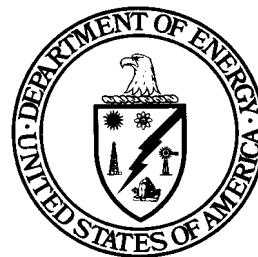


# Direct Sampling Ion Trap Mass Spectrometry (DSITMS)

Characterization, Monitoring, and  
Sensor Technology Crosscutting  
Program



*Prepared for*  
**U.S. Department of Energy**  
Office of Environmental Management  
Office of Science and Technology

December 1998



# Direct Sampling Ion Trap Mass Spectrometry (DSITMS)

OST Reference #69

Characterization, Monitoring, and Sensor  
Technology Crosscutting Program



*Demonstrated at*  
Oak Ridge Reservation  
Oak Ridge, Tennessee  
and  
Savannah River Site  
Aiken, South Carolina

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## ***Purpose of this document***

Innovative Technology Summary Reports are designed to provide potential users with the information they need to quickly determine if a technology would apply to a particular environmental management problem. They are also designed for readers who may recommend that a technology be considered by prospective users.

Each report describes a technology, system, or process that has been developed and tested with funding from DOE's Office of Science and Technology (OST). A report presents the full range of problems that a technology, system, or process will address and its advantages to the DOE cleanup in terms of system performance, cost, and cleanup effectiveness. Most reports include comparisons to baseline technologies as well as other competing technologies. Information about commercial availability and technology readiness for implementation is also included. Innovative Technology Summary Reports are intended to provide summary information. References for more detailed information are provided in an appendix.

Efforts have been made to provide key data describing the performance, cost, and regulatory acceptance of the technology. If this information was not available at the time of publication, the omission is noted.

All published Innovative Technology Summary Reports are available on the OST Web site at <http://OST.em.doe.gov> under "Publications."

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## SECTION 1

# SUMMARY

This report describes the cost, performance, and other key characteristics of an innovative technology for determining the presence or absence, and measuring the concentration, of volatile organic compounds (VOCs) and semi-volatile organic compounds (SVOCs) in groundwater and soil, and in gaseous remediation process streams at hazardous waste sites. This new technology is Direct Sampling Ion Trap Mass Spectrometry (DSITMS) (OST TMS# 69).



Direct sampling ion trap mass spectrometry (DSITMS) introduces sample materials directly into an ion trap mass spectrometer by means of a very simple interface, such as a capillary restrictor or a polymer membrane. There is typically very little, if any, sample preparation and no chromatographic separation of the sample constituents. This means that the response of the instrument to the analytes or contaminants in a sample is nearly instantaneous, and that analytical methods based on DSITMS are fast. Analyses are typically completed in less than five minutes, and the analysis cost is generally fifty percent or less than the amount charged by commercial laboratories using Environmental Protection Agency (EPA) analysis methods.

### Technology Summary

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The broad target problem area for DSITMS is rapid detection and quantitative measurement of VOCs, generally solvents, including chlorinated solvents such as trichloroethylene, perchloroethylene, carbon tetrachloride, and trichloroethane, and SVOCs, in the groundwater, soil, and gaseous remediation process streams at hazardous waste sites.



More specific problem areas where DSITMS is applicable include the following:

- Rapid site characterization to support decisions concerning whether groundwater and/or soil contamination exists at a site;
- Rapid site characterization to support decisions concerning whether, where, and how groundwater monitoring wells should be installed;
- Rapid, high sensitivity, laboratory screening of groundwater samples, providing justification for, and cost savings from, not subjecting uncontaminated samples to the more expensive and time-consuming analysis by the conventional method, EPA Method 8260.

VOCs in water are introduced by purging the sample with helium and routing the purge stream to the DSITMS. VOCs in air, soil gas, and water can be measured in real time or they may be collected on sorbent traps and subsequently analyzed by thermal desorption DSITMS.

DSITMS is applicable to VOCs and SVOCs in a wide variety of sample matrices and it can detect a wide range of those analytes at low-ppb levels. DSITMS is applicable to all 34 VOCs on the EPA target compound list. The DSITMS detection limits are well within the range required by EPA, 1-5 parts per billion for VOCs in water or soil, and 1-100 parts per billion by volume for continuous monitoring of VOCs in air. This versatility and power makes it a good choice for many field-screening applications, including rapid site characterization and rapid source term characterization (Wise et al 1997).

