

Opportunities to Improve Airport Passenger Screening with Mass Spectrometry



Committee on Assessment of Security Technologies for Transportation, National Research Council

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OPPORTUNITIES TO IMPROVE AIRPORT PASSENGER SCREENING WITH MASS SPECTROMETRY

Committee on Assessment of Security Technologies for Transportation
National Materials Advisory Board
Division on Engineering and Physical Sciences

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Preface

The government agency charged with implementing technology for countering terrorist attacks is the Transportation Security Administration (TSA). TSA, and the Federal Aviation Administration (FAA) before it, has invested extensively in the development and deployment of technological and procedural systems to protect the traveling public. In support of its mission, TSA tasked the National Materials Advisory Board (NMAB) of the National Research Council (NRC) with convening a committee that would assess a variety of technological opportunities for protecting the U.S. transportation system. Accordingly, NMAB convened the Committee on Assessment of Security Technologies for Transportation.

STATEMENT OF TASK

TSA prepared for the committee the following statement of task:

This study will explore opportunities for technology to address national needs for transportation security. While the primary role of the committee is to respond to the government's request for assessments in particular applications, the committee may offer advice on specific matters as required. The committee will: (1) identify potential applications for technology in transportation security with a focus on likely threats; (2) evaluate technology approaches to threat detection, effect mitigation, and consequence management; and (3) assess the need for research, development, and deployment to enable implementation of new security technologies. These tasks will be done in the context of current, near-term, and long-term requirements. The committee will perform the following specific tasks:

1. Identify potential applications for technology in transportation security with a focus on likely threats derived from threat analyses that drive security system requirements. Review security system developments structured to meet the changing threat environment. Assess government and commercial industry plans designed to address these threats.
2. Evaluate technology approaches to threat detection, effect mitigation, and consequence management. Delineate the benefits of the insertion of new technologies into existing security systems. Evaluate the trade-offs between effectiveness and cost, including the cost of changing the security system architectures.

3. Assess the need for research, development, and deployment to enable implementation of new security technologies. Review and assess the potential benefit of existing and advanced detection technologies, including scanning technologies, sensing technologies, and the use of computer modeling and databases. Review and assess emerging approaches to effect mitigation and consequence management.

COMMITTEE APPROACH

An overarching goal of the committee is to provide timely reports that meet TSA's priorities for defeating terrorist threats. The committee judged that this could best be done by issuing a series of short reports on chosen technology applications. In consultation with TSA, the committee selected six topics for review, the first of which is the subject of this report:

1. Mass spectrometry for enhanced trace detection
2. Chem/bio sensors and mitigation of threats
3. Viability of aviation countermeasures against shoulder-launched missiles
4. Millimeter wave imaging for explosives detection
5. Machine false alarm reduction
6. Data fusion and integration for airport terminals

This list may be amended during the course of study if significant new threats arise.

As is apparent from the above list, the committee is focusing on aviation security. Many of the technologies considered will also have application in protecting other transportation modes, and deployment in the aviation security arena is viewed as a valuable testbed for gaining experience that might be applied to other transportation situations. Accordingly, although most of the discussion in this report is directed toward aviation security, the committee believes that it could be adapted for bus terminals, train stations, cruise ships, and so on with relatively minor modifications.

These reports are studies of technological capabilities rather than analyses of specific security system instruments deployed to counter threats. The intent is to discuss, describe, and assess the viability of each technology for threat detection, location, and mitigation in the most fundamental sense. Each report will assess the significance of a technology, and if the technology is found to be significant, the report will suggest a phased R&D and implementation scenario that is likely to result in successful deployment.

The February 2004 discovery of the biological poison ricin in a Senate office building in Washington, D.C., highlights the fact that the terrorist's arsenal now includes not only all-too-familiar weapons such as small arms and explosives, but also chemical and biological agents. This expanding arsenal demands that policy makers and transportation authorities consider the deployment of new defensive technologies to respond to the new threats. Because the committee believes that mass spectrometry has the potential to extend the capabilities of current trace detection technologies used at airports to address these new threats, it has chosen to make mass spectrometry the subject of its first report.

This study was conducted under the auspices of the NRC's National Materials Advisory Board. The committee acknowledges the support of the director, Toni Maréchaux, and the board staff. The chair is particularly grateful to key members of the committee, Michael Story and Elizabeth Slate, who, along with the study director, support staff, and publication staff, worked diligently on a demanding schedule to produce this report.

Thomas S. Hartwick, *Chair*

Sandra L. Hyland, *Vice Chair*

Committee on Assessment of Security Technologies for Transportation

Acknowledgment of Reviewers

This report has been reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise, in accordance with procedures approved by the National Research Council's Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making its published report as sound as possible and to ensure that the report meets institutional standards for objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process. We wish to thank the following individuals for their review of this report:

Arnold Barnett, Massachusetts Institute of Technology
Raymond H. Bittel, The Boeing Company
Gary W. Carriveau, Science Applications International Corporation
Matthias Frank, Lawrence Livermore National Laboratory
Gary L. Glish, University of North Carolina, Chapel Hill
R. Kenneth Marcus, Clemson University

Although the reviewers listed above have provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations, nor did they see the final draft of the report before its release. The review of this report was overseen by R. Stephen Berry, University of Chicago. Appointed by the National Research Council, he was responsible for making certain that an independent examination of this report was carried out in accordance with institutional procedures and that all review comments were carefully considered. Responsibility for the final content of this report rests solely with the authoring committee and the institution.

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Acronyms and Abbreviations

APL	Applied Physics Laboratory at Johns Hopkins University
ASMS	American Society for Mass Spectrometry
CBMS	chemical and biological mass spectrometer
DARPA	Defense Advanced Research Projects Agency
DERA	Defence Evaluation and Research Agency (U.K.)
DMNB	dimethylnitrobenzene
DNA	deoxyribonucleic acid
DNT	dinitrotoluene
DOT	U.S. Department of Transportation
EDS	explosive detection system
EGDN	ethylene glycol dinitrate
ESI	electrospray ionization
ETD	explosive trace detector
FAA	Federal Aviation Administration
GC	gas chromatography
HMTD	hexamethylene triperoxide diamine
HMX	cyclotetramethylenetetranitramine
IMS	ion mobility spectrometer
LC	liquid chromatography
MALDI	matrix-assisted laser desorption/ionization
MS	mass spectrometry
MS/MS	multiple stages of mass spectrometry
NG	nitroglycerine

NRC	National Research Council
NT	nitrotoluene
PCR	polymerase chain reaction
PD	probability of detection
PETN	pentaerythritol tetranitrate
Pfa	probability of false alarms
QMS	quadrupole mass spectrometer
RDX	cyclotrimethylenetrinitramine
SASP	small acid-soluble protein
TATP	triacetone triperoxide
TFA	trifluoroacetic acid
TNT	trinitrotoluene
TOF	time of flight
TSA	Transportation Security Administration

Executive Summary

Over the past 20 years, the Transportation Security Administration (TSA)¹—and the Federal Aviation Administration (FAA) before it—invested extensively in the development of systems designed to protect the traveling public from attacks on the commercial aviation system involving explosives. These efforts have resulted in the deployment of two kinds of technologies for screening of baggage and passengers: explosive detection systems (EDSs), which are certified to detect bulk quantities of explosives in checked baggage, and explosive trace detectors (ETDs), which are designed to detect vapor or particles of explosive that would be associated with personal items or carry-on bags as a result of bomb fabrication and transportation. ETDs are also used as one method of resolving alarms from EDSs. An EDS alarm is a more direct indicator of the presence of a potential bomb, since the EDS is designed to detect objects with physical dimensions and densities consistent with threat quantities of explosive materials. The alarm from an ETD, which responds to traces of explosive material, only suggests that a bomb may be present.

In the case of certain explosives, experiments suggest that it is difficult to make a bomb without contaminating persons and things associated with that fabrication. Many of these materials are very sticky, and once a finger has been in contact with the explosive, it is capable of leaving many subsequent fingerprints (on briefcases, clothes, boarding passes, etc.) with detectable amounts of material. The advantages of trace detection are that it can be used on people and baggage without harming them and that it raises minimal privacy issues. This report focuses on opportunities for improving the ability of ETDs to detect terrorist threat materials in transportation—specifically, airport—environments.

Some 7,000 ETDs have been deployed by the TSA in U.S. airports for the interrogation of carry-on baggage for traces of explosives. ETDs are located at passenger checkpoints as well as many other airport venues, and the acquisition of samples involves an operator wiping down surfaces of luggage or carry-on items with a dry pad, which is then most commonly introduced into the sample port of an ion mobility spectrometer (IMS). In the IMS, the target and background molecules in the sample are first ionized and then passed through a drift space, where they are separated based on their mobility. The pattern of separation is compared to a library of known patterns to identify the substance collected. The entire process takes about 1 minute.

¹The Transportation Security Administration, formerly under the Federal Aviation Administration (FAA) in the Department of Transportation, is charged with implementing technology for countering terrorist threats. In March 2003, TSA was placed under the Border and Transportation Security component of the new Department of Homeland Security.

These IMS systems have been in development for decades, and the technology is relatively mature. By limiting the detection requirements to certain classes of explosives and by setting the alarm threshold relatively high so as to reduce the number of false positives, instrument complexity and cost are kept low (less than \$40,000 per instrument) relative to typical laboratory analytical instruments. However, the currently deployed systems have limitations specific to the physics and chemistry of their operation that make them unsuitable for addressing a variety of emerging threats.

LIMITATIONS OF CURRENT TRACE TECHNOLOGY

Trace detection methods are subject to some inherent limitations that are common to all such methods; currently deployed IMS detectors also have some limitations that are more specific to the IMS technology.

Generic Limitations of Trace Detection

Since trace detection methods are not capable of detecting threat quantities of explosive materials directly (as are bulk detection methods), their efficacy is based on the presumption that in the course of preparing and delivering a bomb, the bomb carrier or his personal items will become contaminated with a residue or vapor that is characteristic of the explosive, and that this residue will be available for sampling at a screening point. Their efficacy also depends on the presumption that the threat residue is present in quantities sufficient to be sampled from the person or thing and detected by the deployed ETDs. If any of these presumptions is incorrect, trace detection is not applicable.

Some of the issues that stem from the inferential nature of trace detection are the following:

- *Sampling issues.* As deployed in airports, trace detection equipment depends on blind sampling, whereby an operator attempts to acquire a sample by wiping areas where threat materials are thought most likely to be present. This method may fail to acquire an adequate sample if the bomb was prepared without leaving sufficient residues, if the external surface was cleaned by the terrorist, or—even when explosive residues are present—if the wiping fails to contact the areas of residue.

Another issue related to sampling is that while passenger screening has been the primary justification for trace detection, currently deployed systems sample neither the passenger's body nor his or her clothing for residues of threat materials—but rather only selected personal items and carry-on bags that are likely to have been touched by the passenger. Other than metal detectors, no currently deployed technology screens the passengers themselves. One promising approach for detecting explosive residues that may adhere to a passenger's skin or clothing is the portal sampler.² Portal prototypes have been tested by TSA, but not one has yet been deployed.

- *Alarms due to innocently acquired residues.* The trace detector may alarm if an individual or bag has had some innocent, incidental contact with a threat material in the past. This might occur, for example, if the individual works in the commercial explosives industry; owns a gun or has contact with someone who does; or is taking nitroglycerin heart medication. In this

²A typical portal system performs a nonintrusive sampling of individuals that takes approximately 10 seconds. An individual enters the portal, where jets of compressed air are pulsed to ruffle clothing and detach particles. The volume of air in the portal is then drawn through a preconcentrator device that strains the particles and condensable vapors onto a mesh. This residue is further concentrated and then sent to an analyzer.

case, the detector is functioning as it was designed to, but the alarm does not reflect the individual's one-time proximity to a bomb.

Specific Limitations of Current ETDs

Despite their maturity, IMS-based ETDs also have several specific limitations, discussed below.

- *Vulnerability to higher false alarm rates at lower alarm thresholds.* Current airport IMS systems have an inherently low chemical specificity compared with other analytical instrument systems. In other words, they have a limited ability to distinguish threat substance molecules from interfering molecules that may be in the sample background. As the detection threshold is lowered, this lack of specificity will result in a higher level of false alarms.
- *Limited number of threat agents concurrently detectable.* Current ETDs are designed to detect selected explosives. Because the ionization conditions, dopant gas, and drift time window are optimized for these explosives, IMS systems have limited capability to be reconfigured to concurrently detect new threat materials. As the list of threat materials available to terrorists increases (and assuming the threat scenario is consistent with the expectation of residues), it will be important to develop the capability to concurrently detect a wider range of threat materials.

