Field-Deployable Devices

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Abstract

Reductions in instrument size, weight, and power continue to facilitate the development and application of field-deployable devices for investigative purposes. Portable analytical instrumentation supporting the rapid and reliable identification of two broad categories of compounds - drugs and hazardous materials - are of particular interest to forensic analysts, first responders, and other aligned experts. This article discusses the capabilities and limitations of commonly employed field-deployable devices, along with emerging technologies.

Key Points

- Field-deployable devices provide rapid detection and identification of unknown materials.
- On-site chemical analyses are critical for first responders, HAZMAT, forensic, and security applications.
- Field-deployable device encompass a range of analytical techniques with varying capabilities and limitations.
- Emerging technologies may enable further advancements in miniaturization for on-site forensic investigations.

Introduction

As technologies have advanced, improvements in performance combined with reductions in instrument size, weight, and power (SWaP) have enabled the migration of certain chemical analyses out of the laboratory and into the field. This article focuses on field-deployable devices and instrumentation for on-site or remote (i.e., away from the forensic laboratory) chemical analysis. The rapid detection and identification of unknown materials in the field provides near real-time information critical to personnel and/ or community safety and investigative processes. Devices used in the field have been described by a wide variety of descriptors such as portable, fieldable, handheld, transportable, or compact. Here, "field-deployable" is used and the focus will be on those instrumental devices expressly designed for field use or devices specially modified for field-deployment. Such devices may provide stand-alone analysis (e.g., handheld Raman spectrometer) or be combined with other chemical or instrumental techniques (e.g., gas chromatography - mass spectrometry; GC–MS). Though presumptive chemical tests can also be considered field-deployable, they are discussed in the encyclopedia entry *Presumptive Chemical Tests*, while this article focuses on instrumental components.

Field Needs and Challenges

The most basic requirement for field-deployable devices is maintaining sufficient performance in a reduced instrument package. Instrument size (i.e., handheld up to vehicle transportable), performance requirements, and general benefits or drawbacks afforded by fieldable chemical analysis are application specific. Field-deployable devices operate along a spectrum of discrimination ability from presumptive (indicating the presence of a chemical or chemical class) to confirmatory (enables structural identification of a chemical). Though techniques and devices have been classified as presumptive or confirmatory, factors such as instrument specifications, user expertise, and sample composition can greatly influence chemical indication to identification. A range of testing capabilities are needed, so that a variety of field needs and challenges (time, budget, expertise, etc.) can be sufficiently met. It is common that multiple tests will be employed and/or mandated to confirm the identity of a chemical. For example, when employing a Category A technique (e.g., mass spectrometry or Raman spectroscopy), ASTM E2329 requires an additional second technique from Category A, Category B (e.g., gas chromatography), or Category C (e.g., colorimetry) for identification criteria.

First responders, law enforcement, and hazardous materials (HAZMAT) personnel often employ fieldable instrumentation for rapid identification of unknown chemicals. These analyses generally provide presumptive identifications; however, they are often sufficient to identify hazards and mitigate immediate risks on scene. These techniques include photoionization detection (PID), vibrational spectroscopy (chiefly Raman and Fourier transform infrared), ion mobility spectrometry (IMS), mass spectrometry (MS), and dosimetry. Each commonly employed field-deployable device has capabilities and limitations, as summarized in **Table 1**. In the case of MS, the specific instrument will determine the level of structural information provided. For example, field portable ion trap mass spectrometers allow for MS/MS analysis and detailed structural information through fragmentation spectra. Alternatively, high-pressure mass spectrometers provide poorer resolution and limited differentiation, more analogous to presumptive IMS. Presumptive testing of suspected illicit drugs has long been used by law enforcement to provide probable cause for arrest (Forensic Technology Center of Excellence, 2018). As presumptive tests only provide a cursory identification, subsequent testing is often required. The training and technical knowledge required to properly conduct presumptive tests can range significantly, with the complexity of the analysis dictating training time and user expertise requirements (Forensic Technology Center of Excellence, 2018).

While technological advancements in batteries, device power management and miniaturization, secure Wi-fi, and cellular connectivity have moved laboratory-based instrumentation into the field, their complexity may still require a specialist operator. Advancements in commercial alarm algorithms and compound libraries have aided in reducing the level of expertise required for operation. Alternative workflows have also been employed to allow the use of complex devices onsite with remote data analysis. For example, the NFiDENT project implemented by the Netherlands Forensic Institute (NFI) deployed GC–MS devices at police stations for officer operation (Kloosterman *et al.*, 2015). Resulting data was sent to NFI for further analysis and verification of field results. Similarly, some device vendors offer reachback services to support interpretation of results obtained in the field.

