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Toxicological SciencesJournal homepage: <http://www.ijfmts.com/>**Review Article****Advances in the detection of explosives and chemical weapons: A comprehensive review**Palak Sharma^{1*}, Atul Kumar Dubey¹¹Dept. of Forensic, AP Goyal Shimla University, Shimla, Himachal Pradesh, India**ARTICLE INFO***Article history:*

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ABSTRACT

The persistent threat of explosives and chemical weapons necessitates continual advancements in detection technologies to ensure public safety and national security. This review paper provides a comprehensive overview of recent developments in the field of explosive and chemical weapon detection. Emphasizing the interdisciplinary nature of this research, the paper covers a range of sensing technologies, including ion mobility spectrometry, mass spectrometry, infrared spectroscopy, and biosensors.

The review explores the integration of nanotechnology to enhance the sensitivity and selectivity of detection methods, alongside the application of advanced imaging technologies such as X-ray and Terahertz imaging for non-contact identification of concealed threats. Additionally, it delves into the utilization of biological sensing elements in biosensor platforms, employing enzymes and antibodies to detect specific chemical compounds. Standoff detection capabilities, crucial for ensuring the safety of personnel, are examined, and the paper discusses the ongoing developments in chemical forensics, aiming to determine the origin and composition of explosive or chemical materials. The challenges faced in this field, including the need for high sensitivity, adaptability to different environments, and the detection of emerging threats, are thoroughly addressed. The review concludes by outlining future directions, highlighting the importance of miniaturization, artificial intelligence, and global collaboration in shaping the next generation of detection technologies. This thorough analysis provides insights into current trends, obstacles, and potential solutions in the crucial field of explosives and chemical weapons detection, making it an invaluable tool for scholars, decision-makers, and security experts.

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1. Introduction

An explosive is defined as a material (chemical or nuclear or mechanical) that can be initiated to undergo very rapid, and self-propagating decomposition resulting in the formation of more stable material, liberation of heat or the development of sudden pressure effect. Explosives undergo rapid oxidation reaction. It is the sudden buildup of gas pressure that constitutes the nature of an explosion. The speed at which explosives decompose permits their classification as high or low explosives. The majority of an

explosion's damage is caused by the shock wave that the expanding gases produce.¹

Chemical, nuclear, and mechanical are the three basic kinds. An explosive that relies on a physical reaction, like filling a container to capacity with compressed air, is called a mechanical explosive. These devices are rarely used outside of mining, where the unintended gas release from chemical explosives may be an issue. A nuclear explosive occurs when a large amount of energy can be released through a sustained nuclear reaction that can be triggered almost instantly.

The phrase refers to a variety of products, such as igniters, black powder, pellet powder, ammonium nitrate

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fuel oil (ANFO) mixtures, safety fuses, squibs, mixed binary explosives, and safety fuses. In addition, certain pest control products, fireworks, air bag inflators for cars, specialized industrial tools, fire extinguishers, model rocket engines, and special effects used in the entertainment industry all contain explosives.²

2. Classification

Explosives are categorized into numerous types based on their performance and structure (Scheme 1). In general, explosives are divided into two categories: high explosives, which detonate, and low explosives, which deflagrate. Both categories are then further divided into various forms.

Low Explosives– These explosives deflagrate creating a subsonic wave front that does not reach the speed of sound. The explosion that low explosives may produce is a consequence of the overpressure generated inside a container by the accumulation of gas products from deflagration. Because of the progressive production of these gas products during their deflagration, low explosives are mostly used as propellants, either in pyrotechnics, space rockets or ammunition for firearms.³

High Explosives– These explosives detonate creating a supersonic shock wave that propagates usually exceeding 4000m/s. Three classes are typically subdivided for high explosives according to their sensitivity to explode: primary, secondary and tertiary explosives.