Improving ETD Performance

The committee offers the following finding and recommendation for improving the performance of currently deployed ETDs:

Finding 1: The trace detection systems currently deployed in airports have limited utility for the following reasons:

- **The relatively low chemical specificity of IMS means that the instrument alarm threshold must be set high to avoid excessive false alarms; yet, lower alarm levels are desirable to account for inefficient manual and portal sampling techniques and, possibly, “cleaner” perpetrators.**
- **Detection is dependent on the use of blind sampling methods that cover only a small portion of the bag surface for acquisition of adequate residues for analysis.**
- **Current sampling protocols do not allow for the sampling of explosive residues or vapors that may be associated with a passenger’s skin or clothing.**
- **Currently deployed IMS systems are designed to detect only a specific list of explosives and cannot easily be reconfigured to detect an expanded list of explosive, chemical, and biological threat substances.**

Recommendation 1: To address these deficiencies in the performance of explosive trace detectors, TSA should do the following:

- **Place a high priority on the development and deployment of automated trace sampling hardware.**
- **Decrease the threat alarm threshold for ETDs systematically over time to improve the probability of detection of residues while keeping false alarms at current levels.**

- **Deploy passenger screening portals to enable the detection of explosive traces on passengers' skin and clothing, and assess the acceptability and efficacy of the portals.**
- **Explore new technologies with higher chemical specificity that are capable of detecting a wider range of explosive, chemical, and biological threat materials.**

OPPORTUNITIES TO IMPROVE TRACE DETECTION SYSTEMS WITH MASS SPECTROMETRY

To improve upon the IMS trace detection systems currently deployed in airports across the United States, mass spectrometry (MS) is an obvious candidate to consider. It has become the gold standard for resolving high-consequence analyses involving water, air, and ground pollution; pharmaceutical drug development and manufacture; treaty compliance verification relating to the proliferation of nuclear materials; verification of employee drug abuse for prosecution and job termination; detection of performance-enhancing drugs in horses and athletes; and routine analysis in the chemical, drug, and fuel manufacturing industries.

While mass spectrometers have become one of the analytical mainstays of today's chemistry and biotechnology laboratories, they have historically been large, complex systems that occupied the volume of several file cabinets, were operated by highly trained mass spectrometrists, and sold for around \$250,000. More recently, with demand from lab chemists and technicians for instruments that could be used for routine analysis, automated, self-calibrating, auto-tuning, benchtop units of reasonable size and costing \$50,000 to \$100,000 have become available. These instruments are generally coupled with a gas chromatograph or a liquid chromatograph at the sample inlet to improve chemical selectivity. Indeed, some special-purpose instruments have been miniaturized for mobile applications, though the performance and reliability of these miniaturized systems are still being assessed. In general, however, all of these instruments operate at high vacuum and need professional care and trained operators.

Mass spectrometry is not new to the TSA, which has tested a personnel screener utilizing an MS-based system manufactured by Syagen Technology and a portal developed by Sandia National Laboratories. MS has also been applied by others for the automatic analysis of samples acquired from boarding passes. In the committee's view, such systems could add significantly to future trace detection capabilities for a variety of threat substances in the transportation context.

Mass spectrometers utilize four steps for analysis: (1) vaporize the sample, (2) place an electric charge on sample molecules to form ions, (3) separate the ions based on their charge-to-mass ratio using an electric or magnetic field, and (4) determine the number of separated ions having a particular charge-to-mass ratio. The uniqueness of mass spectrometry lies in its chemical specificity. It directly measures a fundamental property of the target molecule—its molecular weight—and thus provides a highly specific means of identifying the molecule. By contrast, IMS systems measure a secondary and less specific property of the target molecule—the time it takes for the ionized molecule to drift through a tube filled with a viscous gas under an electric field—and the identity of the molecule is inferred from the time vs. intensity spectrum, which is compared with standard spectra in the instrument's database. Since different molecules may have similar drift times, IMS inherently has less chemical specificity than MS.

In fact, the committee estimates that a typical tandem mass spectrometer (two mass spectrometer analyzers arranged in series, or a single trapping spectrometer making tandem analyses in time)—an instrument configuration commonly found in analytical laboratories—has a chemical specificity (or informing power) about 10,000 times greater than that of a typical IMS instrument.

Advantages of MS-Based Detection Systems

As a trace detection technology, MS-based systems have the same generic limitations as all the trace detection technologies discussed above. However, MS-based systems enjoy some advantages over current IMS systems:

- *Lower detection limit while maintaining low false alarm rates.* Given the unpredictable efficiency of sample acquisition, discussed above, it is desirable to reduce alarm thresholds below current levels in order to increase the probability of detecting trace residues or vapor while maintaining passenger throughput. IMS systems have alarm thresholds typically set about 100 times the detection limit; however, lowering the alarm threshold will increase the false alarm rate. MS-based systems should be capable of alarm thresholds 1,000 times lower. Given the committee's estimate that MS-based detectors should have 10,000-fold greater chemical specificity than IMS-based systems, this lower alarm level should be achievable without increasing the rate of false alarms that are due to interfering compounds in the sample background. Note, however, that the lowered detection limit may increase the number of alarms caused by the detection of innocently acquired explosive residues.
- *Broader range of threat substances concurrently detectable.* The flexibility and chemical specificity inherent in MS-based systems make them capable of concurrently detecting a much broader range of threat substances than IMS, including a broader range of explosives, chemical warfare agents, and biological agents. Detection and identification of many of these agents with MS have already been demonstrated under both laboratory and field conditions.

Challenges for MS-Based Detection Systems

MS-based systems face a number of challenges before they can be deployed in airports as trace detectors:

- *Reducing cost and complexity and increasing ruggedness.* The U.S. Army and the Defense Advanced Research Projects Agency (DARPA) have conducted proof-of-principle research and development, testing, and evaluation for both chemical and biological threat analysis using fieldable, rugged, specialized mass spectrometer systems. It is likely that much of the work that these and other entities have done could be used directly or modified for TSA threat scenarios, but TSA needs to focus on its unique needs for a rugged, backbone mass spectrometer that would be useful for many threat detection scenarios. Although extensively used for a variety of laboratory applications, commercially available chemical analysis systems (chromatography followed by two stages of mass analysis, or C/MS/MS) are not designed for an environment as harsh as an airport or other transportation arenas,³ nor are they designed for use by TSA security operators.⁴

³Given the range of airport deployment sites (e.g., baggage rooms, curbside check-in kiosks, passenger checkpoints), an ETD must be able to operate effectively under a variety of adverse conditions, including extremes of temperature, changes in barometric pressure, high humidity, and high levels of dust or other airborne particles. IMS systems have been known to fail under such conditions, and substantial investment may be required to adapt MS-based systems for reliable use in these environments.

⁴Since the configuration of airport instruments is not known at this time, the extent of technical support and operator training is not known and is not addressed in this report.

- *Resolving sampling issues.* The configuration of the sample inlet (chromatograph, if needed), the ionization method, the number of mass analysis stages, and the kind of ion detected will depend on the problem to be solved. Even though modern mass spectrometer systems can be automatically reconfigured based on an analysis just performed (e.g., changing the detection from positive ions to negative ions, or changing which ion is selected in the first stage of an MS/MS system), it is not reasonable to expect that one inlet and one ionization method will serve all threat materials or deployment scenarios. Choosing the most appropriate configurations will take time and additional research. An attempt should be made to select a configuration that is extendable to as many threat scenarios and materials as possible.
- *Improving database robustness.* To identify a target molecule using a mass spectrometer, the spectrum obtained would be compared against a library of reference spectra, and a software algorithm would determine if a match occurred. Such algorithms, formats, and spectral libraries already exist and would form the basis for those used in this application. Once the methods of analysis are chosen, corresponding libraries will need to be augmented. All commercial MS data systems allow libraries to be created based on standard samples of interest. Since the chemical specificity of the analysis technique allows for the elimination of most if not all background signals, it is not necessary to run standards in the presence of all known backgrounds, as is always necessary with IMS.

Getting Started

Reported test results on deployed MS-based trace detectors suggest that these instruments are capable of a low limit of detection as well as a low false alarm rate.⁵ This supports the committee's view that TSA should initiate a vigorous program to take advantage of the opportunities offered by MS-based detector technologies. Thus, if TSA wishes to invest in the improvement of trace detection technologies, the committee offers the following finding and recommendation:

Finding 2: Owing to their lower limit of detection, higher chemical specificity, and chemical flexibility, MS-based trace detection systems have the capability to address many of the limitations of IMS-based systems.

Recommendation 2: TSA should establish mass spectrometry as a core technology for identifying an expanded list of explosives, as well as chemical and biological agents. Specifically, TSA should

- **Create a prioritized list of threat materials that are likely to fit a residue scenario and a second list of materials that are not likely to fit the scenario**
- **Determine appropriate MS sampling procedures, inlet configurations, ionization methods, and analysis strategies for relevant materials on this list.**

A good way to bootstrap this entire process would be to purchase the best field-deployed instrument to gain experience and to test system applications. One option would be for TSA to purchase an instrument such as the one described in Box 2-1 and evaluate its effectiveness in the airport context.

⁵One example is described in Box 2-1.

A Phased Implementation Plan

Full-scale deployment of MS-based detectors in airports cannot occur immediately; it will require a phased approach involving several generations of instruments, as outlined in the following finding and recommendation.

Finding 3: The many trace detection tasks that can be envisioned in airports will require MS-based detection systems with various levels of cost and performance; in some cases, years of R&D and testing may be required to produce MS instruments with the necessary specifications.

Recommendation 3: If TSA wishes to improve its trace detection capabilities, it should deploy MS-based detectors in a phased fashion, with successive generations of instruments addressing lower quantities of an expanded list of threat materials and more sophisticated security tasks. These tasks range from passenger screening at checkpoints to monitoring of the air handling system.

Here, the committee offers just one plausible scenario for such a phased deployment at a large urban airport. The dollar figures are estimates based on the best judgment of committee members familiar with the development of MS apparatus.

- *Phase 1 (1 to 3 years)*. Deploy a limited number of portal sampling systems with both IMS- and first-generation MS-based detectors at airport checkpoints. Compare the performance and reliability of these systems under typical passenger flow conditions.⁶ This would involve the deployment of perhaps 5 to 10 portals costing \$100,000 to \$150,000 each for a large urban airport. The first-generation MS-based portals might incur \$25,000 to \$50,000 more in initial costs compared with comparable IMS portals. Operating costs for an MS-based portal are expected to be \$2,000 to \$5,000 higher per year.
- *Phase 2 (3 to 5 years)*: Develop a second-generation MS instrument with a single geometric configuration that can detect a variety of threat agents, including chemical and biological agents as well as a broader range of explosives. Compare this second-generation instrument with the best available IMS devices at passenger checkpoints and portals to assess suitability and versatility. This would involve deployment of 10 to 20 MS detectors costing perhaps \$100,000 to \$150,000 each.
- *Phase 3 (5 to 10 years)*: Replace current IMS ETDs with fully cost-reduced and automated MS systems that would support both passenger and carry-on screening. This third-generation, automated MS detector would be used in place of IMS in every passenger path and could also be used as an adjunct to EDS x-ray systems in the checked baggage path as well. A major benefit of this device would be to reduce the necessity for hand searches. At a large urban airport, implementation of this phase would mean deployment of perhaps 50 instruments that are assumed to have an initial cost of no more than \$75,000 and an operating cost of less than \$5,000 per year.
- *Phase 4 (>10 years)*: Develop MS-based detectors for use in monitoring for terrorist attacks on the air handling equipment in either a transportation terminal or in the transportation vehicle. This class of instruments is less well-defined than the instruments discussed above, and if biological threats are to be considered, one could expect the cost of this device to exceed the costs of the instruments described above by a factor of between 2 and 3 because of

⁶It would not be necessary to scan each bag with both technologies, as this would result in unacceptable delays for passengers. Rather, the technologies would be evaluated independently based on aggregate performance numbers from similar sets of bags. It would be important to test these technologies under a range of conditions—for example, wintertime/summertime—as well as at various deployment sites—for example, JFK and SFO and any other airports that have unique characteristics.

the added expense associated with sample collection and preparation. In a large urban airport, 5 to 10 instruments might be required, depending upon the extent to which remote sampling could be utilized.

1

Background and Overview

The U.S. transportation system is an attractive target for terrorists because it could allow them to cause immediate harm to large numbers of people and create anxiety for many times more, as well as to cause massive economic disruption in the United States and around the world. The system is vulnerable because its mission is to provide service to people with a minimum of intrusion on privacy and disruption of access. The detection and mitigation of attacks on transportation are made more difficult by the transient nature of the passengers and the fact that passengers often carry large amounts of baggage, making it relatively easy to conceal threat materials. The September 11, 2001, attacks on the Pentagon and the World Trade Center, in which commercial airliners were used as weapons, also broadened the concept of what constitutes a threat to U.S. assets in general and the transportation system in particular.

Based on historical terrorist attacks involving the hijacking and bombing of aircraft, current threat detection measures concentrate on detecting weapons or specific explosives. In the future, such attacks could also involve the use of toxic chemicals, chemical and biological weapon agents, or even nuclear materials.^{1, 2}

CURRENT TECHNOLOGIES TO PROTECT AVIATION SECURITY

FAA and TSA efforts over the past 20 years have resulted in the development and deployment of two kinds of technologies for the screening of baggage and passengers: explosive detection systems (EDSs), which are designed to detect bulk quantities of explosives in checked baggage,³ and explosive trace detectors (ETDs), which are designed to detect vapor or particles of explosive that are collected (sampled) from personal items or carry-on bags. From bomb fabrication and transportation, EDSs are systems that are certified by the FAA as being capable of detecting threat quantities of specified

¹The President's Homeland Security Department Proposal, at <http://www.whitehouse.gov/deptofhomeland/bill/index.html>

²National Research Council. 2002. Making the Nation Safer: The Role of Science and Technology in Countering Terrorism, Washington, D.C.: National Academies Press.