Scenarios, Scenes, and Sample Types

Field-deployable devices are widely used by a variety of users in a range of locations for a plethora of reasons. From crime scenes and combat areas to field hospitals and heritage sites to natural disaster zones, these devices aid in investigations, clinical care, environmental monitoring, conservation, and much more. The versatility of field-deployable devices to assist users across disciplines is perhaps their most significant benefit. Within forensic science, two broad usage categories see significant implementation of field-deployable devices - hazardous material identifications and drugs identification. Both usage categories require methods suitable for the analysis of gas, liquid, and solid samples of varying compositional complexity, including biological fluids. Analysis of biological specimens is methodically covered in toxicology entries such as *Methods of Analysis - Initial Testing, Postmortem Blood*, and *Breath Alcohol*, while this article focuses on non-biological matrices. It has been noted that analysis of breath alcohol content "is the foundation for all forensic on-scene testing" (Kammrath *et al.*, 2021). Breath alcohol testing and employed devices see the widest use, with IR spectroscopy and electrochemical sensors dominating the instrument landscape. While breath alcohol analysis is not specifically covered herein, IR spectroscopy and electrochemical sensors are discussed.

Table 1	Commonly employed field-deployable device categories, capab	ilities, and limitations. The extent of certain capabilities or limitations
may be inst	strument dependent	

Technology	Capabilities	Limitations
Photoionization and flame ionization detectors	 Sensitive Low cost Handheld Gas/vapor detection Continuous operation Used alone or as detector for GC 	 No solid or liquid analysis Poor selectivity Provides little-to-no structural information Susceptible to water vapor interference (PIDs) Only certain gasses detected PIDs cannot detect methane FIDs cannot detect ammonia
Raman spectroscopy	 Nondestructive Noncontact options Ease of use Minimal startup time (1–2 min) Rapid analysis Provides structural information Spectral libraries No consumables Analysis through glass Solid and liquid analysis Little-to-no sample preparation 	 Poor(er) sensitivity Difficulty with mixtures No gas/vapor analysis Fluorescence interference Ignite sensitive materials
Fourier transform infrared spectroscopy	 Nondestructive Noncontact options Ease of use Rapid analysis No consumables Provides structural information Spectral libraries Popular for solid and liquid analysis Little-to-no sample preparation (ATR) 	 Poor(er) sensitivity Difficulty with mixtures Not routinely employed for gas/vapor analysis Long startup time (10's of min.) Only detects IR-active components
lon mobility spectrometry	 Rapid analysis Sensitive Ease of use Solid, liquid, and gas/vapor analysis Provides physical/chemical characteristics 	 Long startup time (10–30 min) Direct sample interaction Potential for overload Destructive analysis Resolution limits selectivity Susceptible to environmental conditions Provides little-to-no structural information
Mass spectrometry	 Rapid analysis Sensitive Spectral libraries Provides structural information (MS/MS) Solid, liquid, and gas/vapor analysis 	 Long startup time (10 min) Direct sample interaction Potential for overload Destructive analysis High(er) cost Libraries dependent on ionization scheme May require understanding of technology
Gas chromatography-mass spectrometry	 Sensitive Mixture separation and identification Provides structural information Spectral libraries Solid, liquid, and gas/vapor analysis 	 Long startup time (10's of min.) Long analysis (10's of min.) Direct sample interaction Potential for overload Destructive analysis High(er) cost

Hazardous materials identification

Hazardous materials (HAZMAT) are categorized in several ways, with the National Fire Protection Association (NFPA) 472: Standard for Competence of Responders to Hazardous Materials/Weapons of Mass Destruction Incidents, defining these materials as "matter (solid, liquid, or gas) or energy that when released is capable of creating harm to people, the environment, and property. This includes weapons of mass destruction, as defined in 18 U.S. Code, Section 2332a, as well as any other criminal use of hazardous materials, such as illicit labs, environmental crimes, or industrial sabotage" (Federal Emergency Management Agency, 2019). Scenarios requiring fieldable hazardous material analysis fall largely into (1) industrial, workplace, and environmental incidents and

(2) criminal or malicious actions. The emergency response to HAZMAT incidents typically follows a defined risk-based response process that includes evaluation and treatment protocols, employing specific equipment at each stage. Guided by established protocols, training, and experience, first responders assess the scene, engage in planned response actions aimed at stabilizing the incident, and continuously monitor incident progress. Field-deployable devices provide valuable information at each stage, with such devices categorized in, and often selected from, the U.S. Federal Emergency Managements Agency's (FEMA's) Authorized Equipment List to meet a range of samples (i.e., solid, liquid, gas) and scenario needs. The Authorized Equipment List details approved equipment types for use by emergency and homeland security professionals (Occupational Health & Safety, 2003). On-site incident assessments may use a variety of techniques from the less specific (such as colorimetric tests or gas monitors), to more specific (e.g., Raman spectroscopy or mass spectrometry). Early assessments of a scene will inform first responders to the nature of potentially hazardous materials and aid in steering law enforcement and/or regulatory actions, material cleanup/remediation, and forensic investigations.

Criminal and malicious actions using hazardous materials often categorically fall into chemical, biological, radiological, nuclear, and explosives (CBRNE) incidents and applications. These areas are of significant forensic and national security interest. More specifically, security applications are generally concerned with screening, detection, and identification of harmful agents or pre-blast explosives. The operational concepts are application specific. In general, vehicles, cargo, containers, and individuals are screened for hazardous materials, explosives, synthesis precursors, drugs, and other contraband materials. The focus for field-deployed instrumentation targeting chemical or explosive threats, for example, is the detection and identification of residual contamination on various items which provides an indication of prior handling or contact with the bulk materials. Chemical detection in this scenario often initiates further, and more thorough, examination of a flagged item or person; and more generally, denial of entry or access.