The DSITMS instrumentation is field transportable, rugged, and relatively easy to operate and maintain. It can be operated in a small van, a four-wheel-drive vehicle, or a SCAPS truck, permitting it to be as close as possible to sampling and/or direct push operations, as shown in the photograph above. SCAPS stands for the Tri-Services (U.S. Army, Navy, and Air Force) site characterization and analysis cone penetrometer system (Davis et al. 1997). The cone penetrometer can be used for soil gas sampling, with direct sampling into the DSITMS. In addition, a cone penetrometer can be used to push a hollow pipe below the water table, creating a mini-well. A small diameter bailer can be dropped down the inside of the pipe and used to collect groundwater samples for quick screening by DSITMS at the surface. Alternatively, a specially designed, *in situ* sparging probe can be inserted into the pipe and used to purge VOCs directly from the groundwater. The VOCs are brought to the surface through a transfer line and are directly sampled into the DSITMS in the same manner as soil gas. The advantages of the *in situ* sparge technique are that it is fast and it eliminates the need to collect and handle samples. Comparison of results using *in situ* sparging versus the analysis of discrete samples by laboratory GC/MS has been favorable (Wise and Guerin 1997).

### **Potential Markets**

- According to a recent market assessment (Sigmon, 1998), groundwater remediation is in progress at an estimated 4000 to 5000 DNAPL-contaminated U.S. sites, with about 350 being added each year. Roughly, this means characterizations of the problem situations are being completed at about the rate of 350 sites per year. This includes both private- and public-owned sites; all are potential candidates for DSITMS characterization. DOE, DoD, and NASA sites comprise the bulk of the potential market at federally owned sites.
- DSITMS is applicable to VOCs and SVOCs in a wide variety of sample matrices and it can detect a wide range of those analytes at low-ppb levels. This versatility and power makes it a good choice for many field-screening applications, including rapid site characterization and rapid source term characterization (Wise et al. 1997).



- Because of its high sensitivity and speed, DSITMS is useful for laboratory screening of groundwater samples. Because most such samples do not have VOC contamination above the DSITMS and EPA Method 8260 MDLs, the results from the faster, cheaper DSITMS analysis can provide justification for not subjecting most samples to the slower, more costly baseline analysis method (EPA Method 8260). This application would be suitable for any analytical laboratory that currently uses Method 8260 to perform a large number of analyses for VOCs in groundwater. The expected cost savings compared to baseline for this application are addressed in Section 5 of this report.
- Furthermore, for screening purposes, it is not always necessary to analyze for a full suite of compounds to support valid conclusions regarding the presence of absence of contamination. This is so because certain contaminants commonly co-occur at hazardous waste sites. In fact, it is possible to confidently screen for the presence of the 37 most common VOCs by monitoring for only 15 specific analytes (Wise et al. 1997).
- A good working relationship between the site regulator, site manager, and DSITMS applier, a relationship that is open to the regulatory acceptability of the DSITMS results, is essential for successful utilization of DSITMS.

## Demonstration Summary

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Numerous applications/demonstrations of DSITMS have occurred at DOE and DoD sites in the period covered by this report, from April 1993 through November 1997. Information concerning the location, purpose, and dates of many of those applications/demonstrations are tabulated in Appendix C. The key features of DSITMS that favored its application at those sites are:

- applicability for field analysis
- ability to provide analysis results with little or no sample pretreatment
- ability to provide analysis results for VOC concentration levels in groundwater that are at or below the level of regulatory concern
- ability to provide analysis results without false negatives
- ability to complete VOC analysis of a sample every 3 to 5 minutes, thus supporting expedited site characterization and the use of dynamic work plans for site characterization
- ability to provide analysis results for site characterization in a manner that favorably competes technically and economically with baseline methods.

This report focuses closely on three of those demonstrations/applications to illustrate three distinctly different application scenarios and the DSITMS performance and cost benefits in each. The three scenarios are:

- Use of DSITMS for rapid laboratory screening of water samples for site characterization (groundwater contamination) investigations.
- Field screening of groundwater to rapidly characterize the location, nature, and extent of VOC contamination and/or to characterize migration of contaminated groundwater.
- Laboratory screening of water samples to reduce the cost of periodic groundwater quality monitoring.

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Davis is a leader in the development, testing, and application of probes for cone penetrometer application (thermal desorption and hydrosparge probes for VOCs in soil and groundwater). He has typically used these probes with a DSITMS.

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### **Patent and Licensing Information**

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### **Other**

All published Innovative Technology Summary Reports are available on the OST Web site at <http://em-50.em.doe.gov> under "Publications." The Technology Management System, also available through the OST Web site, provides information about OST programs, technologies, and problems. The OST Reference # for the Direct Sampling Ion Trap Mass Spectrometer is 69.