a. Primary Explosives are extremely sensitive to different weak stimuli (such as heat, spark or friction) by which detonation initiates. In general, primary explosives are not particularly powerful. Because of these properties, they are usually used in little amounts as detonators of secondary high explosives. Some typical primary explosives are mercury fulminate, silver fulminate, lead azide, cuprous acetylide, lead picrate, lead styphnate, diazodinitrophenol, tetrazoles, NG, TATP and HMTD.⁴

b. Secondary explosives typically need a powerful shock to trigger them, and they are essentially insensitive to mild stimuli. The majority of secondary explosives have detonation velocities greater than 6000 m/s, making them incredibly powerful. Secondary explosives include the most common explosives used in the military field such as RDX, PETN, HMX, TNT, 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), tetryl, picric acid, CL20 and NC.⁵

c. Tertiary explosives are an additional category that is occasionally added to the classification in order to distinguish and include those insensitive explosives that are frequently used for demolition and mining operations and have detonation velocities that are lower than those of military secondary explosives. ANFO, ANAI and dynamite compositions are common examples of tertiary explosives.⁶

3. Chemical Weapons

"A chemical substance which is intended for use in military operations to kill, seriously injure, or incapacitate people because of its physiological effects" is how the North Atlantic Treaty Organization defines a chemical agent. Conventional chemical weapons and biological weapons, like plague or anthrax, are viewed as two extremes of a spectrum, with "chemicals of biological origin," like ricin or botulinum toxin, lying in the middle. Chemical weapons can be categorized based on how they work, how long they stay active in the environment (persistence), and how lethal they are.⁷

A biological toxin, a variety of chemical agents, and microbiological toxins are among the substances that have been or could be used as weapons of mass destruction or terrorist agents. A biological terrorism agent of the highest priority is Clostridium Botulinum toxin, according to the US Centers for Disease Control and Prevention (CDC). Second most important are the toxins produced by Staphylococcus enterotoxin B and Clostridium perfringens, as well as the toxin derived from Ricinus communis, or castor beans. Priority chemical agents are those that have been used as weapons in the past, are accessible to potential terrorists, have the potential to cause significant morbidity and/or mortality, have the potential to cause public panic and social unrest, and require special action for public health preparedness, among other criteria.⁸

4. Methods to Detect Explosives and Chemical Weapon

Many different techniques are used to detect explosive materials and devices, such as mines and improvised explosive devices (IEDs) and range from metal detectors and sniffer dogs, still probably the most effective and versatile method, to fixed and portable X-ray systems and analytical techniques, most notably ion mobility spectrometry (IMS).⁹

Infra-red Spectroscopy- Infrared spectroscopy has played an important role in laboratory studies of the characterization of highly energetic materials. Contributions of IRS in the area of HEM lab-based detection and characterization were reviewed by Steinfeld and Wormhoudt¹⁰ up to 1998, and the area was later updated by Moore in 2004 and 2007.¹¹

The absorption spectroscopy method known as FT-IR involves passing infrared light through the sample. While some wavelengths may simply pass through the sample unaffected, others may be absorbed. A certain amount of energy is absorbed by particular molecular bonds, and these energy losses correlate to the peaks that are recovered during an analysis. For materials with polar covalent bonds, FT-IR absorptions are robust and yield excellent, understandable results.

Raman Spectroscopy- Developed in the 1960s, Raman-based LIDARs (light detection and ranging) are an active mode optical remote sensing technology that measures the characteristics of scattered light to determine distance and inelastically scattered signals from contaminant gases and vapors in the atmosphere.¹²

Raman is a type of vibrational spectroscopy where a sample is exposed to a single wavelength laser. The material in question can be identified by the laser energy, which breaks the bonds in the molecule and produces or "scatters" measurable light. Based on the underlying chemistry of an unknown substance, Raman is very effective at obtaining a trustworthy and accurate identification of that substance. Devices gather the material's molecular spectrum, and internal chemo metric algorithms use this information to determine the material's chemical composition by comparing the obtained spectrum to those that are already stored in the device. Certain devices can also detect explosive precursors present in mixtures.