In addition, emergency and forensic response to criminal or malicious actions are commonly concerned with hazardous material mitigation and investigation. These scenarios often follow incidents and target chemical release, post-blast compounds, and degradation or decomposition products of hazardous materials. Chemical analysis and identification under post-blast type conditions must often handle complex matrices and contaminants. Clandestine laboratories, which straddle both device usage categories of HAZMAT and drugs identifications, can present a broad range of challenges often necessitating additional or expanded protocols and response teams. The response or investigation of clandestine laboratories expands beyond drug synthesis to synthesis of chemical or biological agents or fabrication of improvised explosive devices. For scene specific discussions, please see entries such as *Clandestine Laboratories, Clandestine Explosive Laboratories, Improvised Explosive Devices*, and *Explosions*.

Drug identification

Drug detection and identification, as with HAZMAT incidents, relies heavily on presumptive testing in the field to support responder safety and provide investigative assistance. A variety of testing techniques from the most presumptive to confirmatory are employed to assess incidents and items of interest, with field results routinely used as probable cause for search and seizure. Color-based chemical tests are routinely used for presumptive testing, as explored in the encyclopedia entry *Presumptive Chemical Tests*. On-site assessment of suspected drug material informs time-sensitive decisions including search and seizure, detainment of persons, and required personal protective equipment (PPE). On-site forensic investigation of suspect materials also aids in reducing overall analysis times by providing fast diagnostic examinations that can clarify in-laboratory workflow. Though field-deployable drug detection often focuses on regulated and scheduled compounds, detection and identification of precursors, synthesis products, and adulterants can provide important information for first responders and investigators.

Device Categories

Here, field-deployable devices will be categorized and discussed in the context of their fundamental method of detection or identification. These basic analytical technologies and devices have exhibited broad application to many classes of analytes and widespread or common deployment by emergency responders, law enforcement, crime scene investigators, or checkpoint personnel. Discussion on principles of operation, capabilities, challenges, and supporting references will be highlighted. Table 1 contains a high-level overview of each technology's detection or identification capabilities and limitations.

Photoionization and Flame Ionization Detection

Photoionization detectors (PID) are handheld field-deployable devices that measure volatile organic compounds and related gases or vapors. These simple and inexpensive devices use photons generated from an ultraviolet lamp to ionize gas or vapor molecules present in sampled air. The resulting ion current is measured and digitally converted to a concentration. PIDs provide sensitive detection in the parts per million (ppm) to sub parts per billion (ppb) concentration ranges. The rapid and efficient detection of PID devices enables continuous operation and monitoring modes. PIDs are often employed by emergency responders early in the tiered scene assessment or mounted on vehicles for plume mapping. Though most commonly used as stand-alone handheld devices, photoionization detection has also been used as the gas detector for gas chromatography-based separations. PID devices can detect a range of toxic and hazardous compounds relevant to first responders and investigators, however their compound coverage is limited to compounds with certain ionization energies (e.g., PIDs cannot detect methane from natural gas). Similarly, correction factors are required for accurate measurements of gasses other than the calibration gas. The general nature of the detection scheme provides poor specificity and selectivity between similar gasses or mixtures. PIDs are also susceptible to interference from water vapor or quenching from other gasses or vapors present in the area.

Flame ionization detectors (FIDs) represent a similar class of field-deployable devices targeting flammable and/or toxic gasses and vapors, specifically hydrocarbons (e.g., methane, propane, etc.) and other organic compounds. FIDs are employed as both a simple, inexpensive stand-alone instrument for first responders and detection scheme for gas chromatography. Contrary to PIDs, a hydrogen-air flame is used to combust the entrained sample gas/vapor. An FID measures the current of generated ions migrating through an electrostatic field. This current is directly proportional to the concentration of all organic ionizable species in the sample, however no differentiation between substances is achieved. Comparatively, FIDs cannot detect inorganic compounds, e.g., ammonia, but also do not experience the same detrimental effects of environmental moisture as PIDs. Select instruments combine FID and PID into a single portable device. Critical device overviews and evaluations on commercially available PIDs and FIDs provide valuable information from a practitioner point of view. Such reports have been conducted as part of the System Assessment and Validation for Emergency Responders (SAVER) program administered by the U.S. Department of Homeland Security (DHS) (Department of Homeland Security, 2014, 2013, 2015).

Vibrational Spectroscopy

Enabling non-invasive analysis, vibrational spectroscopy techniques have found widespread use in a variety of fields requiring nondestructive and/or direct sampling of target materials. The category of vibrational spectroscopy includes several techniques, with midinfrared (mid-IR) and Raman spectroscopy devices being extensively employed for forensic, HAZMAT, and/or national security applications (Forensic Technology Center of Excellence, 2018; Chalmers *et al.*, 2012b; Kammrath *et al.*, 2021; Department of Homeland Security, 2016a, 2021). While the mid-IR wavenumber range of 400 cm⁻¹ to 4000 cm⁻¹ overlaps with the general operating range for Raman spectrometers of 200 cm⁻¹ to 4000 cm⁻¹, each technique depends on different adsorption phenomena discussed in-depth elsewhere in this encyclopedia including *Spectroscopy: Basic Principles* and *Spectroscopic Techniques*. Briefly, for a molecule to be IR active there must be a change of dipole moment during a normal mode of vibration of a molecule, while Raman requires a change in polarizability (Chalmers *et al.*, 2012a). Those species that do not undergo the required changes in dipole moment or polarizability are, respectively, not IR-active or Raman active. IR incorporates a broadband light source, while Raman requires monochromatic light that is typically supplied by a laser. Both IR and Raman spectroscopy provide structural information to support compound identification.