³Small versions of EDS machines are also being developed to replace current x-ray equipment for screening of personal luggage. The deployment of such small bulk detectors (whether based on computed tomography or some other technology) at passenger checkpoints in the future would probably affect the role played by trace detectors at such checkpoints.

explosives. Currently, the two certified EDS systems are both based on x-ray computed tomography technology. Since this report focuses on trace detection, these systems are not discussed further here.

Some 7,000 ETDs have been deployed by the TSA in U.S. airports.⁴ They are deployed in various venues: at passenger checkpoints, in baggage rooms to resolve alarms from EDS machines, in terminal lobbies together with EDS machines; at curbside check-in kiosks; at remote baggage screening locations, including hotels; at ticket counters where bags are screened; and at lobby drop-and-go points.

This report does not comment on the manner in which ETDs should be deployed—for example, in the checked baggage stream instead of at passenger checkpoints. Rather, it focuses on the potential of mass spectrometry to improve the performance of ETDs, wherever they may be deployed.

The majority of current ETDs are ion mobility spectrometers (IMSs), which utilize an ionizing source, a drift spectrometer, a detector, and an alarm and data presentation processor. Chemical identification is accomplished by tailoring the ion chemistry in the ion source for the material(s) to be detected (along with molecules likely to be present that might interfere with the analysis) and passing the resulting ions through a drift space, where they are separated based on their mobility.

ETDs are deployed at various airport locations, where operators acquire samples by wiping down surfaces of luggage or carry-on items with a pad, which is then introduced into the IMS sample port. For trace detection to be useful for aviation security, these objects or persons would have to be contaminated by residue from the preparation and delivery of the explosive device.

Experiments suggest that it is difficult to fabricate a bomb containing certain explosives without contaminating persons and things associated with that fabrication. Many of these materials are very sticky, and once a finger has been in contact with the explosive, it is capable of leaving many subsequent fingerprints (on briefcases, clothes, boarding passes, etc.) with detectable amounts of material. Of course, since each subsequent fingerprint will contain less material than the previous one, the actual amount specified as an alarm amount for the trace detection system is a bit arbitrary; however, the lower the limit of detection of the device, the higher the probability that a residue will be detected.

The IMS systems used for trace explosives detection in airports have been in development for decades, and the technology is relatively mature. In the committee's judgment, only incremental advances in the technology's performance can be expected in the future. By limiting the detection requirements to a specific set of explosives and by setting the detection limit relatively high, instrument complexity and cost are kept low (~\$40,000) relative to typical laboratory analytical instruments.

The advantages of trace detection are that it can be used on people and baggage without harming them and that it raises minimal privacy concerns. In addition, it can be deployed in passenger screening areas because of its relatively small size and low cost. The 7,000 or so units now deployed also have a deterrent value.

LIMITATIONS OF CURRENT TRACE TECHNOLOGY

An ideal trace system would be capable of inexpensively detecting a specific threat substance and distinguishing it from a complex background on a time scale appropriate for terminating the threat and mitigating the impact on people, property and flight operations. Unfortunately, there is no system that is widely deployable and able to identify all threat substances in real time.

Since trace detection methods do not detect threat quantities of materials directly (as do bulk detection methods), their efficacy presumes that in the course of preparing and delivering a bomb, the terrorist and/or his personal items will become contaminated with a residue or vapor that is uniquely characteristic of the explosive, and that this residue will be available for sampling at a screening point. It also presumes that the threat residue is present in quantities sufficient to be sampled from the person or

⁴TSA Fact Sheet.

thing and detected by deployed ETDs. If these presumptions are incorrect, trace detection is not applicable. The indirect nature of trace detection means that a positive detection does not confirm the presence of a threat amount of explosive, nor does a negative result confirm the absence of an explosive.

Generic Limitations

Trace threat detection techniques as deployed in airports are subject to a number of generic limitations that stem from the indirect nature of the detection: These include sampling issues and false alarms triggered by innocently acquired residues.

Sampling Issues

As deployed in airports, trace detection equipment depends on blind sampling, whereby an operator attempts to acquire a sample by wiping areas where threat materials are thought most likely to be present. This method may fail if the bomb is prepared without leaving residues, if the external surface has been cleaned, or—even when explosive residues are present—if the wiping fails to contact the areas of residue.

Another limitation is that while passenger screening has been the primary justification for trace detection, in currently deployed systems neither the passenger's body nor his or her clothing is sampled for residues of threat materials—only selected personal items and carry-on bags that are likely to have been touched by the passenger are sampled. Other than metal detectors, there is no currently deployed technology for screening the passengers themselves. One promising approach for detecting explosive residues that may adhere to a passenger's skin or clothing is the portal sampler.⁵ Portal prototypes have been tested by TSA and a draft Acceptance Test Plan issued,⁶ but no portal has yet been deployed.

Finally, a trace detector may alarm if an individual or bag has had some innocent, incidental contact with a threat material in the past. This might occur, for example, if the individual works in the commercial explosives industry or has contact with someone who does, or is taking nitroglycerin heart medication. In this case, the detector is functioning as it was designed to, except that an alarm does not reflect the presence of a bomb—again, a limitation of trace detection.

Specific Limitations of Current ETDs

Despite their maturity, ETDs as currently deployed in airports also have several specific limitations, discussed below.

Vulnerability to Higher False Alarm Rates at Lower Alarm Thresholds

Current airport IMS systems use a combination of ionization chemistry, dopants, and negative ion sensing to detect specific explosives and have an inherently lower chemical specificity than many other analytical techniques—for example, mass spectrometry (see Chapter 2). In other words, they have a limited ability to distinguish threat substance molecules from interfering molecules that may be in the sample background. Given the uncertainty surrounding the amount of explosive residue that may be

⁵A typical portal system provides a nonintrusive sampling of individuals that takes approximately 10 seconds. An individual enters the portal, where jets of compressed air are pulsed to ruffle clothing and detach particles. The volume of air in the portal is then drawn through a preconcentrator device that strains the particles and condensable vapors onto a mesh. This residue is further concentrated and then sent to an analyzer.

⁶R.T. Chamberlin and S. Brunk. 2002. Acceptance Test Plan for Explosive Trace Detection Portals, DOT/TSA/AR. December.

present on a bag and current sampling techniques, which sample only a small fraction of the bag's surface, the current level of alarm should be reduced to increase the probability of detection.

Unfortunately, with a technique such as IMS, which has relatively low chemical specificity, as the alarm threshold is lowered, the number of false alarms will increase when innocent materials are misidentified as threat materials.

False alarms bog down a security system by increasing the time required to screen individuals and requiring use of additional equipment and personnel to meet departure schedules. They also degrade the performance of a screening system by creating a sense among operators that all alarms are false. In extreme cases, responses could include shutting down buildings, clearing airports, and preparing for the isolation and treatment of a significant population. It is important to balance the consequences of an alarm with the certainty of identification: High-impact consequences demand high-certainty identification. As the alarm threshold for trace analyzers is lowered, either to increase the probability of detection or to accommodate situations where there is less threat material available, it will be important to increase the chemical specificity of the device to avoid increasing false alarms.

Limited Number of Threat Agents Concurrently Detectable

Technology development has focused on specific classes of explosives almost exclusively, in part because these materials are readily distinguishable from typical background materials and in part because these kinds of explosives were thought to be the most readily available to those who want to harm the aviation system. As a result, current ETDs are only able to detect certain explosives. They have little if any capability for simultaneously detecting other threat substances, including other classes of explosives and chemical and biological threats. Further, IMS systems cannot be reconfigured to concurrently detect a broad palette of these new threat substances. As the list of threat substances available to terrorists increases (and assuming the threat scenario is consistent with the expectation of residues), it will be important to develop the capability for concurrently detecting a wider range of threat substances.

Summary

Trace explosives detection as practiced in airports today is a system of limited effectiveness and significant vulnerabilities. Nevertheless, ETDs are the only technology currently available for screening passengers and their carry-on luggage for selected threat materials. With the proliferation of knowledge about how to synthesize a variety of explosives as well as chemical and biological agents, and the known interest in these substances on the part of terrorist groups, new analysis techniques are needed that could reliably detect a wide range of threat substances in lower quantities without increasing the rate of false alarms in high-consequence situations.

FOCUS AND STRUCTURE OF THIS REPORT

If, despite the limitations detailed above, trace detection technology continues to be relied upon for passenger and baggage screening, the committee believes that there are alternative technologies that would greatly increase the probability of detection at acceptably low false alarm rates. In particular, this report focuses on the potential role for mass spectrometry to improve trace detection capabilities now deployed in airports for the growing variety of threat materials. Mass spectrometry was selected because, in the committee's opinion, it has the greatest potential for addressing the deficiencies in the current trace techniques over the next 5 to 10 years.

Chapter 2 discusses the capabilities of mass spectrometers and the potential opportunities and challenges that they present for the trace detection of threat agents. Chapter 3 discusses R&D priorities

that need to be addressed before such instruments could be deployed in an airport setting and suggests one possible phased strategy for such deployment.

2

Mass Spectrometry for Trace Detection of Threat Agents

Mass spectrometry (MS) is an obvious candidate to consider for improving the IMS-technology-based trace detection systems currently deployed in airports across the United States. It has become the gold standard for resolving high-consequence analyses involving water, air, and ground pollution; pharmaceutical drug development and manufacture; treaty compliance verification relating to proliferation of nuclear materials; verification of employee drug abuse for prosecution and job termination; detection of performance-enhancing drugs in horses and athletes; and routine analysis in the chemical, drug, and fuel manufacturing industries.¹

While mass spectrometers have become one of the analytical mainstays of today's chemistry and biotechnology laboratories, they have historically been large, complex systems that occupied the volume of several file cabinets, were operated by highly trained mass spectrometrists, and sold for around \$250,000. The generalized use of the instruments by lab chemists and technicians has led to automated, self-calibrating, auto-tuning, benchtop units of reasonable size costing \$50,000 to \$100,000. These instruments are generally coupled with a gas chromatograph (GC) or a liquid chromatograph (LC) at the sample inlet to further enhance chemical selectivity. Some special-purpose instruments have been miniaturized for mobile applications,² though the performance and reliability of these miniaturized systems are still being assessed. In general, however, all of these instruments operate at high vacuum, and they need professional care and trained operators.

Mass spectrometry is not new to the TSA; as a result of a TSA program focusing on the use of MS technology, researchers concluded that "there are no major technical barriers to its use in the field for trace detection scenarios, provided effective sampling and introduction procedures for the specific application are employed."³ Currently, the TSA is testing a personnel screener utilizing an MS-based system from Syagen Technology and a portal from Sandia National Laboratories.⁴ MS has also been

¹ M.A. Grayson, ed. 2002. *Measuring Mass: From Positive Rays to Proteins*. Philadelphia: Chemical Heritage Foundation.

² For a rather extensive listing of portable/mobile mass spectrometers see <http://www.gcms.de/#Time-of-Flight>.

³ S.A. McLuckey, D.E. Goeringer, and K.G. Asano. 1996. *High Explosives Vapor Detection by Atmospheric Sampling Glow Discharge Ionization/Tandem Mass Spectrometry*. Report No. ORNL/TM-13166. Oak Ridge, Tenn: Oak Ridge National Laboratory.

⁴ Jack A. Syage, Karl Hanold, Charles Rhykerd, Frank Bouchier, and Kevin Linker. 2002. MS-based explosives detection portal for passenger screening. *Proceedings of the 50th ASMS Conference on Mass Spectrometry and Allied Topics*, Orlando, Fla. June 2-6.

applied by others for the automatic analysis of samples acquired from boarding passes (see Box 2-1).⁵ In the committee's view, such systems have the potential to add significantly to future trace detection capabilities for a variety of threat substances in the transportation context, as discussed below.

PRINCIPLES OF MASS SPECTROMETRY

Mass spectrometers use four steps for analysis: vaporizing the sample; placing an electric charge on sample molecules to form ions; separating the ions based on their charge-to-mass ratio using an electric or magnetic field; and, finally, determining the number of separated ions having a particular mass-to-charge ratio (i.e., producing a "mass spectrum"). Some mass spectrometers that operate in this fashion are called quadrupole mass spectrometers (QMS), sector field mass spectrometers, and ion trap mass spectrometers. In a time-of-flight (TOF) mass spectrometer, ionized sample molecules in a vacuum are accelerated in a straight line so that they fly down an evacuated tube. By measuring how long the ions take to reach a detector at a fixed position and by taking into account the length of the flight, one can determine the mass-to-charge ratio and the number of ions detected at each sequential mass.⁶

Several varieties of hybrid and single analyzer mass spectrometers are used for analysis. One of the most common for utilizing multiple stages of mass spectrometry (MS/MS) is a combination of three quadrupole structures in sequence (triple quadrupole) and an ion-trap mass spectrometer. Increased chemical specificity is achieved in the triple quadrupole configuration because the first mass spectrometer can be used to select a single mass corresponding to the compounds of interest in the sample (targeted analysis), rejecting all the other compounds of differing molecular weight that could interfere with the detection and identification. Ions having the desired mass are then collided in the second quadrupole, and the resulting fragment ions are analyzed in the third quadrupole. This multiple mass analysis technique provides information about the structure of the original molecule and confirms the detection of the target compound. This same chemical specificity can be achieved in a single-ion-trap mass spectrometer by holding the ions of interest in a three-dimensional ion trap, colliding them with neutral gas molecules, collecting the fragments, and sweeping the fragments in order of ascending mass out of the trap for detection.