Time-of-Flight Mass Spectrometry (TOF-MS) - Time-of-Flight Mass Spectrometry (TOF-MS) is a powerful analytical technique widely used in various fields, including the detection of explosives. TOF-MS measures the time it takes for ions to travel from the ion source to the detector based on their mass-to-charge ratio (m/z). Ions are generated by ionization techniques such as laser ablation, electron impact, or photo ionization. The ions are then accelerated in an electric field and their time of flight is measured. The mass of the ions can be ascertained because lighter ions arrive at the detector sooner than heavier ions. Recent advances in LC/MS technology have led to the availability of Time-of-Flight (ToF) LC/MS systems. These offer a higher degree of analyte information because of their high resolution and capacity to gather precise mass data down to sub-ppm levels. This significantly increases the confidence in analyte identification by limiting the possible number of candidate compounds.¹³

Ion Mobility Spectrometry (IMS) - In airports across the US, ion mobility spectrometry has emerged as the most effective and popular technology for detecting traces of nitro-organic explosives on carry-on luggage and handbags. The effective ionization method, atmospheric pressure chemical ionization (APCI) reactions in negative polarity, provides the low detection limits. Ion mobility spectrometry (IMS) is an instrumental technique that combines two separate principles to react quickly to trace amounts of chemicals in gas or vapor forms. Sample vapours in IMS are transformed into ions at atmospheric pressure, and the characteristics of those ions in weak electric fields are determined by their gas phase mobilities.¹⁴

Nanomaterials based sensors- Ion mobility spectrometry (IMS), mass spectrometry (MS), and gas chromatography (GC) are the most widely used methods for detecting trace explosives nowadays; however, the

majority of these instruments are large, costly, and involve labor-intensive processes. These limitations result in sparse deployment of such equipment and decrease the overall protection against explosive-based terrorism. One technique that can potentially address many of the demands for reproducible onsite detection of explosives is that of electrochemical sensors, which can be low cost, portable and specific. In particular, electrochemical sensors possess many advantages for use in field-deployable detection of explosives, including high sensitivity and selectivity, speed, wide linear range, compatibility with micro-fabrication, minimal space and power requirements, and lowcost instrumentation.¹⁵ Recent years have seen a major increase in interest in nanomaterial-based sensors because of their special qualities, which can be used to detect explosives and chemical weapons with great sensitivity and selectivity. Sensor platforms perform better in terms of sensitivity, selectivity, and response time when nanomaterials are integrated into them. To further enhance the functionality of explosive and chemical weapon detection systems, research in this area is still being conducted, investigating novel nanomaterials and sensor architectures. The potential for improving the capabilities of security and defence systems when nanotechnology and conventional sensor technologies are combined is substantial.¹⁶

Quantum Dots- Semiconductor nanocrystals known as Quantum Dots (QDs) have special optical and electrical characteristics. Their small size, tunable emission wavelengths, and high surface area make them attractive for various applications, including the detection of explosives and chemical weapons. These can be used in:

1. Fluorescence based detection
2. Optical sensing platforms
3. Surface functionalism
4. Multiplexed detection
5. Nanocomposites
6. Conjugation with nanomaterials
7. Time resolved detection
8. Real time monitoring

Quantum dot-based sensing technologies continue to be an active area of research, and advancements in material design, surface chemistry, and sensor architectures contribute to the ongoing improvement of their performance in the detection of explosives and chemical weapons.¹⁷

Enzymatic Biosensors- Enzymatic biosensors are analytical devices that incorporate enzymes as the recognition element to detect specific target analytes. In the context of explosives and chemical weapons detection, enzymatic biosensors offer advantages such as high specificity, sensitivity, and the ability to work under mild conditions. A novel biosensor based on ion-selective field effect transistors (ISFETs) was created to detect explosives. The biosensor's identifying component, *Escherichia*

coli nitroreductase (NTR), was employed to provide high sensitivity and specificity towards nitroaromatic compounds. The NTR-catalyzed reduction of multiple nitroaromatic compounds, coupled with the oxidation of nicotinamide adenine dinucleotide phosphate (NADPH) from its reduced form to NADP⁺, was detected analytically by the ISFET-based device. Spectrophotometric analysis was used to characterise the catalytic properties of nitroreductase. The enzyme nitroreductase exhibited peak activity in response to tetryl and trinitrotoluene, with corresponding Michaelis constants of 70 and 91 μM . Self-assembly was used to covalently attach the enzyme to the ISFET surface. Asymmetric spacer 3-maleimidobenzoic acid N-hydroxysuccinimide ester and symmetric spacer glutaric dialdehyde were used in the comparison of two SiO₂-surface immobilization techniques. The immobilized nitroreductase's enzymatic activity increased when the symmetric spacer was used. Rapid analytical response, low-cost mass-production technologies, and seamless integration into portable devices are the key features of this biosensor, which enables quick assay and online explosive detection. Portable analytical instruments can readily integrate the microfluidic system and the enzyme-functionalized CMOS-compatible ISFET chip.¹⁸