Mid-IR spectroscopy

The majority of commercially-available IR spectrometers are Fourier transform (FT) rather than dispersive instruments (Chalmers *et al.*, 2012a,b; Kammrath *et al.*, 2021; Forensic Technology Center of Excellence, 2018; Thermo Fisher Scientific Inc., 2008–2015). Modern portable FTIR devices incorporate sampling accessories like attenuated total reflection (ATR), require minimal sample preparation, and support direct analysis of liquids or solids. A range of such ATR FTIR field-deployable devices were featured in the 2016 DHS SAVER *Portable Infrared Spectroscopy Chemical Detectors Assessment Report* (Department of Homeland Security, 2016a) and 2018 US National Institute of Justice (NIJ) *Landscape Study of Field Portable Devices for Presumptive Drug Testing* (Forensic Technology Center of Excellence, 2018). Given the common use of ATR FTIR devices in the field, it is worth noting that this technique requires direct contact between the sample and the internal reflection element. The reflection of IR radiation, along with sample induced attenuation of IR radiation resulting in spectral bands, occurs along the sample-element interface. Both ATR FTIR and transmission FTIR require "sufficiently thin" samples, which is ultimately device specific (Kammrath *et al.*, 2021). The penetration of IR radiation is wavelength dependent and spectral band intensity is influenced by sample thickness (Shimadzu, 2021; Kammrath *et al.*, 2021; PerkinElmer, 2005b).

Due to the differences between measuring reflectance and transmission, ATR FTIR spectra and transmission FTIR spectra can be markedly different. This makes the use of technique specific libraries critical to sample identification work. FTIR is routinely used to study gases, though a gas cell is required (Kammrath *et al.*, 2021; Thermo Fisher Scientific, 2018). A recent review of portable spectrometers for forensic use noted that FTIR devices were "not usually deployed for vapor/gas detection" (Kammrath *et al.*, 2021). There are a number of field-deployable FTIR devices available, including handheld devices like the Agilent 4300 Handheld FTIR spectrometer, with select devices designed with HAZMAT and/or forensic work in mind (Department of Homeland Security, 2016a). Widely used for a range of chemical threat applications, portable FTIR instruments offer a number of benefits as summarized in Table 1. While FTIR provides structural information useful for molecule identification, those species that are not IR active are "invisible". Water, especially due to its strong absorption peak corresponding to an OH stretch (3700 cm⁻¹ to 3100 cm⁻¹), can "drown out" sample bands of interest in the same region in transmission FTIR (Water, 2021; Wilkinson *et al.*, 2013). In ATR FTIR, this effect is significantly lessened or avoided as IR radiation travels along the sample - element interface rather than penetrating through a bulk solution (Parikh *et al.*, 2014).

Raman spectroscopy

Raman instruments typically employ a laser, detecting inelastically scattered light reflected from the sample and measuring wavelength shifts between incident and scattered light (Kammrath *et al.*, 2021; Department of Homeland Security, 2021; Wilkinson *et al.*, 2013). These shifts - either to a longer (Stokes shift) or shorter (anti-Stokes shift) wavelength - results in characteristic spectra for compounds. As in IR spectroscopy, where particular functional groups give rise to characteristic absorbance bands, there are characteristic Raman shifts for functional groups. A number of commercially available portable Raman instruments are routinely used for forensic, HAZMAT, and/or national security applications. The aforementioned 2018 NIJ landscape study (Forensic Technology Center of Excellence, 2018), along with the 2021 DHS SAVER *Handheld Raman Spectrometer Market Survey Report* (Department of Homeland Security, 2021), feature several fieldable Raman spectrometers such as the Field Forensics HandyRam II. Raman devices benefit from a lack of sample preparation or device-to-sample contact requirements. As with FIIR devices, Raman instruments are typically deployed for analysis of solids and liquid samples, with gas analysis minimal-to-non-existent in field applications of focus herein (Cocola *et al.*, 2020; Kammrath *et al.*, 2021; Department of Homeland Security, 2021). Field-deployable Raman devices are capable of analysis through plastic and glass containers, which are weak Raman scatterers under typical run conditions (Kammrath *et al.*, 2021; PerkinElmer, 2005a; Department of Homeland Security, 2021). Direct analysis of suspect material without opening its container is a significant benefit. Water is also a weak Raman scatterer, thus avoiding the challenge it presents for FTIR spectroscopy (Kammrath *et al.*, 2021; PerkinElmer, 2005a; Department of Homeland Security, 2021).