⁵ Richard Sleeman, Samantha L. Richards, William R. Stott, William R. Davidson, John G. Luke, Brendan J. Keely, I. Fletcher, and A. Burton. 2002. The detection of explosives residues on aircraft boarding passes. Proceedings of the 50th ASMS Conference on Mass Spectrometry and Allied Topics, Orlando, Fla. June 2-6.

⁶Superficially, the operation of the TOF MS resembles the IMS system—in both cases, the intensity of ions is measured as a function of their flight/drift time down a tube. In the case of TOF, however, the tube is evacuated, and the flight time is a function of the ion's momentum (mass at a fixed energy)—a fundamental property of the ion. In the case of IMS, the ion's drift time through a viscous gas is measured. This depends on the ion's size as well as other factors and is not a fundamental property of the ion.

BOX 2-1

Deployed Mass Spectrometry-Based Trace Explosives Detector

The U.K. company Mass Spec Analytical, Ltd., in collaboration with Transport Canada and the Oak Ridge National Laboratory, has developed and deployed the Scentinel tandem mass spectrometer for use in customs, police, and airline security applications (Figure 2-1). For the airline security application, Scentinel has been used to detect traces of explosive residues on luggage or on passenger boarding passes. The company has successfully used a similar system in the detection of drug traces on paper money, with the analyses offered as evidence in hundreds of court cases.

In one configuration of the Scentinel system, boarding passes are fed into the analyzer and chemical traces on the passes are vaporized with pulsed infrared lamps. The vapor is ionized and enters a tandem mass spectrometer (MS/MS) for staged analysis. For each pulse, the MS/MS analyzer is tuned to detect a specific ion that is characteristic of a particular target substance (e.g., a parent or compound-specific primary ion in the first analysis and the NO₂ ion in the second mass analysis for confirmation of the primary ion as an explosive). Each boarding pass can be interrogated up to 20 times—that is, checked for up to 20 target substances. The method is faster than manual swabbing, requires less manpower than current trace detection methods, and analyzes the entire boarding pass.

According to the manufacturer, the deployed unit is robust and sensitive to picogram levels of explosive. It has been tested in various sampling configurations, including residual explosive contaminants on boarding passes and on the exterior surfaces of packages and luggage. In these tests, the manufacturer claims that the Scentinel system had a 98 percent detection rate with no false alarms. Throughput is high; up to 1,000 boarding passes per hour could be analyzed (approximately one every 4 seconds), with no interference from background. Data were obtained for the explosives RDX, PETN, TNT, HMX, NG, DMNB, TATP, and HMTD.

The committee has not had access to Transport Canada's report, nor has it seen the equipment to determine the adequacy of the tests or the robustness of the instrument for airport deployment. Questions remain regarding the threat scenario: for example, are hands of the passenger (and therefore the boarding pass) the most likely contamination site? However, the reported analytical results, as well as the reported limit of detection at low false alarm rates, supports the committee's recommendation that TSA should initiate a vigorous program to take advantage of the opportunities offered by MS-based detector technologies.

Additional chemical specificity can be attained by preseparation of target molecules from a complex mixture using chromatography in tandem with MS (C/MS or C/MS/MS). C/MS is generally accepted as the final word in a variety of applications that require high confidence in the identification of a substance. Laboratory-based mass spectrometers, especially when used in combination with other separation methods such as chromatography, have the ability to identify and quantify targeted chemicals based on molecular weight and structure in very complex mixtures at picomole (10^{-12} mole) to attomole (10^{-18} mole) levels.

As noted above, any mass spectrometer requires a method of forming ions from the molecules in the sample. The highest chemical specificity and (usually) sensitivity are achieved if the ions formed are those of the molecule itself (molecular weight) rather than fragments of the molecule. Two common methods of soft ionization achieve this: matrix-assisted laser desorption/ionization (MALDI) and

electrospray ionization (ESI). In MALDI, the sample is mixed with a larger quantity of an organic molecule (the matrix), which is selected for its ability to efficiently absorb radiation from a laser. When the dried sample-matrix mixture is exposed to a laser beam, the matrix absorbs the laser energy and transfers it to the sample, typically forming positive ions with a single charge. In ESI, a sample in a liquid is continuously aerosolized into a fine spray near a needle maintained at high electrical potential, and the droplets take on a charge from the electric field. As the charged droplets evaporate, the charge is transferred to organic molecules in the sample, forming molecular ions that can be separated in the MS.

Comparison of Informing Power of MS and IMS

The uniqueness of mass spectrometry lies in its chemical specificity. Because it directly measures a fundamental property of the target molecule—its molecular weight—it affords a highly specific means of identifying the molecule. By contrast, IMS systems measure a secondary and less specific property of the target molecule—the time it takes for the molecule to drift through a tube filled with a dense gas—and the identity of the molecule is inferred by reference to calibration standards. Since different molecules may have similar drift times, IMS inherently has less chemical specificity than MS.

Since there is no quantitative calibration of airport IMS systems⁷ and no systematic reporting of screened objects and alarms, there are no reliable data with which to properly assess the current IMS instrumentation in terms of probability of false alarms and probability of detection. Instead, another method of comparison is adopted here (described below) that might be used in the future for comparisons of technologies when operational data are unavailable.

The chemical specificity of an instrumental method can be quantitatively estimated on a consistent basis using a metric called “informing power.” In a discussion of the informing power of tandem mass spectrometry (MS/MS), Yost and Fetterolf⁸ use information theory to give figures of merit for chemical resolution of various analysis techniques. The committee has estimated the informing power of IMS using the same method (see Appendix A) and compares it with the previously calculated informing power of MS/MS systems in Table 2-1. The informing power of the tandem QMS/QMS configuration is on the order of 10,000 times greater than that of IMS.

The substitution of an MS/MS analyzer for the analyzer of an ion mobility spectrometer with the same ionization technique would yield an informing power (chemical specificity) increase of approximately 10,000. The higher chemical specificity of MS means that significantly smaller quantities of target molecules can be detected in the presence of relatively large quantities of background molecules. This enables the detection threshold to be lowered without increasing the false alarm rate.

TABLE 2-1 Comparison of the Informing Power of IMS and MS Analytical Techniques

Technique	Informing Power P_{inf} (bits)	Approximate Increase in P_{inf} IMS (order of magnitude) ^a
IMS	1×10^3	1
QMS	1.2×10^4	10
Capillary GC-QMS	6.6×10^6	10,000
QMS/QMS	1.2×10^7	10,000
Capillary GC-QMS/QMS	6.6×10^9	10,000,000

^a Informing power of IMS is estimated by the committee to be on the order of 1,000, as discussed in Appendix A. Remaining values in this table are from Yost and Fetterolf, 1984.

⁷NRC. 2002. Assessment of Technologies Deployed to Improve Aviation Security: Second Report, Progress Towards Objectives. Washington, D.C.: National Academy Press.

⁸R.A. Yost and D.D. Fetterolf. 1984. Added resolution elements for greater informing power in tandem mass spectrometry. *Int. J. of Mass Spectrometry and Ion Processes* 62: 33-49.

MS Target Molecule Identification Strategies and Analysis Times

Identification Strategies

In the case of trace detection in the airport scenario, the problem of identification is made easier in that there are only a few hundred threat compounds and/or organisms that might conveniently be used by terrorists. Thus, one does not have to determine the identity of an unknown substance from scratch but rather must determine whether it contains one of these ~200 compounds or organisms. If a mass spectrometer is used, the spectrum obtained would be compared electronically against a library of reference spectra, and a software algorithm would determine if a match occurred. These algorithms and spectral libraries already exist for electron ionization, though it is not a foregone conclusion that electron ionization will be the ionization method of choice. These libraries may be searched for over 300,000 reference spectra; typically, two measures of confidence in the spectral match are given as part of a search report. If GC or LC is also used, the chromatographic elution time can be used to further increase the confidence of the identification. If MS/MS is used, each molecule of interest would be identified by two or three masses: that of the parent (molecular weight) ion (or parent less some known ion loss), indicative of the molecular weight, and the masses of one or two ions that result from intentional fragmentation of the parent ion, for confirmation. These ions would be determined by running standards.

With highly energetic molecules such as explosives or with the complex macromolecules that are present in microorganisms, the process of preparing, vaporizing, and ionizing the sample often causes the target molecule (and background molecules as well) to break up into fragments. This tendency is minimized by the use of soft ionization (see above for two common methods), but the effect can also be utilized in the collision (fragmentation) process of MS/MS analysis to confirm the identity of the material. The pattern of fragments formed is characteristic of the structure of the parent molecule or organism, and under appropriate conditions this spectrum and the molecular weight can be used to identify the target molecule/organism by comparing them to the reference library. This detection strategy makes MS/MS systems much more flexible than IMS systems. If additional threat agents become a concern, the MS/MS molecular species and reference library can be expanded to accommodate them.

Analysis Time

In the airport context, the time required for acquisition and analysis of a sample is a critical factor in determining where and in what circumstances the trace detection technique can be used. The current system of IMS trace detectors for explosive residues on passenger carry-on bags takes on the order of 1 minute from sample acquisition to final analysis. It is probable that an MS or MS/MS-based system would take about the same amount of time or slightly longer, because for explosives, the sample collection and preparation requirements for IMS and MS are essentially the same.

Once a sample has been acquired by wiping or collecting as with IMS, the time required to acquire a mass spectrum can be made short (on the order of 1 second), and the electronic analysis of the resulting spectrum takes about the same amount of time. However, in some cases (e.g., biological analysis), sample collection and preparation, as well as pre-separation of complex mixtures, might add significantly to the analysis time. Gas or liquid chromatography used as a pre-separator at the MS inlet might add several seconds to several minutes to the analysis time⁹; however, by using an MS/MS configuration, the chromatographic separation on the front end may be avoided, saving significant analysis time. Preparation of complex biological samples for MS analysis (e.g., lysing cells and digesting polypeptides) may also add considerable time to the analysis of potential biological agents. There is

⁹A short column transfer line chromatograph would add 1 second; a 6-foot capillary column would add 30 seconds to 5 minutes, depending on how much chemical specificity is required from the chromatography.

considerable literature on the sampling and ionization of explosive material,¹⁰ but the optimum methods for vaporizing and ionizing the specific combinations of threat materials likely to be encountered remain to be determined.

Sampling Strategies

The same dry wiping techniques used with current IMS systems can also be used with MS-based detection systems. However, as discussed in Chapter 1, automated sampling (either of hand luggage or in a portal arrangement) would be better because it would avoid the many uncertainties of manual sampling. Any automated sampling system would incorporate a condensation or concentration step to counteract the air flow dilution (such a step is now included in portal sampling systems).

OPPORTUNITIES TO IMPROVE CURRENT TRACE DETECTION SYSTEMS WITH MASS SPECTROMETRY

As a trace detection technology, MS-based systems may have the same generic limitations as all trace detection technologies, discussed in Chapter 1. The threat preparation and delivery scenario must predict a high probability that threat residue will be deposited on items to be interrogated. The sampling method must effectively access the residues if present. This trace technique is unable to distinguish innocently acquired, but real, explosive compounds such as might be found on persons who take nitroglycerin heart medication or on, say, hunters, law enforcement personnel, and mining engineers, from explosive compounds on individuals who prepared bombs. However, as discussed below, MS-based systems can address several of the specific limitations of current IMS systems.

Lower Detection Threshold with Lower False Alarm Rate

Given the unpredictable efficiency of sample acquisition, discussed above, and the possibility that a terrorist would try to minimize the presence of threat substance residues on his or her hands and luggage, it is desirable to reduce alarm thresholds below current levels to increase the probability of detection of trace residues or vapor. Whereas IMS systems have alarm levels in excess of 1 nanogram of explosive, MS-based systems should be capable of alarm levels on the order of 100 picograms. Given the 10,000-fold greater chemical specificity of MS compared with IMS (see above), this lower alarm level should be achievable without increasing the false alarm rate due to interfering compounds in the sample background.¹¹ While the lowered detection limit may increase the number of alarms caused by detection of innocently acquired explosive residues, the higher chemical specificity of MS-based systems might enable these systems to compensate for this problem. For example, nitroglycerin pharmaceuticals will contain other characteristic compounds that can be detected in the mass spectrum and used to distinguish medication residues from explosive residues, avoiding false alarms raised by heart patients.