## SECTION 2

### TECHNOLOGY DESCRIPTION

Direct Sampling Ion Trap Mass Spectrometry (DSITMS) involves the continuous real-time monitoring of volatile organic compound (VOC) analytes as they are introduced into an ion trap mass spectrometer (ITMS). VOCs from water or soil samples are introduced by purging the sample with helium and routing the purge stream into the ITMS. VOCs in air may be monitored in real-time or may be analyzed by collection on solid sorbent traps followed by thermal desorption into the ITMS. Thermally stable SVOCs can also be determined by thermal desorption from the sample. Little or no sample preparation is required; chromatographic separation is not required. A key benefit is the very short analysis time. A visual indication of the kinds and quantities of pollutants present is available immediately and sufficient data are accumulated for quantitation of VOCs in water or soil in five minutes or less. Air monitoring can be performed in real-time. The technology is applicable to the determination of VOCs in groundwater, soil, and air.

VOCs in water can be quantitatively determined to concentrations of 5-10 ppb (parts per billion) depending on the analyte. Response is linear over at least four orders of magnitude. Instrument detection limits are approximately 0.5 ppb for most analytes. Detection and quantitation limits are 2-3 times larger for soils compared to water. Continuous real-time air monitoring detection limits are 50-100 ppbv (parts per billion by volume). The mass detection limit for analytes introduced by thermal desorption is approximately 50 picograms. The concentration detection limit depends on the sample size analyzed. The principal applications include screening without false negatives and quantitative analysis. Costs per sample are generally 50% or less of standard methods. Analyses can be performed in the field or in the laboratory.

#### Technology Description

Early DSITMS instruments were based on commercially available Finnegan MAT or Teledyne ion trap mass spectrometers; these were modified by addition of a direct sampling inlet designed by Oak Ridge National Laboratory personnel. The instruments were further modified for field and mobile use by replacing the instrument base, vacuum pump, and roughing pump (Wise et al. 1993). According to W. M. Davis, the U.S. Army Engineers, Tulsa District, recently acquired a DSITMS instrument by purchasing a Varian Saturn ion trap mass spectrometer and having it modified by ORNL personnel (Haas 1998b). Both laboratory-based and field-transportable versions of the instrumentation are available.

Figure 2.1 provides a schematic illustration of the main components and functions of the DSITMS technology. In the illustration, headspace vapor containing VOCs from a contaminated sample (or a helium stream containing VOCs sparged from a sample) are pulled into the mass spectrometer chamber (from atmospheric pressure through the capillary restrictor). There, the VOCs are ionized, mass analyzed in the ion trap (Mass Filter), and detected. The detector signals produce a mass spectrum as shown at the bottom of Figure 2.1.

Figure 2.2 shows a typical DSITMS capillary restrictor inlet comprised of a 25-cm length of 50 to 150 micrometer ID deactivated fused silica capillary that can be heated to more than 200 °C. The splitter on the atmospheric pressure end of the capillary permits the use of sampling modules that



require gas flows greater than the capacity of the restrictor. The splitter also enables the simultaneous collection of archival samples on sorbent cartridges.

Figure 2.3 shows some examples of sample introduction modules that can be attached to a capillary restrictor inlet by means of a quick-connect fitting. These modules permit the use of DSITMS for analysis of VOCs and SVOCs in air, water, and soil.