Raman scattering is a small portion (1 part in 10⁶ or less) of the scattered light resulting from irradiation, impacting sensitivity and typically requiring the presence of more sample (Chalmers *et al.*, 2012a; Wilkinson *et al.*, 2013; Department of Homeland Security, 2021). Surface enhanced Raman spectroscopy (SERS) offers increased sensitivity and selectivity, along with a lower limit of detection, compared to its parent technique (Fikiet *et al.*, 2018; Chalmers *et al.*, 2012a; Department of Homeland Security, 2021). The "trade-offs" are sample preparation and contact requirements, shifting toward those of ATR FTIR. In SERS, a compound is typically placed on a suitable gold or silver surface. Under specific excitation conditions, compound - surface interactions can result in increased Raman scattering up to several orders of magnitude (Muehlethaler *et al.*, 2016; Fikiet *et al.*, 2018; Chalmers *et al.*, 2012a; Pilot *et al.*, 2019). SERS also addresses another challenge of Raman spectroscopy, which is possible fluorescence interference with emission bands masking the weak Raman band. In traditional Raman spectroscopy, shifting to longer excitation wavelength laser source and/or lower lasing power was enacted to manage fluorescence interference (Department of Homeland Security, 2021; Kammrath *et al.*, 2012). SERS attachments or kits for deployable Raman devices are commercially available, such as the Metrohm Mira DS.

Ion Mobility Spectrometry

Ion mobility spectrometry (IMS) has long maintained a role in fieldable chemical analysis due to its sensitive detection and reasonable cost. IMS instrumentation in general is relatively small, with units extending from lightweight and transportable benchtop models (e.g., 9–20 kg [20 lbs to 45 lbs]) to handheld models (e.g., 3–5 kg [7 lbs to 12 lbs]). Chemical analysis by IMS starts with the direct sampling of vapor analyte or the conversion of solid or liquid analytes to the gas phase, typically by thermal desorption. Gas phase analytes are then ionized and separated based on the mass, charge, and cross-sectional area of the resulting ions. Ionization has long been achieved with the use of reactant gases and a radioactive ⁶³Ni source. However, more recent instrumentation has moved away from radioactive sources and toward corona discharge or photoionization schemes. Reactant ion chemistries are often employed to target specific species for improved IMS detection performance. The resulting analyte ions are introduced to a drift region in pulses by a gating electrode. Ions traverse the drift tube under the influence of an electric field and in some cases a counterflow drift gas. The drift time of the separated ions is measured as an ion current impacting a Faraday plate.

IMS occurs under ambient pressures, eliminating the need for expensive and bulky vacuum pumps, unlike mass spectrometry. The drift velocity of ions can be susceptible to changes in the environmental conditions (i.e., temperature and pressure) and often requires consumable desiccant to dry the environmental air used as the drift gas. Internal calibration and verification standards can be used to maintain system performance. While analysis by IMS is rapid (on the order of seconds), the startup time to achieve steady state temperature and pressure can be lengthy (10–30 min). The ease of use and extensive commercial alarm algorithms have helped establish IMS as a major technology for screening applications that require a pass/fail indication, frequently conducted by non-technical personnel. Most common instrument libraries focus on explosives and/or drugs, however, libraries including toxic chemicals/gases and chemical warfare agents are also available. In addition, many compound libraries are user customizable.

ASTM standards on seized drug analysis and SWGDRUG recommendations classify IMS as a Category B analytical technique, providing selectivity through chemical and physical characteristics of the compound (Scientific Working Group for the Analysis of Seized Drugs, 2019; ASTM International, 2017). The limited resolution and selectivity of IMS can also lead to false positive results. IMS is a sensitive technique (typically nanogram or below range) but can be susceptible to overloading by concentrated samples or background, which may require extensive cleaning or clear-down times. And like any ion-based analytical technique, there is the potential for false negatives due to signal suppression and other matrix effects from background or contaminant components of a sample. In this scenario, these components are preferentially ionized, suppressing the potential signal from target analytes.

Mass Spectrometry

Mass spectrometry is a powerful analytical technique with high sensitivity and selectivity, capable of delivering confirmatory chemical identification (Brown *et al.*, 2020). A range of mass analyzers enable high mass resolution (e.g., time-of-flight or Orbitrap) or provide fragmentation and structural information (e.g., triple quadrupole). These advanced instruments are almost exclusively confined to the laboratory. Though many of the analytical techniques discussed in this article have been frequently employed for fieldable chemical analyses in forensic applications, mass spectrometry has not yet seen widespread deployment. This has largely been attributed to the significant electronics and vacuum system requirements. Most often, miniaturized mass

spectrometers for fieldable applications are ion traps or single quadrupole mass analyzers. In addition to potential differences in the mass analyzer, commercial mass spectrometers offer a variety of methods for solid, liquid, or gas sample introduction. Samples are converted to the gas phase, ionized, and separated based on mass-to-charge ratio (m/z). Sample introduction can be direct gas collection, thermal desorption of wipe collected- or solid phase microextraction (SPME) collected-samples, or electrospray-based.