¹⁰See, for example, Jehuda Yinon, 1999, *Forensic and Environmental Detection of Explosives*, New York: John Wiley & Sons.

¹¹This report considers the effect of substituting one trace detection technology (MS) for another (IMS) on the probability of detection and the false alarm rate. By fusing data from complementary detection technologies, one can reduce false alarm rates with no degradation in the overall system detection probability. However, an analysis of the costs and benefits of such multimodal detection systems is beyond the scope of this report.

Broader Range of Threat Substances Detectable

As discussed in Chapter 1, currently deployed IMS trace detectors are designed to detect specific explosives only. The flexibility inherent in MS-based systems should make them capable of detecting a much broader range of threat substances, including other improvised explosives, chemical warfare agents, and biological agents.

Explosives

The efficacy of mass spectrometry in detecting explosives is well established. Jehuda Yinon, an internationally known forensic scientist and author of many papers and several books¹² on detection of terrorist materials, concluded as follows:

We have studied several groups of explosives, including TNT, nitrate ester explosives (such as nitroglycerin and PETN) and inorganic oxidizers (such as ammonium nitrate). We have found that the analytical method of choice for identification and characterization of all studied explosive residues -from the point of view of sensitivity and selectivity- is LC/MS.¹³

McDonald et al.¹⁴ have reported a gas chromatography/mass spectrometry (GC/MS)-based laboratory method for confirming nine nitrogen-containing explosives (EGDN, DMDB, NG, PETN, RDX, HMX, NT, DNT, and TNT) by their molecular weight at subnanomole amounts using methylene chloride chemical ionization and detection of negative ions. (This is nearly the same ion source chemistry as is used in IMS.) The time for analysis was less than 10 minutes. Another approach that substitutes glow discharge ionization¹⁵ and another stage of MS for GC (in order to reduce the analysis time to seconds) is being tested by the TSA in a portal form.¹⁶

Picogram quantities of explosive residues on packages and luggage, as well as on passenger boarding passes, have been detected using the portable tandem MS detector described in Box 2-1 and shown in Figure 2-1.

Chemical Warfare Agents

Similar approaches taking advantage of the versatility of mass spectrometry have been used to detect chemical warfare agents, and commercial spectrometers are offered for both military and industrial use.^{17,18,19,20} Presentations have been given documenting the detection in drinking water of 42 of the 48

¹²See, for example, Jehuda Yinon, 1999, *Forensic and Environmental Detection of Explosives*, New York: John Wiley & Sons.

¹³Jehuda Yinon and Xiaoming Zhao. 2002. Tracking the terrorists: Identification of explosive residues in post-explosion debris by LC/MS methods. Proceedings of the 50th ASMS Conference on Mass Spectrometry and Allied Topics, Orlando, Fla. June 2-6.

¹⁴J.G. McDonald, K. Mount, and M.L. Miller. 2003. Mass spectral confirmation of nitro-based explosives using negative chemical ionization mass spectrometry with alternate reagent gasses. 51st Conference of the American Society for Mass Spectrometry, Montreal.

¹⁵S.A. McLuckey et al. 1993. Atmospheric Sampling Glow Discharge Ionization and Triple Quadrupole Tandem Mass Spectrometry for Explosives Vapor Detection. Oak Ridge National Laboratory, TM-12434.

¹⁶J.A. Syage, K.A. Hanhold, and M.A. Hanning-Lee. 2001. Mass Spectrometry Based Personnel Portal Screening System. Proceedings of the Institute of Nuclear Materials Management, 42nd Annual Meeting, Indian Wells, Calif. July 15-19.

¹⁷Inficon, at <http://www.inficon.com/products/family.cfm?id=f00323>.

¹⁸Bruker Daltonics, at <http://www.gcms.de/download/cbms.pdf>.

¹⁹Agilent, at <http://pubs.acs.org/subscribe/journals/ancham-a/74/free/902smith.pdf>.

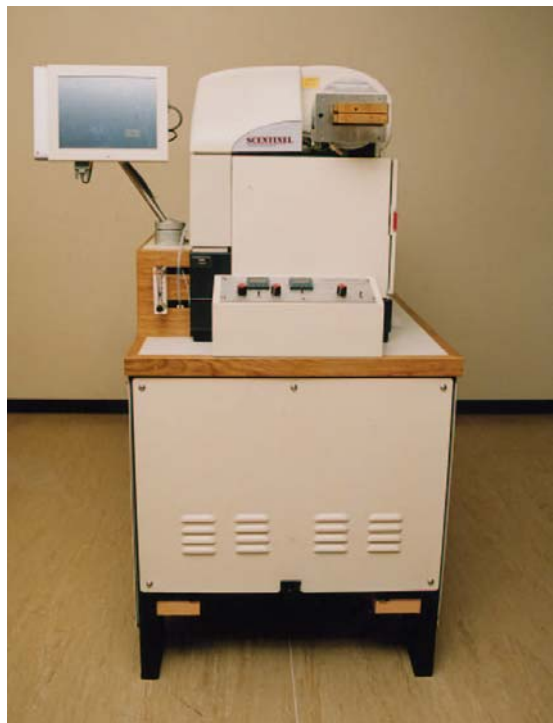


FIGURE 2-1 The as-deployed Scentinel mass spectrometer trace explosives analyzer. SOURCE: Mass Spec Analytical, Ltd.

compounds listed on Chemical Weapons Convention schedules.²¹ These studies used a low-pressure photoionization/ion trap/TOF mass spectrometer.²² IMS spectrometers have not been considered for these diverse analysis needs.

Biological Agents

Biological agents pose a greater challenge to MS-based detection systems because the target bioagents must be detected against a complex background of naturally occurring microorganisms and other aerosols found in the environment. Sample preparation is likely to be more complex with biological samples, and it is not yet clear which types of instruments will be best suited to the analysis. If the analysis focuses on whole proteins, TOF spectrometers with large mass ranges may be required; if detection of characteristic polypeptides or unique amino acid sequences is the goal, MS/MS and small spectrometers might be used. Single-particle aerosol mass spectrometers are also being developed that can analyze the composition of individual aerosol particles in real time.^{23,24} Only further research on these issues will determine which, if any, MS technology will be appropriate. The encouraging thing is that

²⁰Syagen Technology, at <http://www.syagen.com/FrameSt3.htm>.

²¹http://www.cwc.gov/treaty/annex_chem/annonchem_html#A-1.

²²M.D. Evans, E.R. Beckley, K.A. Hanold, and J.A. Syage 2003. Chemical weapons screening of water samples by photoionization MS. 51st Conference of the American Society for Mass Spectrometry, Montreal. June 8-12.

²³M.V. Johnston. 2000. Sampling and analysis of individual particles by aerosol mass spectrometry. *Journal of Mass Spectrometry* 35: 585-595.

²⁴D.T. Suess and K.A. Prather. 1999. Mass spectrometry of aerosols. *Chem. Review* 99: 3007-3035.

mass spectrometry has already shown significant capabilities for biological identification.^{25, 26}

A paper by Randolph Long²⁷ of Edgewood Arsenal—an Army laboratory that has been conducting and funding research on chem/bio detection for more than 30 years—compares the three current contenders for the detection of chemical and biological agents and bioactive peptides and toxins: immunoassays; assays based on nucleic acid sequence; and mass spectrometry. In contrast to immunoassays, which are specific to a single agent and take 15-20 minutes, and assays based on nucleic acid sequence, which use polymerase chain reaction (PCR) amplification and detection with DNA arrays, mass spectrometry was characterized as follows:

Mass spectrometry represents the third major contender for biological identification. Principal advantages of mass spec include potential for full spectrum detection of chem and bio agents to include mid-spectrum materials for which biological approaches are inadequate. Mass spectrometry also relieves a major logistical concern associated with biosensor approaches, namely, the dependence on agent-specific reagents and assays. There is in fact a reasonably mature mass spectrometer of recent vintage fielded for military applications, the Chem Bio Mass Spectrometer. Next generation MS approaches such as ESI and MALDI targeting principally protein and peptide biomarkers are emerging as contenders for enhanced biological differentiation. Major issues that require resolution will be database robustness and sensitivity.

Biological agent analysis will require considerable chemical specificity, and MS/MS configurations will be incorporated. MS/MS systems with a single-analyzer, ion trap mass spectrometer have been implemented by Oak Ridge National Laboratory in the chemical and biological mass spectrometer, Block II (CBMS).²⁸ The CBMS was developed with funds from the U.S. Army and the Department of Energy for use in chemical and biological warfare. It consists of an ion-trap MS/MS mass spectrometer with chemical ionization source and three specific inlets to handle various sample types to be analyzed.²⁹ Biodetection for bacterial, viral, and toxin targets was accomplished by concentrating particles in a respirable range (2-10 μm) into a quartz pyrolysis/thermolysis tube, where, after the addition of a derivatization reagent, the sample is thermolyzed. The mass spectra of the liberated chemical biomarkers are then processed to determine if targeted biological agents are present in the sample. Viruses and toxins are typically distinguished on the basis of protein fragments, while bacteria are distinguished on the basis of their fatty acid methyl ester profiles.³⁰

Another extensive program developing mass spectrometry for chemical and especially biological detection is being conducted at the Johns Hopkins University Applied Physics Laboratory (APL). With funding from DARPA as part of a systems approach to the detection of threats in the environment, APL has built and is testing an integrated chemical and biological detection system based on a miniaturized

²⁵M.P. McLoughlin, W.R. Allman, C.W. Anderson, A.A. Carlson, J.J. DeCicco, and N.H. Evancich. 1999. Development of a field-portable time-of-flight mass spectrometer system. *Johns Hopkins APL Technical Digest* 20(3): 326-334.

²⁶W.H. Griest, M.B. Wise, K.J. Hart, S.A. Lammert, C.V. Thompson, and A.A. Vass. 2001. Biological agent detection and identification by Block II chemical biological mass spectrometer. *Field Analytical Chemistry and Technology* 5(4): 177-184.

²⁷S.R. Long. 2002. Detection, identification, and analysis of chemical and biological agent materials. *Proceedings of the 50th ASMS Conference on Mass Spectrometry and Allied Topics*, Orlando, Fla. June 2-6.

²⁸K.J. Hart, M.B. Wise, W.H. Griest, and S.A. Lammert. 2000. Design, development and performance of a fieldable chemical and biological agent detector. *Field Analytical Chemistry and Technology* 4(22-3): 93-110.

²⁹A bio/air inlet for 2-10 μm aerosols sampled from the ambient air by the bioconcentrator; a chem/air inlet sampled by heated capillary line; and a chem/ground inlet for ground sampling of liquid and/or solids from a heated ground sampler.

³⁰S.A. Lammert, W.H. Griest, M.B. Wise, K.J. Hart, A.A. Vass, D.A. Wolf, M.N. Burnett, R. Merriweather, and R.R. Smith. 2002. A mass spectrometer-based system for integrated chemical and biological agent detection—The Block II CBMS. *Proceedings of the 50th ASMS Conference on Mass Spectrometry and Allied Topics*, Orlando, Fla. June 2-6.



FIGURE 2-2 Miniaturized mass spectrometer for bio-chem defense. The Johns Hopkins University Applied Physics Laboratory (APL) has developed a miniaturized time-of-flight mass spectrometer built into a suitcase-sized container for analyzing solids, liquids, and gases in the field. SOURCE: JHU/APL.

TOF mass spectrometer utilizing electron impact ionization for vapors and laser desorption-ionization for higher molecular weight threats (bioregulators, toxins, and microbes; see Figure 2-2).^{31, 32}

Recent reports from Purdue University suggest that the identification of whole proteins from complex mixtures can be accomplished with lysated cells (*E. coli*) and mass spectrometry alone, using no chromatography or other preparation step.³³ For targeted biomolecules, this raises the possibility of significant reductions in sample preparation time.

CHALLENGES FOR MASS SPECTROMETRY-BASED TRACE DETECTION SYSTEMS

MS-based systems face a number of challenges before they can be deployed in airports as trace detectors, discussed further below.

Reduce Cost and Complexity, Increase Ruggedness

As noted above, the U.S. Army and DARPA have conducted proof-of-principle research and development, testing, and evaluation for both chemical and biological threat analysis using fieldable, rugged, specialized mass spectrometer systems. It is likely that much of the work these and other agencies have done to develop equipment concepts could be used directly or modified for TSA threat scenarios, but TSA needs to focus on its unique needs for a rugged, backbone mass spectrometer that would be useful for many threat detection scenarios.

³¹ R.J. Cotter, R.D. English, B. Warscheid, A. Hardy, and B.D. Gardner. Miniaturized time-of-flight mass spectrometers for bioagent detection and identification. Submitted for publishing.

³² See a series of articles in the Johns Hopkins APL Technical Digest, Vol. 20, No. 3 (1999).

³³ G.E. Reid, H. Shang, J.M. Hogan, G.U. Lee, and S.A. McLuckey 2002. Gas-phase concentration, purification, and identification of whole proteins from complex mixtures. *J. Am. Chem. Soc.* 124: 7353-7362.