Immunoassays- Analytical methods known as immunoassays employ the unique binding affinity of antibodies to antigens in order to identify and measure target molecules. Immunoassays provide high sensitivity and selectivity in explosives detection. It has been demonstrated that CL-LFIA and CL-ELISA are sensitive, selective, and accurate enough to be utilised in forensic processes. These methods can be highly helpful in identifying the samples that require more costly and time-consuming forensic confirmation. Numerous analyses are possible because each assay only requires a small amount of solution. This method yields faster results and saves time and money because only samples that test positive for immunoassays are examined for confirmation, which ultimately leads to resource optimization. These are the qualities that criminal investigators always want to see. Immunoassays were useful for identifying post-transfer residues on hands as well as post-blast residues in soil and target materials.¹⁹

X-ray Imaging- The combination of two areas of X-ray physics that date back to the early 1900s is known as X-ray diffraction imaging. The first branch deals with radiography, as demonstrated by the well-known X-ray image of Roentgen's wife's hand. The diffraction pattern of copper sulphate, which was shown in Max von Laue's 1914 Nobel Physics Prize lecture, serves as an illustration of the second branch of X-ray diffraction (XRD). It shows the distinctive interference peaks, or spots, that arise when an X-ray beam interacts with atoms arranged in a regular lattice structure. The so-called "killer application," which detects

and identifies explosives (and drugs) whose illegal use poses a serious risk to society, has sparked the development of XDI. Technological developments over the years, especially in the areas of multi-foci, high-radiance X-ray sources, and pixilated energy resolving semiconductor detectors, have made advancements in XDI possible. Undoubtedly, the introduction of computed tomography (CT) had a significant impact on the growth of XDI. The first observation and accurate interpretation of the dominant contribution of coherent X-ray scattering, the foundation of XRD, to the small-angle X-ray signal in the diagnostic radiology energy range occurred in CT.²⁰

Terahertz Imaging- The potential of terahertz (THz) detection for imaging of explosives, chemical and biological agents, and concealed weapons has drawn more attention in recent years. This interest is primarily fueled by three factors.

1. (a) Since most non-metallic and non-polar materials easily transmit terahertz radiation, THz systems can "see through" barriers like packaging, corrugated cardboard, clothes, shoes, book bags, etc. to investigate potentially hazardous materials inside.
- (b) THz spectra are a useful tool for fingerprinting and, consequently, identifying a variety of materials that are of interest for security applications, such as explosives and chemical and biological agents.
- (c) Both the operator of the THz system and the suspect being scanned by it are at minimal or no risk to their health from terahertz radiation.

Effective methods for the quick detection and identification of these threats are needed as chemical and biological agents, plastic explosives, fertiliser bombs, and weapons of mass destruction and terrorism grow more common, and as the trafficking of illicit drugs becomes a more significant national security concern. Using THz electromagnetic waves to spectroscopically detect and identify concealed materials based on their distinctive transmission or reflectivity spectra in the range of 0.5–10 THz is one suggested method for locating, detecting, and characterizing concealed threats.²¹

Isotope Ratio Mass Spectrometry (IRMS) - The technique of isotope ratio mass spectrometry (IRMS) exhibits the capability to distinguish between samples that originate from distinct sources. The powerful analytical method known as isotope ratio mass spectrometry (IRMS) is used in many different fields, including explosives detection. IRMS can be used to analyse stable isotopic compositions of elements in explosive materials or related residues, but it is not a direct method for detecting explosives. Most of the forensic community's research on AN to date has focused on

methods for identifying and detecting AN. Stable isotope analysis using IRMS is a potent technique that is frequently used in conjunction with more comprehensive analytical methods for explosives identification and detection. Furthermore, extensive databases of stable isotopic compositions connected to different explosives and their sources must be available for IRMS to be effective in explosive detection. The study of stable isotope analysis in explosive detection is a constantly developing field with the goal of enhancing the analytical techniques' sensitivity and specificity.²²