As technology continues to advance and miniaturize, the field-deployment of mass spectrometry will become more and more practical (Evans-Nguyen *et al.*, 2021). Current portable mass spectrometers are expensive relative to other techniques discussed here (e.g., Raman spectroscopy or ion mobility spectrometers). Mass spectrometer operation and spectra interpretation often requires technical expertise or experience. However, systems providing simplified operation and spectral interpretation based on library matching and specific alarm algorithms are seeking to address this hurdle. Similarly, though many mass spectral libraries are available, a compound's mass spectrum or "fingerprint" depends on the system's ionization scheme, mass analyzer, and other parameters. For example, softer ionization schemes such as atmospheric pressure chemical ionization (APCI) often yields intact molecular ions, while harsher electron ionization (EI) results in fragment ions.

The sensitivity and structural information afforded by mass spectrometry enables trace level detection (i.e., invisible to the naked eye) and confirmatory identification. ASTM and SWGDRUG classify mass spectrometry as a Category A analytical technique, however, this is dependent on the selectivity provided by the specific instrument and analysis. For example, the reduction in resolution for high-pressure mass spectrometry (discussed below) does not provide sufficient selectivity for differentiation of compounds with similar structures or similar masses. The sensitivity of mass spectrometry also yields a propensity for overloading from "dirty" field samples and a susceptibility to matrix effects or signal suppression. In some cases, sample preparation or separation can alleviate these difficulties. Incorporating a separation technique, such as gas chromatography, aids in addressing limitations posed by complex mixtures.

Gas chromatography-mass spectrometry

GC-MS has long been a robust laboratory instrument for chemical analysis with large spectral libraries (e.g., NIST Mass Spectral Library). GC-MS instrumentation has also been ruggedized for fieldable analysis, but has traditionally been limited to toxic chemicals and chemical warfare agents (volatile compounds). The gas chromatography component inherently increases analysis time for appropriately resolved separation. In addition, the startup time is also lengthened to achieve steady-state temperatures for operation. GC-MS shares many of the same attributes and hurdles as mass spectrometry alone, including sensitive analysis, high(er) cost, and potential for overload from concentrated samples. GC-MS provides confirmatory identification of compounds by combining two orthogonal techniques, Category B: GC and Category A: MS. The U.S. National Urban Security Technology Laboratory conducted an assessment of GC-MS instrumentation for the U.S. DHS Science and Technology Directorate SAVER program (Department of Homeland Security, 2020). The report assesses the capability, deployability, maintainability, and usability of three GC-MS instruments.

High-pressure mass spectrometry

Recent instrumentation developments and commercialization of high-pressure mass spectrometers also have the potential to play a role in field-deployed forensic analyses. These instruments operate at high(er) pressures, relieving some of the bulky vacuum pump requirements and higher costs of traditional mass spectrometry. While the reduced vacuum requirement enables more fielddeployable and portable instrumentation, it also yields poorer resolution and selectivity. High-pressure mass spectrometry is generally not considered a confirmatory technique and requires more complex algorithms for interpretation and compound identification, similar to ion mobility spectrometry.

Radiological Equipment

First responders and investigators may also require instrumentation focusing on the detection of ionizing radiation. Fielddeployable radiological equipment covers a number of devices that meet the measurement needs for personal safety, interdiction, and investigative purposes. Dosimeters are radiation detectors employed for personal safety, measuring the accumulated dose an individual receives. Though commonly used for industrial or occupational monitoring purposes, dosimeters may be deployed in certain HAZMAT or CBRNE scenarios. Alternatively, survey meters measure the exposure rate of radiation and are used for locating and measuring source intensity as opposed to passive monitoring. Finally, radionuclide isotope identifiers provide exposure measurements and the emitting radionuclide identity. The National Urban Security Technology Laboratory has conducted similar assessments of radiological equipment and dosimeters for the U.S. DHS under the SAVER program (Department of Homeland Security, 2012, 2016b). Details of devices and their capabilities, such as detectable radiation type(s), measurement units, and range (i.e., background radiation to lethal), are thoroughly reviewed.

Emerging Technologies for Portability

Emerging technologies for portability encompass new(er) technologies exhibiting field-deployability, promising technologies not yet demonstrating widespread use and/or commercialization, along with enabling technologies that provide miniaturization avenues for existing techniques. This section will discuss select examples of technologies to demonstrate the frontiers of portability but is not intended to be all-inclusive.

Ambient Ionization Mass Spectrometry

Initially introduced and developed as a class of laboratory sample introduction methods, ambient ionization mass spectrometry techniques enable rapid analysis of samples in their native environment. Ambient ionization MS removes traditional sample preparation requirements to directly analyze samples on various surfaces or items. The list of ambient ionization sources is continuously growing, but they can generally be classified as (1) solid-liquid extraction, (2) plasma desorption, (3) laser ablation, or (4) multimode and hybrid techniques (Feider *et al.*, 2019). The applicability of specific ambient ionization platforms for field-deployable use depends largely on their mode of operation. For example, laser-based techniques are typically reserved for laboratory work. Similarly, solvent and gas consumable requirements must be accounted for in the transition to portable instrumentation. The analytes of interest for a specific scenario will also play a role in identifying the most appropriate technique or class of techniques.

These ambient ionization techniques can largely be coupled with any mass spectrometer containing an atmospheric pressure inlet. In combination with the reduction in mass spectrometer size (discussed in the Mass Spectrometry device category section), the versatile capabilities of ambient ionization techniques directly position ambient MS for field-deployability. The overall sensitivity, specificity, and other figures of merit will be dictated predominantly by the mass analyzer. A number of ambient ionization MS combinations have demonstrated utility for on-site forensic analyses. However, robust and rigorously validated systems have yet to break through into widespread use for fieldable analysis. Further advances in the burgeoning area may provide unique instrumentation for field-deployable forensic analysis.