Although extensively used for a variety of laboratory applications, commercially available chemical analysis systems (C/MS/MS) are not designed for an environment as harsh as an airport or other transportation arenas, nor are they designed for use by TSA security operators.³⁴ Given the range of airport deployment sites (e.g., baggage rooms, curbside check-in kiosks, passenger checkpoints), an ETD must be able to operate effectively under a variety of adverse conditions, including extremes of temperature, changes in barometric pressure, high humidity, and high levels of dust or other airborne particles. IMS systems have been known to fail under these adverse conditions, and substantial investment may be required to adapt MS-based systems for reliable use in these environments. MS-based systems can be robust, however, as demonstrated by contract laboratories in which millions of environmental analyses are run around the clock, with several mass spectrometers overseen in their automatic operations by technicians.

The costs of laboratory instruments depend on their complexity and the volume produced. GC/MS instruments that sell in the thousands of units per year are offered at about \$50,000. LC-ion trap machines and TOF machines cost from \$100,000 to \$250,000 and are sold in quantities of hundreds per year. The annual maintenance contracts typically cost about 10 percent of the purchase price per year in a laboratory setting.

Once an analyzer configuration is selected, the operational, cost/benefit, and functional requirements can be specified, test protocols issued, and bids solicited from companies with MS product history to supply a rugged and cost-effective product or design. Cost goals must be given, but there are limits of design and pricing that depend on volume. To keep costs as low as possible, it would be desirable to involve multiple vendors in the design and production of an MS-based ETD system.

Resolve Sampling Issues

The configuration of the sample inlet (chromatograph, if needed) and the ionization, mass analysis, and ion detection methods will depend on the problem to be solved. It is not reasonable to expect that one inlet and ionization method will serve all threat materials or all threat scenarios. It is moreover possible to have more than one inlet or ion source in or attached to the MS. Ion trap analyzers, in particular, can perform several different types of mass spectrometer scans (MS/MS/MS...) and change the polarity of detected ions, all based on information from the previous scan. As can be seen from the examples so far, several different configurations have been chosen for solutions to chem/bio problems: systems utilizing gas or liquid chromatography, chemical vs. electrospray ionization, ion trap or TOF, MS/MS or MS alone, and positive/negative ion detection, among others. Choosing the most appropriate configurations will take time, expertise, in-depth knowledge of the manufacture of mass spectrometers, and perhaps additional research. A significant attempt should be made to select configurations that are extendable to as many threat scenarios and substances as possible.

Several groups and companies are working on related problems, and these efforts must be considered. For example, R.G. Cooks at Purdue University is leading an initiative on multiplexing and miniaturizing ion trap mass spectrometers.³⁵ These devices (Figure 2-3)³⁶ are ion traps and hence have MS/MS capability. They are miniaturized and have a single vacuum system; they are, however, the only devices having separate mass spectrometers and separate ion inlets, allowing different ionization and sample handling techniques.

³⁴Since the configuration of fielded instruments is not known at this time, the extent of technical support and operator training are not known and not addressed in this report.

³⁵L.S. Riter, R.J. Noll, Y. Peng, G.E. Patterson, A. Guyman, and R.G. Cooks. 2002. MSⁿ capability of a miniature cylindrical ion trap mass spectrometer. Proceedings of the 50th ASMS Conference on Mass Spectrometry and Allied Topics, Orlando, Fla. June 2-6.

³⁶Personal correspondence including presentation materials by Amy Tabert and Professor Cooks, 2002.

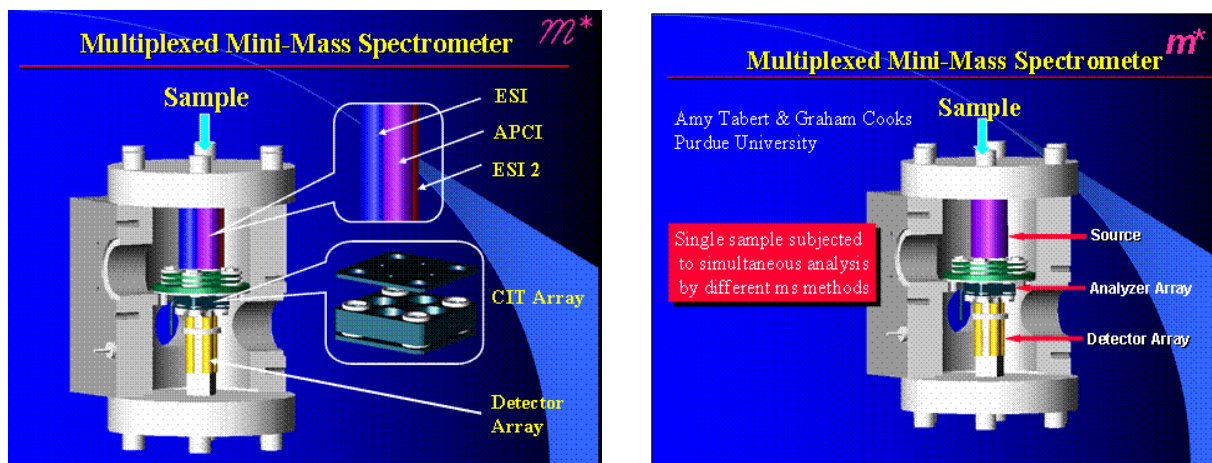


FIGURE 2-3 Miniaturized mass spectrometer with inlet configuration enabling a single sample to be analyzed by several different MS techniques. SOURCE: Courtesy of R.G. Cooks, Department of Chemistry, Purdue University.

Automated Sampling

The Achilles heel in trace detection is improper manual sampling. To fit in better with current in-line baggage handling systems, ETDs with automated sampling systems will be needed. Two approaches are being developed. One uses a laser pulse to desorb particles from the bag; these are subsequently collected. The other uses pulsed air jets to dislodge particles. These approaches have the potential to automatically and systematically sample a large percentage of carry-on and checked baggage without relying on an operator. If successful for carry-on materials, a major flaw and bottleneck in passenger screening could be eliminated. The actual capabilities and understanding of these approaches need further funding and optimization, with deployment once they have been shown to be justified.

Portal Sampler Development

Passenger screening has been the primary reason for the development of trace detection. However, in currently deployed systems, neither the passenger's body nor his or her clothing is sampled for residues of threat materials—only personal items and carry-on bags that are likely to have been touched by the passenger are sampled. Other than metal detectors, there is no currently deployed technology for screening passengers per se. Clearly, one scenario for bringing down an airplane is a suicide attack in which the terrorist straps an explosive or other threat material to his or her body. Such a device should be detectable by a portal sampler.

Passenger portals based on IMS technology for sampling and detection have been tested and are commercially available. As noted earlier, TSA has evaluated an MS-based portal system. Passenger portal systems will, however, require lower alarm thresholds in the future to compensate for the inefficiency of sample collection.

The TSA has an opportunity to directly compare MS technology with existing IMS technology in passenger screening portals. Deployment of both IMS and MS types with lower alarm levels would be a good test of mass spectrometry's ability to detect at lower levels with fewer false positives than current technology. The probability of detection should be compared with the probability of false alarms at lower alarm thresholds for each technology in an airport scenario, and each technology should be characterized for operational and security adequacy. Concurrent studies could determine (1) the expanded list of threat materials that MS could address and (2) the extent of alarm level reduction.

In the committee's view, MS-based portals represent the lowest-cost pathway to demonstrating the utility of MS-based detection. Portals with IMS-based detectors and portals with MS-based detectors should be compared side-by-side to determine the relative probability of detection and the probability of false alarms as alarm levels are lowered.

Improve Database Robustness

To identify a target molecule using a mass spectrometer, the spectrum obtained would be compared against a library of reference spectra, and a software algorithm would determine if there is a match. Such algorithms, formats, and spectra libraries already exist and will form the basis for those used in this application. Once the methods of analysis are chosen, corresponding libraries will need to be augmented. All commercial MS data systems allow libraries to be created based on standard samples of interest. Since the chemical specificity of the analysis technique allows for eliminating most if not all background signals, it is not necessary to run standards in the presence of all known backgrounds, as is always necessary with IMS.

There are several commercial algorithms available for searching spectra libraries of both chemical and biological compounds. These algorithms need to be customized and tested with the libraries using spectra obtained in the actual airport environments to better understand their robustness and sensitivity. As has been seen in other technology implementations for civil aviation security, such real-world tests are critical to the assessment and success of the technology.

FINDINGS AND RECOMMENDATIONS

Based on the discussion above, the committee offers two sets of findings and recommendations:

Finding 1: The trace detection systems currently deployed in airports have limited utility for the following reasons:

- **The relatively low chemical specificity of IMS means that the instrument alarm threshold must be set high to avoid excessive false alarms; yet, lower alarm levels are desirable to account for inefficient manual and portal sampling techniques and, possibly, “cleaner” perpetrators.**
- **Detection is dependent on the use of blind sampling methods that cover only a small portion of the bag surface for acquisition of adequate residues for analysis.**
- **Current sampling protocols do not allow for the sampling of explosive residues or vapors that may be associated with a passenger's skin or clothing.**
- **Currently deployed IMS systems are designed to detect only a specific list of explosives and cannot easily be reconfigured to detect an expanded list of explosive, chemical, and biological threat substances.**

Recommendation 1: To address these deficiencies in the performance of explosive trace detectors, TSA should do the following:

- **Place a high priority on the development and deployment of automated trace sampling hardware.**

- **Decrease the threat alarm threshold for ETDs systematically over time to improve the probability of detection of residues while keeping false alarms at current levels.**
- **Deploy passenger screening portals to enable the detection of explosive traces on passengers' skin and clothing, and assess the acceptability and efficacy of the portals.**
- **Explore new technologies with higher chemical specificity that are capable of detecting a wider range of explosive, chemical, and biological threat materials.**

Finding 2: Owing to their lower limit of detection, higher chemical specificity, and chemical flexibility, MS-based trace detection systems have the capability to address many of the limitations of IMS-based systems. Several development efforts are under way at universities and in the private sector to commercialize miniaturized, low-cost MS systems that can detect a range of threat materials.

Recommendation 2: TSA should establish mass spectrometry as a core technology for identifying an expanded list of explosives, as well as chemical and biological agents. Specifically, TSA should

- **Create a prioritized list of threat materials that are likely to fit a residue scenario and a second list of materials that are not likely to fit the scenario.**
- **Determine appropriate MS sampling procedures, inlet configurations, ionization methods, and analysis strategies for relevant materials on this list.**

TSA should execute an orderly program for development, testing, and deployment of mass spectrometry-based systems for residue threat scenarios that involve the expanded threat list. Rugged, miniaturized MS-based trace detection systems should be developed for use in an airport environment in order to achieve lower alarm thresholds without increasing false alarm rates and to provide versatility for threat substances not now detected.

A good way to bootstrap this entire process would be to purchase the best field-deployed instrument to gain experience and to test system applications. One option would be for TSA to purchase an instrument with the capabilities of the Scintinel instrument described in Box 2-1 and evaluate its effectiveness in an airport setting.

In Chapter 3, the committee suggests one possible example of an orderly program for development, testing, and deployment of mass-spectrometry-based systems.

3

Strategy for Improving Trace Detection Capabilities

Explosive trace detectors have become a part of the layered, system-of-systems aviation security structure in use at various airport locations. Dogs are used to screen a number of items, from foodstuffs to bombs; IMS systems are used to screen carry-on bags; and metal detectors and x-ray systems screen for concealed weapons. Each detection technique has strengths and weaknesses, and, as discussed in Chapter 2, the committee believes that mass spectrometry will find use as an adjunct for many of these detection systems. Again, the key advantages of mass spectrometry are the improvement in chemical specificity (enabling a lower alarm threshold while maintaining a low false alarm rate) and its applicability to a variety of threat substances. Security advantages accrue directly from these features, including faster diagnosis of potential threats, greater capability for detecting new threat species, and improved instrument performance—especially under unfavorable background conditions. MS also offers a standard against which to evaluate the performance of existing IMS instruments.

Chapter 2 explored the potential advantages of MS-based trace detection systems in detail. This chapter offers one plausible scenario for integrating MS instruments into an airport security system, as part of an overall effort to improve trace detection capabilities. It envisions a phased introduction process that involves several generations of MS-based systems, adaptations that will be necessary for these systems to function in an airport checkpoint and screening context, and future technological developments that might allow the instruments to address broader security issues, such as monitoring of the air handling system.

PHASED DEPLOYMENT OF MASS SPECTROMETRY-BASED DETECTION INSTRUMENTS

Below, the committee describes an evolution of various generations of mass spectrometers that would provide increasingly capable trace detection systems and at the same time decrease costs and improve functionality. The deployment is assumed to take place in a large urban airport; the estimates provided for instrument costs are rough, based on committee members' experience with the research, development, and commercialization of analytical instruments.

As noted in Chapter 2, current sampling methods that involve wiping selected carry-on baggage are time consuming, prone to operator error, and incomplete in coverage. There have been proposals to automate this process using lasers or other methods of safely dislodging material from the entire bag. If these efforts are successful, they would greatly enhance trace detection utilizing any technology. Development of engineering prototypes and agreement on specifications for the final product might take

1 to 2 years, with deployment not likely before year 3. This development should be concurrent with any existing and new trace technology efforts and coordinated with them.