Chemical Signature Analysis- Chemical signature analysis is a method for detecting explosives that entails locating and examining distinctive chemical signatures connected to particular explosive materials. The primary explosive compound as well as any secondary and trace compounds created during the production or handling process can all be found in these signatures. The objective is to distinguish between various explosive kinds and possibly locate their origin. The ability to work at standoff is one of the advantages of radiation techniques, but it is still difficult to quickly detect explosives at safe standoff distances. This method is distinct from the main nuclear approaches, which include quantitative analysis (e.g., prompt- and inelastic-scatter gamma-ray production based on neutron interrogation) and/or imaging (using either photon or neutron interrogation). This method does not use quantitative analysis or imaging, but rather makes use of both photon and neutron interrogation. The method, which we refer to as signature-based radiation scanning (SBRS), does not try to further characterize the internals of a target; instead, it only detects whether a target contains explosives. The method uses a template-matching technique that yields a single figure-of-merit whose value is used to discriminate between targets that are safe and targets that are explosive. Verification of the validity of SBRS has been done through experimentation and simulation.²³

Laser-Induced Breakdown Spectroscopy (LIBS) - Laser-induced breakdown spectroscopy is one optical method for explosives detection that shows promise (LIBS). LIBS is a spectroscopic analysis method that determines the sample composition based on elemental and molecular emission intensities by analyzing light emitted from laser-generated micro plasma. Because LIBS has the inherent ability to detect and analyze a wide variety of chemical species in real-time, in situ, and with minimal damage, it holds particular promise for the identification and detection of explosives. Because the first laser shot has the potential to ablate all or most of the residue, LIBS's capacity to detect trace amounts of materials with a single shot is particularly crucial for residue detection. The following characteristics of LIBS:

1. No sample preparation is required;
2. It is very sensitive, e.g. only a very small sample is required (nanograms–picograms) for production of a usable LIBS spectrum;
3. It is fast, providing real-time (<1s response);
4. LIBS sensors can be made rugged and field-portable;
5. All components (i.e., laser, detector, computer, etc) can be miniaturized; and
6. LIBS offer the flexibility of point detection or standoff mode operation

Since every element in the periodic table has distinctive atomic emission lines that emit in the UV, VIS, and NIR spectral regions, LIBS can be used to determine the elemental composition of any target material thanks to recent advancements in broadband detectors (multispectrometers or echelle).²⁴

5. Conclusion

In conclusion, the integration of cutting-edge technologies, interdisciplinary research, and the creation of novel methodologies have resulted in notable advancements in the detection of explosives. The ongoing need for strong and trustworthy techniques to combat security threats is what motivates these developments. By combining cutting-edge methods, new technology, and interdisciplinary cooperation, the field is best positioned to defend against possible dangers. Future prospects for improving explosives detection methods' efficiency, speed, and reliability are bright as long as research and development efforts continue.

6. Discussion

Enhancing global security protocols through technological advancements in explosives and chemical weapons detection are critical steps. Modern technologies like mass spectrometry, spectroscopy, and sophisticated imaging techniques have significantly increased the detection capability. Owing to their exceptional sensitivity and specificity, these methods can detect chemical agents and explosive compounds—even in trace amounts—quickly. Furthermore, interdisciplinary research collaborations have aided in the development of novel detection techniques like aptamer-based sensors and nanostructured materials that improve detection sensitivity and selectivity. The continuous threat posed by terrorism and the proliferation of chemical weapons underscore the criticality of the advancement of detection technologies. The field's future appears bright, with improvements expected to further improve detection efficiency, speed, and reliability. Nevertheless, some challenges persist, such as the need for detection systems that are able to identify and react to novel threats and the shifting tactics of hostile actors. In order to mitigate these risks and ensure the safety and security of communities worldwide, it is imperative that research and development expenditures be sustained, and

1. No sample preparation is required;

that government agencies, business, and academia continue to collaborate.

7. Source of Funding

None.

8. Conflict of Interest

None.

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