Chromatographic and Electrophoretic Separations

In addition to ion mobility spectrometry, a number of other separations have demonstrated use for field-deployed chemical analysis. These technologies include various chromatographic, electrophoretic, and related separations. ASTM standards and SWGDRUG recommendations generally classify separations as Category B analytical techniques because they provide chemical selectivity. However, separations lack structural information produced by techniques such as mass spectrometry. Similar to many of the traditionally laboratory-based methods, technical advancements in miniaturization have benefited potential fieldable applications. Techniques such as high-performance liquid chromatography (HPLC) and nano LC have experienced miniaturization leading to portable devices. Portable LC systems have benefited from advancements in the miniaturization of liquid handling pumps, miniaturized capillary columns, microfabricated monolithic columns and micro-pillar array columns, 3D printed stationary phases, and advancements in detectors (Rahimi *et al.*, 2020; Sharma *et al.*, 2015). The reductions in instrumentation size and cost necessary for field-deployability have also led to reductions in consumable reagents and generated waste. However, the reductions in size may also lead to an increase in susceptibility to channel clogging or system overpressurization.

Advances in instrumentation, microfabrication techniques, and lab-on-a-chip systems have also led to miniaturization of capillary electrophoresis(CE) separations both in traditional capillary or microchip form. In addition to advancements in the analytical device itself, advancements in portable and rapidly replaceable liquid storage and handling are enabling field-deployability (Araujo *et al.*, 2018; Patel and Lurie, 2021). Like many of the separations discussed here, selectivity and resolving power will be a function of the specific instrument, method (e.g., capillary zone electrophoresis versus isotachophoresis versus gradient elution moving boundary electrophoresis), and sample being analyzed. CE generally requires shorter analysis times than LC, but longer than IMS and MS. Recent systems have been developed for analysis of specific classes of compounds (e.g., drugs vs inorganic oxidizers). In addition, field-deployable microchip electrophoresis has been applied to forensic analysis of DNA for genotyping applications. The microchip and microfluidic technologies enable sample preparation, including DNA extraction, purification, and amplification, prior to separation and detection (Bruijns *et al.*, 2016). Further details of DNA analysis can be found in encyclopedia entries *DNA Extraction and Quantification* and *Capillary Electrophoresis in Forensic Genetics*. Many of the advances in miniaturized liquid handling (i.e., microfluidics, lab-on-a-chip, centrifugal microfluidics, μPADs [microfluidic paper-based analytical devices], etc.) have also enabled more complete sample handling and preparation for numerous other detection schemes (e.g., electrochemical, and colorimetric, fluorescence).

Electrochemical Sensors

Electrochemical techniques are naturally amenable to miniaturization and exhibit field portability. These sensors measure the voltammetric response to electroactive compounds that have been specifically calibrated for detection. Electrochemical devices are often low cost and enable rapid detection with minimal sample preparation. However, beyond the basic commonality of electrochemical detection, this class of devices includes a range of designs and sensing elements, including conventional three-electrode cells, screen-printed electrodes, room temperature ionic liquids, solid hydrogel electrolytes, competitive immunosensors, aptamers, disposable paper-based devices, and more. Often, the sensing element of the device dictates the detection specificity and sensitivity. Ongoing advancements in novel sensing materials and chemistry may provide further applicability of electrochemical devices for field-deployable forensic analysis (Brown and Dennany, 2019).

Electrochemical sensors have seen repeated application to explosives detection (e.g., nitroaromatics, nitrate esters, nitramines, and peroxides), as well as demonstrations in other forensic areas such as illicit drugs, novel psychoactive substances, synthetic cannabinoids, and gunshot residues, among others. The state of samples (i.e., solid, liquid, vapor) may play a role in the devices capabilities and need or not for sample preparation to account for the matrix. Developments in disposable sensors aid in eliminating carryover or contamination difficulties. Though amenable to miniaturization, electrochemical devices require frequent

calibration and may exhibit poor stability depending on environmental and other conditions. In addition, they often perform best when used to target specific and select analytes, limiting applicability.

Colorimetry

Colorimetry is typically defined as the science of measuring color and color appearance with a colorimeter, an instrument for taking such measurements (Colorimetry - Glossary, 2021). The use of color-based chemical tests, which are typically designed to yield a measurable color change and have been developed for a vast array of chemical species, makes colorimetry a widely applicable technique. Color-based chemical tests of particular interest to forensic, HAZMAT, and/or national security professionals - ranging from single reagent spot tests to colorimetric papers and tubes - are discussed in the encyclopedia entry, Presumptive Chemical Tests. The pairing of color-based chemical tests and colorimeters has long been deployed in the lab and field in a variety of disciplines. Colorimeters have traditionally been categorized as either (1) spectrophotometers measuring transmittance or reflectance as a function of wavelength or (2) tristimulus devices that measure color based on light passing through three primary (red, green, and blue) filters (Choudhury, 2014). Light emitting diodes (LED), emitting narrow bands of light, are incredibly popular light sources in both benchtop and portable colorimeters, with commercially available devices often marketed as enabling measurement at specific wavelengths such as the Orion AOUAfast AO4000 Colorimeter with wavelength options of 420, 520, 580, and 610 nm (OrionTM AQUAfastTM AQ4000 Colorimeter and Accessories, 2021). Field-deployable broad range spectrophotometers are also widely available, such as the Hach DR1900 Portable Spectrophotometer with an wavelength range of 340-800 nm (DR1900 Portable Spectrophotometer, 2021). Tristimulus colorimeters have long featured in field work and are a goto device for a number of disciplines, with a variety of deployable devices commercially available such as the handheld Konica Minolta CR-410 Chroma Meter (2017).