Phase 1: Introduce Portals with Both IMS-Based and First-Generation MS-Based Detectors (1 to 3 Years)

The rationale for current trace detection systems is to screen passengers for the presence of explosive residues or vapors. However, for reasons of safety and respect for personal privacy, sampling is limited to the wiping of hard objects (computers, briefcases, and carry-ons) that the passenger has touched—passengers themselves may not be subjected to radiation, have their skin or clothing wiped, or be otherwise touched by an operator. Thus, current sampling methods might fail to detect traces of a bomb or other threat substance that adhere to a terrorist's skin or clothing.

One option for sampling the passenger directly without raising safety or privacy issues is to introduce portals in which the passenger walking through is subjected to a puff of air intended to dislodge particles of threat materials from skin or clothing and to collect and concentrate the resulting air sample. Research and development already conducted by the TSA, the national laboratories, and private industry have resulted in several portal prototypes, and models of the portals that use IMS or MS-based detection have been tested by the TSA. Issues that remain to be resolved include the appropriate limit of detection, the acceptable rate of false positives, and especially, passenger acceptance and restrictions on passenger flow. These issues need to be resolved by testing in an actual airport environment.

Operational tests of these units in selected airports could begin within 1 year. Testing could likely be completed in an additional 6 months to 1 year, with final specifications and testing protocols formulated in the second or third year. While the IMS-based detectors in these portal systems are essentially the same as those currently deployed for bag screening, the MS version would require additional development and testing to make it more rugged and suitable for installation in a concourse environment. The MS equipment must be designed in accordance with human factors principles for both interface design and operator training. Addressing these issues might delay wider deployment of these first-generation MS-based systems for an additional year. It would be very important that the specifications for the MS system include lower limits of detection, and the design should anticipate that future models will be programmed for analysis of additional threat materials. This dual deployment would allow comparison of MS and IMS technology in terms of false positives and probability of detection at a lower detection limit. With a simple coupon inlet, this machine could also be configured to help resolve alarms from existing ETDs, as well as any other unresolved alarms from suspicious materials that are not covered by ETDs or dogs.

These portals are expected to be deployed at a limited number of security checkpoints. For a large urban airport, between 5 and 10 MS-based portals might be deployed at a cost of \$100,000 to \$150,000 per portal, an increment of \$25,000 to \$50,000 in initial costs over the comparable IMS portal. Operating costs for the MS-based portal are expected to be \$2,000 to \$5,000 higher per year than those for the IMS portal.

Phase 2: Expand the List of Threat Materials That Can Be Detected (3 to 5 Years)

As discussed in Chapter 2, the combination of chromatography and MS has the ability to identify almost all types of organic molecules, and identification of the current list of threat materials covered by IMS in a single C/MS instrument configuration has been demonstrated.¹ However, covering an expanded list of target compounds with a minimum number of configurations of chromatography, ionization, mass

¹J.G. McDonald, K. Mount, and M.L. Miller. 2003. Mass spectral confirmation of nitro-based explosives using negative chemical ionization mass spectrometry with alternate reagent gasses. Presented at the 51st American Society for Mass Spectrometry Meeting, Montreal. June 8-12.

analysis, and detection will require additional development. Selecting the list of probable threat compounds and working out the methods for optimum instrumental configurations will require 1 or 2 years. Once defined, these configurations would then take another 1 or 2 years of instrument development to withstand the rigors of airport use prior to deployment. This second-generation MS detector would be designed to detect multiple threat agents from the beginning and would have to have a lower cost and better reliability than the first-generation systems.

Once developed, the second-generation MS detectors could be compared with the best available IMS devices at passenger checkpoints and portals.² They could be used to probe suspicious carry-on items. If available, dogs are often utilized to resolve this type of threat, which in extreme cases may require evacuation of the terminal to ensure safety. However, dogs are trained on only a small number of specific materials, and chemical and biological threats are not currently in their repertoire.

For a large urban airport, 10 to 20 second-generation instruments might be deployed at an initial cost of \$100,000 to \$150,000 per instrument. The incremental purchase and operating costs for these instruments relative to IMS instruments would likely be comparable to these costs for first-generation instruments, since there will also be cost reduction efforts with IMS systems.

The committee believes that this second-generation detection system could be deployed in the 4 or 5 years. Even were it not to be widely deployed because of cost or complexity, this system would serve as a gold standard against which to compare alternative technologies.

Phase 3: Replace Current IMS ETDs with Automated MS Systems (5-10 Years)

In this class of third-generation, automated MS instruments, the cost is assumed to be sufficiently low to permit use of a mass spectrometer in every passenger path. With automatic sampling, this device would be an add-on to the x-ray system currently in use for carry-on bags. With additional automatic sampling, this detector could be used in the checked baggage path as well.

A major benefit of this device would be to reduce the need for hand searches. Hand searches are expensive and slow down the overall throughput rate of carry-on and checked baggage. Procedures vary from airport to airport for handling the great variety of packed items, including foodstuffs, that trigger alarms. The success of the hand search requirement is also highly dependent on personnel training, and neither the hit rate nor the false alarm rate has been well established.

Once the advantages of the third-generation MS instruments are demonstrated, it could be decided whether this technology should be widely used in place of IMS. Prior to widespread deployment, the instrument would likely need to be redesigned to achieve a cost reduction of at least 50 percent, with improved reliability to match that of the much less complicated IMS technology. If the portal concept proves to be scientifically, economically, and socially acceptable, it would likely replace all procedures for sampling items the passenger has touched.

At a large urban airport, implementation of this phase would mean deployment of ~50 instruments that are assumed to have an initial cost of no more than \$75,000 and an operating cost of less than \$5,000 per year. If the superiority of the MS technique is sufficient, the needed R&D effort might well be undertaken by industry and would likely be completed within 2 years.

²For an adequate comparison, it would not be necessary to scan each bag with both technologies, as this would result in unacceptable delays for passengers. Rather, the technologies would be evaluated independently based on aggregate performance numbers from similar sets of bags. It would be important to test these technologies under a range of conditions—for example, in wintertime and summertime—as well as at various deployment sites—for example, JFK, SFO, and any other airports that have unique characteristics.

Phase 4: Environmental Monitoring (>10 years)

As future threats emerge, one can imagine attacks on the air handling equipment in either a transportation terminal or in the transportation vehicle. One concept of operations might involve the use of less sophisticated triggering detection devices that would provide immediate emergency rerouting or cessation of air movement and that would then activate the environmental monitoring MS device to identify the species that created the event.

This class of instruments is less well defined than the instruments discussed above and is only at the concept stage. For environmental monitoring, MS operation would feature a data path to a central control point and/or feed-forward warnings to checkpoints or other strategic posts to facilitate airport shutdown and evacuation. This is a scenario in which the false alarm rate must be very low, so that the performance of this mass spectrometer would have to be well established. If biological threats are to be considered, one could expect this device to be two or three times as expensive as the instruments described above owing to the added expense of sample collection and preparation.

In a large urban airport, 5 to 10 instruments might be required, depending on how much remote sampling could be utilized.

FINDING AND RECOMMENDATION

Finding 3: The many trace detection tasks that can be envisioned in airports will require MS-based detection systems with various levels of cost and performance; in some cases, years of R&D and testing may be required to produce MS instruments with the necessary specifications.

Technology development schedules depend strongly on government involvement, and the instrument costs and deployment times mentioned here are based on the committee's best judgment of the difficulty of the detection task and practical issues associated with producing high-quality, field-usable instruments.

Recommendation 3: If TSA wishes to improve its trace detection capabilities, it should deploy MS-based detectors in a phased fashion, with successive generations of instruments addressing lower quantities of an expanded list of threat materials and more sophisticated security tasks. These tasks range from passenger screening at checkpoints to monitoring of the air handling system.

In conclusion, this report has examined the potential of one promising technology—mass spectrometry—to improve trace detection capabilities of explosives as well as chemical and biological threat agents in the aviation environment. Here, the committee has offered just one plausible scenario for deployment of MS systems. Subsequent committee reports will examine additional technologies and defensive strategies for addressing a wide range of terrorist threats.

Appendixes

Appendix A

Estimation of the Informing Power of an Ion Mobility Spectrometer

The idea of informing power comes from information theory (or entropy). H. Kaiser (1978, reprinted from a 1974 publication) provided an introduction to the use of information theory for evaluating methods in analytical chemistry. Fitzgerald and Winefordner (1975) also described the concept and provided applications to molecular absorption, conventional phosphorimetry, and time-resolved phosphorimetry. Fetterolf and Yost (1984) determined the informing power of various tandem mass spectrometry configurations, including GC/QMS, QMS/QMS, GC/QMS/QMS (see Table 2-1).

The informing power, P_{inf} , of a measuring device is the number of bits required to encode the information potentially available from the device. Supposing, for example, that the device can report one of S possible values, the informing power of the device is $\log_2(S)$. If the device has a parameter x that can be varied over k possible values x_1, \dots, x_k , and the device is capable of reporting $S(x_i)$ measurement values at x_i , then the informing power is summed over the k settings, producing

$$P_{\text{inf}} = \sum_{i=1}^k \log_2 S(x_i)$$

Because of the log term, greater gains can typically be achieved by increasing the number of values for x than by increasing $S(x)$.

If the parameter x can be varied continuously, then P_{inf} can be reformulated by introducing the concept of resolution for the parameter x , defined as $R(x) = x/\delta x$, where δx is the smallest distinguishable difference in x for practical purposes. As introduced by Kaiser, the informing power becomes

$$P_{\text{inf}} = \int_{x_a}^{x_b} R(x) \log_2 [S(x)] x^{-1} dx$$

There might be a number of simplifications to this expression. It might be that $S(x)$ is constant, $S(x) \equiv S$, for example when S is fixed by characteristics of the detector. Or, the resolution might be constant, $R(x) \equiv R$. Another common possibility is that δx is constant. If $S(x) \equiv S$ and $R(x) \equiv R$, then

$$P_{\text{inf}} = R \log_2(S) \ln\left(\frac{x_b}{x_a}\right)$$

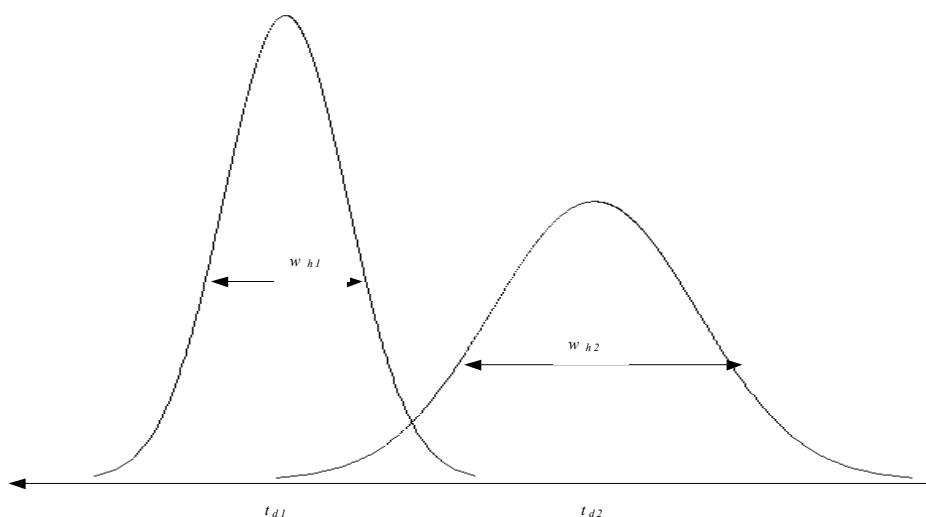


FIGURE A-1 The resolution of two peaks in an IMS spectrum depends on the separation of their drift times and the width of the peaks at half intensity. An important quantity that governs whether two different substances are distinguishable by the drift time is the width of the intensity peaks. This width is quantified by w_h , the width at half the maximum height of the distribution. Two drift times, t_{d1} and t_{d2} , are distinguishable if $|t_{d1} - t_{d2}| > \frac{1}{2}(w_{h1} + w_{h2})$.

(For chromatographic devices, another common measure of device capability is the number of theoretical plates, N , which is related to the resolution by $R = (N/5.55)^{1/2}$. The number of theoretical plates is often reported as a constant.)

This general expression for P_{inf} is easily extended to devices for which multiple parameters can be varied—e.g., for two parameters, x and y :

$$P_{\text{inf}} = \int_{x_a}^{x_b} \int_{y_a}^{y_b} R_y(y) R_x(x) \log_2[S(x, y)] y^{-1} x^{-1} dy dx$$

where it is assumed here that the resolution for y does not depend upon the value of x .

