or humid conditions. There must also be as little downtime as possible due to maintenance, and the cost to maintain the system should not be excessive.

Both GC-CLD and IMS are unprotected from dust, dirt, and water vapor entering the system. This is a serious problem for traditional IMS, as the dryer or desiccant requires frequent changing, resulting in increased downtime and cost. In addition, persistent contamination leads to a loss of instrument sensitivity over time.

ITMS systems resolve these issues with patented regenerating dryers that do not require changing, and a semi-permeable membrane that protects systems from dirt, dust, and humidity. With high usage, GC-CLD systems require costly



Smokeless powder is often detected by IMS systems in the negative mode because it contains nitroglycerine. A peak in the positive mode gives the screener further information about the substance for which they may conduct a hand-search. This more precise identification may also help resolve the alarm by generating questions that reveal a legitimate use for the substance, such as sport shooting or military training.[7]

Technology Comparison Summary Matrix

	GC-CLD	IMS	ITMS
Sensitivity	•••	•••	••••
Selectivity	•••	•••	•••
Range of Compounds Detected	•	••	••••
Logistics	••	••	••
Reliability/Maintainance	•	••	••••

•••• Excellent ••• Good •• Fair • Poor

replacement of the chemical modules approximately every 3-6 months, which may be nearly as expensive as a brand-new desktop ITMS or IMS detector.

While all three use similar sampling consumables, the GC-CLD also requires gas bottle replacement. The ITMS and IMS devices require dopants, depending on the application.

ITMS Improvements Over IMS Technology

Compared to IMS technology, ITMS can deliver increased sensitivity, flexibility, and practicality for security applications.

ITMS can detect extremely low concentrations of electrophillic vapors such as explosive vapors. The ionization chamber in the ITMS detector is a field-free region where both negative and positive ions are allowed to build up by the action of the beta particles on the dopant gas. The high density of electrons produces a high probability of ionization of the dopant gas molecules, which in turn collide with the target molecules. An electric charge is then transferred to the target molecules because of their extremely high charge affinity, and the overall result is high ionization efficiency. In traditional IMS, ions discharge onto the shutter grid, and a high percentage of the ions can be lost. With ITMS, ions are accumulated and then compressed into a pulse, increasing the density and collected current by a factor of 30 or more.[4,5,6]

ITMS technology features a semi-permeable membrane that excludes dust and dirt. This critical improvement makes the system more sensitive to the target substance, and enables continued operation and sensitivity in harsh field environments.

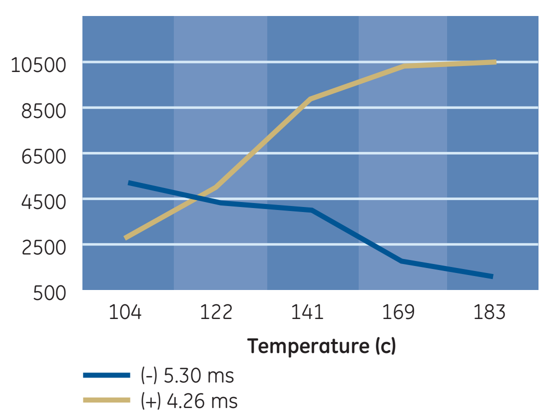
In addition to providing a charge medium, the specific chemicals chosen as dopants can reduce the chances of ionizing non-target substances. The dopants accept charge from the low energy beta particles, reducing the chance that molecules with charge affinities lower than that of the dopant will accept charge. The target contraband molecules will accept the charge more readily than the dopants due to their higher affinity for the charge. This process can reduce the amount of possible interferences from non-target molecules because the detector recognizes only charged species.[4,5,6]

Finally, ITMS allows simultaneous detection and analysis of target positive and negative ions, making it possible to effectively screen for low concentrations of multiple substances with a single sample. It works this way: most narcotics have a positive charge affinity, and most explosives have a negative charge affinity. However, there are some crucial exceptions.

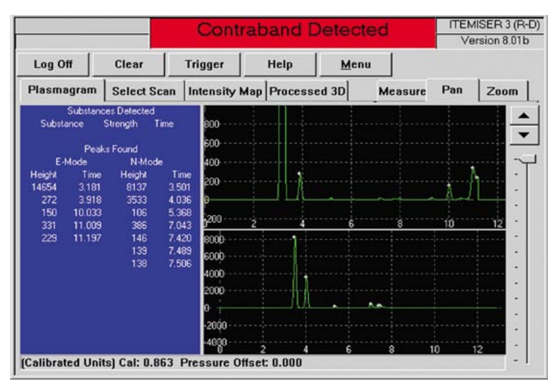
Certain explosives have a positive affinity molecule and would not be detected with traditional IMS in single-mode operation for explosives. ITMS incorporates precision engineered high-speed switching systems that alternate from positive to negative ion mode in milliseconds. Detection limits for real-world samples in ITMS in vapor sampling mode are in the picogram (billionths of a gram) range.[7] Clearly, its speed and detection sensitivity make ITMS greatly preferable to traditional IMS.

Summary

Delivering unsurpassed explosives and narcotics detection, ITMS can be an outstanding alternative to GC CLD and IMS for today's demanding security needs. With its innovative trap and membrane design, ITMS can identify the most challenging substances while withstanding the rigors of real world use. The combination of superior detection effectiveness, selectivity, versatility and reliability in a flexible detector design can make ITMS technology a good candidate for checkpoint security and screening personnel, packages, baggage, vehicles, mail, cargo and other applications.



TATP Response vs. Temperature



The ITMS detector was used to monitor both the positive and negative mode peaks as a function of temperature. As you can see, the negative mode peak gets smaller as the detector temperature approaches the normal operating temperature of an IMS or ITMS system. By monitoring both modes, the ITMS detector retains sensitivity and has more information to make a positive identification.[7]

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