Though colorimeters bring color clarity and quantitation abilities to color-based tests, the use of colorimeters in the field lags far behind portable IR and Raman devices judging from recent reviews of field portable devices for forensic, HAZMAT, and/or national security applications mentioned herein. Digital image colorimetry (DIC), incorporating portable imaging devices like smartphones and color space (e.g., red-green-blue, RBG) analysis, is poised to expand the use of color measurement devices in the field (Fang *et al.*, 2016; Fan *et al.*, 2021; Shin *et al.*, 2017; Jain *et al.*, 2021; Tiuftiakov *et al.*, 2021; Merli *et al.*, 2019; Fernandes *et al.*, 2020; Krauss *et al.*, 2016; Oliveira *et al.*, 2018). DetectaChem, a commercially available bundle of color-based test kits and DIC via a smartphone application called MobileDetect, is currently marketed for the assessment of suspected drugs and explosives (Kammrath *et al.*, 2021; DetectaChem, 2019). In the recent review *Forensics in hand: new trends in forensic devices* (de Oliveira *et al.*, 2018), smartphones for colorimetry featured prominently for detection of explosives, drugs, and other chemicals of forensic interest. The modification and "upcycling" of near ubiquitous devices such as colorimeters, fluorometers, and other detector types, is promising for a variety of applications. However, colorimetry does not provide structural details like vibrational spectroscopy or mass spectrometry, limiting its use along the presumptive to confirmation spectrum.

Lateral Flow Immunoassays

Long used for the detection of compounds in biofluids (e.g., urine, blood, saliva), recent developments in lateral flow immunoassays have targeted illicit drugs, specifically fentanyl and analogs. Similar lateral flow immunoassays have also been developed for other drugs such as Δ^9 -tetrahydrocannabinol or biological threats such as *Bacillus anthracis*. Though mainly demonstrated in research settings, lateral flow immunoassays are easy to use by nontechnical personnel, disposable, and relatively inexpensive. Early demonstrations have used lateral flow immunoassays for supervised injection facilities, drug checking services, and drug supply surveillance programs (Karamouzian *et al.*, 2018; Krieger *et al.*, 2018; Green *et al.*, 2020). Sample preparation for these tests is limited to dissolving solid samples into a buffer liquid and depositing onto the assay strip or dipping the strip in the resulting solution. Interpretation of results is also straightforward and similar to colorimetric tests. Lateral flow immunoassays exhibit sensitive detection for the targeted analyte; however they can also be susceptible to both false negatives from matrix effects and false positives due to cross reactivity.

Conclusion

Current field-deployable devices provide first responders and forensic investigators critical tools for preliminary identification of unknown materials and potential hazards. The variety in information provided, capabilities, and limitations of these techniques often enables complimentary coverage of scene and scenario needs. These needs are amplified by the ever-expanding and evolving list of target compounds encountered on-site. Detection of new target compounds relies on continuing to grow and curate technique specific compound libraries. In general, there is no single field-deployable device solution for all potential needs.

As the role of first responders and law enforcement in on-site scene assessment increases, technologies have become more geared toward use by nontechnical operators. This has led to novel workflows that involve sending data electronically to laboratory-based forensic scientists for further analysis and verification. In parallel, improving capabilities of field-deployable devices has also begun to enable on-site analyses by forensic scientists that may replace traditional laboratory analyses. These approaches and technologies must be rigorously verified and their reliability evaluated for adjudication. Similarly, a full

accounting of the uncertainties, limitations, and performance characteristics associated with field-deployable devices must be undertaken.

Further, as computational and statistical methods advance, chemometrics and machine learning will play an important role in supporting the forensic scientist and interpretation of data generated by field-deployable devices. The rigorous application of statistics to evaluation of forensic evidence critically supports proper interpretation. The Center for Statistics and Applications in Forensic Evidence (CSAFE) was established in 2015 to provide the forensic community with educational resources and tools for applying statistics to evidence. In addition, CSAFE also supports open-source databases and learning opportunities, including the potential role of machine learning in forensic science (CSAFE, 2020, 2017).

Disclaimer

These opinions, recommendations, findings, and conclusions do not necessarily reflect the views or policies of NIST or the United States Government. Certain commercial equipment, instruments, or materials are identified in this paper in order to specify the experimental procedure adequately or provide a device example. Such product mentions are not intended to imply recommendation or endorsement by NIST, nor do they imply that the materials or equipment identified are necessarily the best available for the purpose.

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