For ion mobility spectrometry (IMS), the output is the intensity and the variable parameter (x) is the drift time. The critical quantities, then, are the resolution of the drift time and the precision of the intensity measurements. The resolution of the drift time quantifies the degree of separation required to distinguish different peaks. At drift time t , the resolution is given by $R(t) = t/w_h(t)$, where $w_h(t)$ is the width of the peak at half maximum intensity, as shown in Figure A-1. (See, for example, Asbury and Hill, 1999; Matz, Tornatore, and Hill, 2001; Clemmer and Jarrold, 1997; Dugourd, Hudgins, Clemmer, and Jarrold, 1997.) The literature supports the assumption that the drift time resolution is constant, $R(t) \equiv R$. Matz et al. report that R is about 30 for commercial IMS instruments and use $R = 36$ in their calculations. Asbury and Hill report that for a typical IMS device, the number of theoretical plates rarely exceeds $N = 5,000$, which corresponds to $R = 30$.

The number of intensity values that can be reported, S , is also constant. Fetterolf and Yost use $S = 2^{12}$ for mass spectrometry. For IMS, the value of S appears to be less well defined. Often a 12-bit analog-to-digital converter is used, which would imply $S = 2^{12}$ at first glance. However, in practice the number of reproducible intensity values is much less, perhaps as low as 2^4 (Knapp 2003).

Finally, the value of P_{inf} depends upon the range of drift times observed. One commercial IMS used in aviation security reports a range of approximately 0 to 15 ms. The literature indicates considerable variation in the drift times observed, depending (as one would expect) on the application and construction of the device (dopant gas, length of drift tube, voltage, gate width, and so on).

The value of P_{inf} for IMS, then, is approximately

$$P_{inf} = 36 \log_2(2^4) \ln(15/0.3) = 36 * 4 * 3.9 = 562$$

For the comparative calculations in Table 2-1, the value used for P_{inf} for IMS is 1,000.

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Appendix B

Biographies of Committee Members

Thomas S. Hartwick, *Chair*, is retired manager of satellite payload program and system design activities at TRW. Dr. Hartwick has many years experience as manager of various organizations in the aerospace industry and previously worked at Hughes Aircraft Company and the Aerospace Corporation. His areas of research include sensors and imaging, with specialization in optical communications, far-infrared lasers and their applications, and laser heterodyne radiometry. Since leaving the aerospace industry in 1995, Dr. Hartwick has served on a number of academic, government, and industrial boards in a technical management role. Dr. Hartwick was chair of the NRC Panel on Assessment of Technologies Deployed to Improve Aviation Security.

Sandra L. Hyland, *Vice Chair*, is with Tokyo Electron Massachusetts, where she is responsible for process support to integrated circuit manufacturing facilities along the East Coast. Her group analyzes technology trends and customer data to determine hardware and process needs for manufacturing current and next-generation computer chips, including both capability and cost-reduction considerations. Dr. Hyland was previously an integration engineer for IBM's radiation-hardened computer chip manufacturing facility and managed a processing facility for the Jet Propulsion Laboratory to assess various materials for their potential as solar-cell substrates. She was also a staff officer for the National Materials Advisory Board, where she managed committees on aviation security and the design of U.S. paper money. She has a Ph.D. in materials science from Cornell University and M.S. and B.S. degrees in electrical engineering from Rutgers, the State University of New Jersey, and Rensselaer Polytechnic Institute, respectively.

Cheryl A. Bitner is program director for electronic warfare trainers, maintenance trainers, gunnery system trainers, and on-board (embedded) trainers at AAI Corporation. She has over 21 years of industry experience in providing training and simulation products for government as well as commercial customers and has a strong background in cost and schedule control techniques. Her responsibilities include ensuring positive program performance, strategic planning, manpower management, and personnel development. Ms. Bitner is a certified project management professional (PMP) and is a member of the National Training and Simulation Association (NTSA). She has published a cost and benefit analysis of piloting and navigational team trainers and contributes to the AAI Training Systems Newsletter. Ms. Bitner completed the advanced program management course at the Defense Systems Management College in 1989 and holds an M.S. in engineering science and a B.S. in computer science from Loyola College.

Donald E. Brown is chair of the Department of Systems Engineering of the University of Virginia. His research focuses on data fusion and simulation optimization, with applications to intelligence, security, logistics, and transportation. He has developed decision support systems for several U.S. intelligence agencies and was previously an intelligence operations officer for the U.S. Army. Dr. Brown is coeditor of *Operations Research and Artificial Intelligence: The Integration of Problem Solving Strategies* (Kluwer Academic Publishers, 1990) and *Intelligent Scheduling Systems* (Kluwer Academic Publishers, 1995) and is an associate editor for the journal *International Abstracts in Operations Research*. He has been president, vice president, and secretary of the Systems, Man, and Cybernetics Society of the Institute of Electrical and Electronics Engineers (IEEE). He is past chairman of the Technical Section on Artificial Intelligence of the Institute for Operations Research and Management Science and was awarded that society's Outstanding Service Award.

Colin G. Drury is professor of industrial engineering at the University at Buffalo and executive director of the Center for Industrial Effectiveness, where he has worked extensively in integration of ergonomics/human factors into company operations, resulting in increased competitiveness and job growth for regional industry and two Project of the Year awards from the National Association of Management and Technical Assistance Centers (NAMTAC). Since 1990 he has headed a team applying human factors to the inspection and maintenance of civil aircraft, with the goal being error reduction. Dr. Drury performed a study for the Air Transport Association evaluating the FAA's modular bomb set and the use of this bomb set in training and testing security screeners. Dr. Drury is a fellow of the Human Factors and Ergonomics Society, the Institute of Industrial Engineers, and the Ergonomics Society. In 1981 he was awarded the Bartlett Medal by the Ergonomics Society, and in 1992 the Paul Fitts Award by the Human Factors and Ergonomics Society. He has a Ph.D. in production engineering from Birmingham University, specializing in work design and ergonomics. Dr. Drury served on the NRC Panel on Assessment of Technologies Deployed to Improve Aviation Security.

Patrick Griffin is a senior member of the technical staff at Sandia National Laboratories and was chair of the NRC Panel on Assessment of Practicality of Pulsed Fast Neutron Analysis for Aviation Security. At Sandia, he performs research in radiation modeling and simulation, neutron effects testing, radiation dosimetry, and radiation damage to materials. He is active in the standardization community and is the current chairman of the American Society of Testing and Materials (ASTM) subcommittee E10.05 on nuclear radiation metrology.

Jiri (Art) Janata is a professor of chemistry at Georgia Institute of Technology. Dr. Janata was previously associate director for materials and interfaces in the Environmental Molecular Science Laboratory at Pacific Northwest National Laboratory. His research areas include analytical chemistry, electrochemistry, chemical sensors, bioinstrumentation, biophysical chemistry, fundamentals of materials science, micromachining, and instrumental analysis. Professor Janata has organized and chaired numerous symposia and conferences in his field, including Gordon Research Conferences on electrochemistry (January 1995), nuclear waste and energy (September 1996), and Chemical Sensors and Interfacial Design (July 1998). He is on the editorial boards of three journals: *Biosensors*; *Sensor Technology*; and *Talanta*. He is on the advisory board of *Analytical Chemistry* and associate editor for *Field Analytical Chemistry and Technology*. Dr. Janata has received numerous awards for his research (Alexander von Humboldt Senior Scientist Prize, 1987; Outstanding Research Award, University of Utah, 1990 (declined); Heyrovsky Medal, Czechoslovak Academy of Sciences, 1990; finalist medal, Science pour l'Art 1992, Moët Hennessy & Louis Vuitton, 1992; and Outstanding Achievement Award, Electrochemical Society, October 1994) and has been a visiting professor at many outstanding universities around the world (Wolfson College, Oxford University 1986/1987; Ecole Polytechnique Fédérale de Lausanne, 1990; and Tokyo Institute of Technology, 1995).

Len Limmer retired as deputy executive director of operations at the Dallas/Fort Worth International Airport, where he was responsible for the management of the airport's three operating departments: Operations, Public Safety, and Maintenance. He has held high office in numerous Texas and national associations concerned with public safety in large metropolitan areas. Mr. Limmer served on the NRC Panel on Assessment of the Practicality of Pulsed Fast Neutron Transmission Spectroscopy for Aviation Security and the NRC Panel on Assessment of Technologies Deployed to Improve Aviation Security.

Harry E. Martz, Jr., is the leader for the nondestructive evaluation research and development thrust at Lawrence Livermore National Laboratory. Dr. Martz has extensive background in the use of computed tomography and x-ray radiography (technologies commonly used in explosives detection) to perform nondestructive evaluation. His current projects include the use of nonintrusive x- and gamma-ray computed tomography techniques as three-dimensional imaging tools to understand material properties and to assay radioactive waste forms. Dr. Martz has served on several NRC committees and panels dealing with the general topic of aviation security. In addition, he chaired the NRC Panel on Technical Regulation of Explosives Detection Systems.

Richard McGee is a retired electronics engineer with 35 years in the area of ballistics at the Army Research Laboratory, Aberdeen Proving Ground. Currently working part time as a senior scientist contractor at ARL, Dr. McGee is an experienced researcher with extensive expertise in millimeter-wave, infrared, radiometry, radar, smart munitions, and sensor-based system engineering and integration. He conducted field experiments to characterize near-Earth propagation of millimeter waves (10 mm to 1 mm wavelength) in turbid and tactically hostile environments and designed, fabricated, and field tested brassboard smart munition sensors. Additionally, he has designed and fabricated instrumentation to measure millimeter radiometric and radar signatures of red and blue combat vehicles and signatures of various terrains. Some new projects of his look at microwave and millimeter-wave holography, development of algorithms for multispectral fusion target recognition, and SAR and ISAR high-resolution instrumentation radars (3.2 mm and 2.2 mm). Dr. McGee is highly skilled in system integration and engineering for smart munitions with a working knowledge of sensors, warheads, guidance and control, aerodynamics, lethality performance analysis and high acceleration survivability.

James F. O'Bryon is retired deputy director, Operational Test and Evaluation (OT&E), Live Fire Testing, Office of the Secretary of Defense, at the Pentagon. Mr. O'Bryon served in various positions within the DDR&E, USD(A&T), before his position as director of OT&E. All of these positions involved overseeing and directing test and evaluation activities for the Secretary of Defense, primarily examining test plan adequacy, test execution, vulnerability/lethality, and application of tactics and doctrine to these issues. Mr. O'Bryon has testified to various committees of the Congress on defense issues as well as drafting the Secretary of Defense's reports on system survivability and lethality vulnerability. He has served on more than a dozen committees addressing such things as directed energy, ozone-depleting compounds, and modeling and simulation.

Richard L. Rowe is retired chief executive officer of MCMS, a \$550 million electronics contract manufacturing company. His experience includes sensor technologies applied to aviation security, as well as new technologies in optics and radio frequency and electronic sensors and switch products. He has over 20 years of experience in the electronic sensors and switch products industry. Prior to his work in the electronics industry he was with the U.S. Army for 6 years. He has a master's degree in engineering administration from the George Washington University, Washington, D.C., and a bachelor's degree in engineering and applied sciences from the U.S. Military Academy. He has served on the board of various electronics industries and was awarded the Honeywell Lund Award, a major leadership award, in 1987.

Eric R. Schwartz is director of Advanced Vehicle Systems Technology at the Boeing Company's Phantom Works. In this role he leads R&D activities for advanced commercial and military aerospace vehicle systems and subsystems. This includes technology development for crew systems, vehicle systems, flight management systems, software integration, and subsystems. He is also responsible for aviation security technologies such as chem/bio detection and mitigation and for aircraft protection. Mr. Schwartz has experience in threat analysis, bomb blast effects, and blast testing of hardened luggage containers. He has performed Boeing and National Transportation Safety Board investigations and managed engineering analyses on terrorist bombing events on aircraft. He is a recognized expert on the structural and systems effects of threats against commercial aircraft and has presented numerous papers to the FAA, NASA, AIAA, U.S. Department of Defense, and international aviation authorities. Mr. Schwartz has participated in several government committees and advisory boards, including the National Research Council's Panel on Assessment of Technologies Deployed to Improve Aviation Security and the FAA Aviation Security R&D Advisory Committee and served as deputy director of the AIAA Technical Committee. He has also served on the NASA Aviation Safety Executive Council, the European JAA Future Aviation Safety Team, the IATA Aviation Security Committee, and the NATO R&D Advisory Group for Aircraft Survivability.

Elizabeth H. Slate is an associate professor in the Department of Biometry and Epidemiology at the Medical University of South Carolina. One of her more recent grants was from the Semiconductor Research Corporation/NSF for methods of modeling stochastic processes in semiconductor manufacturing. Dr. Slate has a diverse statistical analysis background and both academic and industrial experience. She is active in many statistics-related societies, such as the American Statistical Association, and is the chair elect of the American Statistical Association Subsection on Statistical Computing. Dr. Slate served on the NRC Panel on Assessment of Technologies Deployed to Improve Aviation Security.

Michael Story is retired from Thermo Electron Corporation. Mr. Story was involved in the research, design, and commercialization of mass spectrometers for 37 years and is a cofounder of the Finnigan Corporation. He was a member of previous NRC committees on commercial aviation security (1988-1993) and chaired the Panel on Test Protocol and Performance Criteria. He is a member of the NRC Committee on Commercial Aviation Security and the Panel on Assessment of Technologies Deployed to Improve Aviation Security.