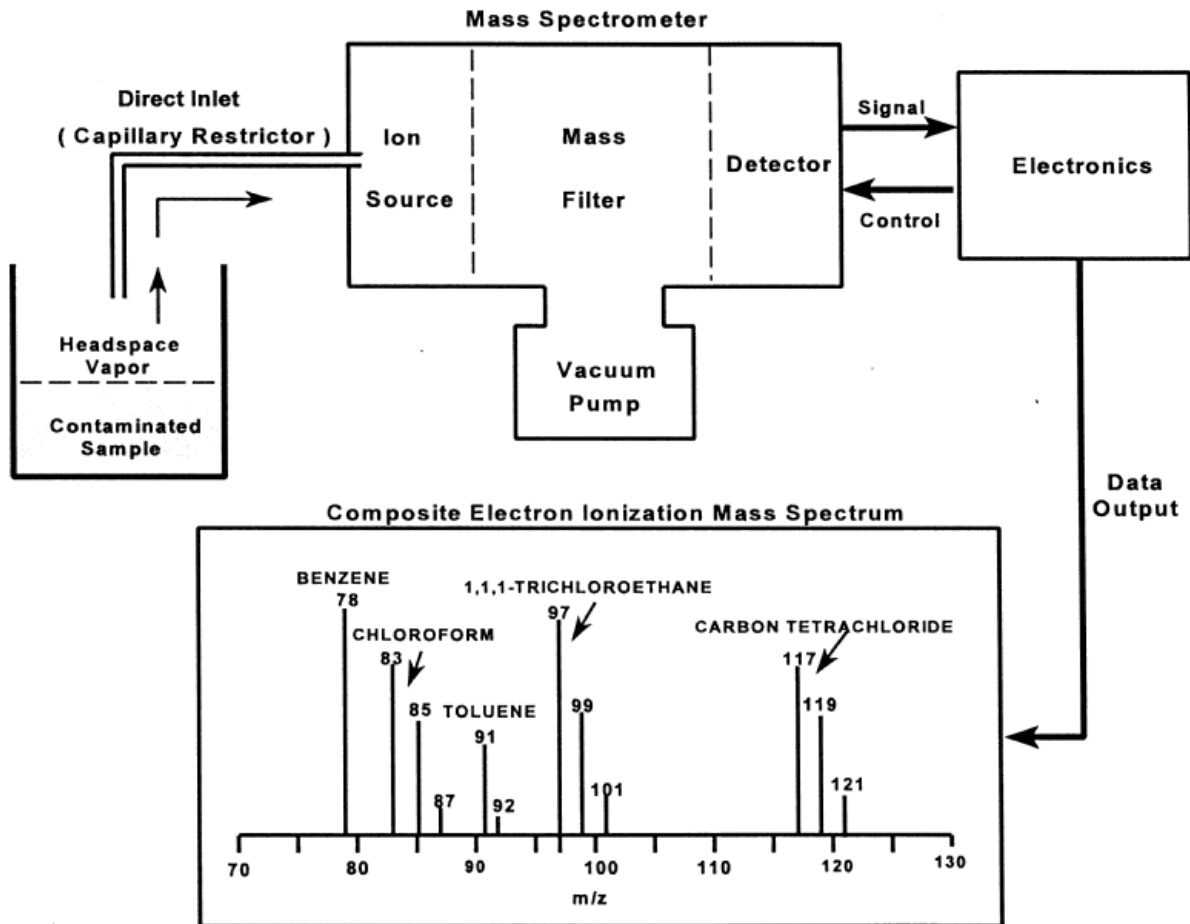


Figure 2.1. Schematic of a direct sampling mass spectrometer equipped with a capillary restrictor and used for the measurement of VOCs in the headspace vapor of a contaminated sample (Wise et al. 1997).

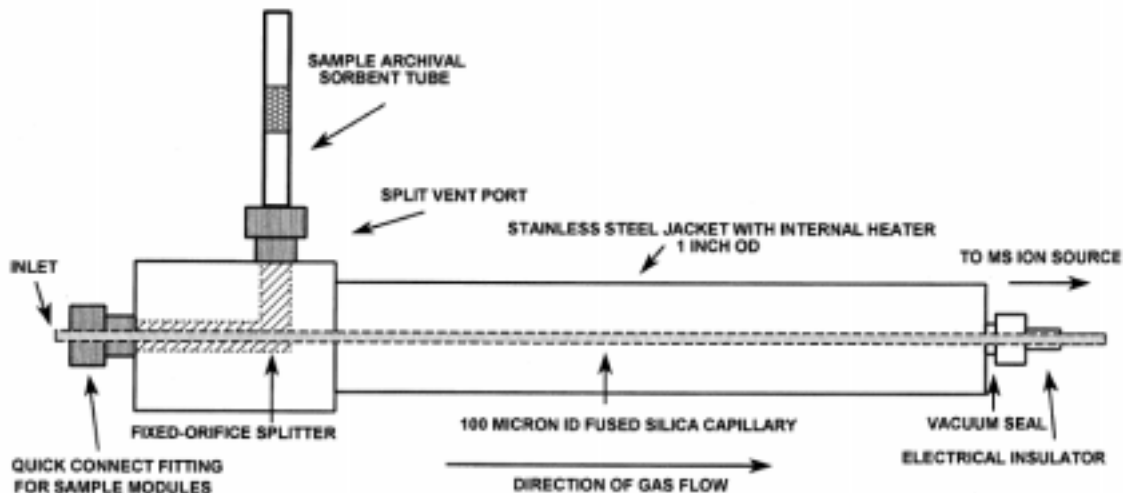


Figure 2.2. A typical capillary restrictor inlet for DSITMS (Wise et al. 1997).

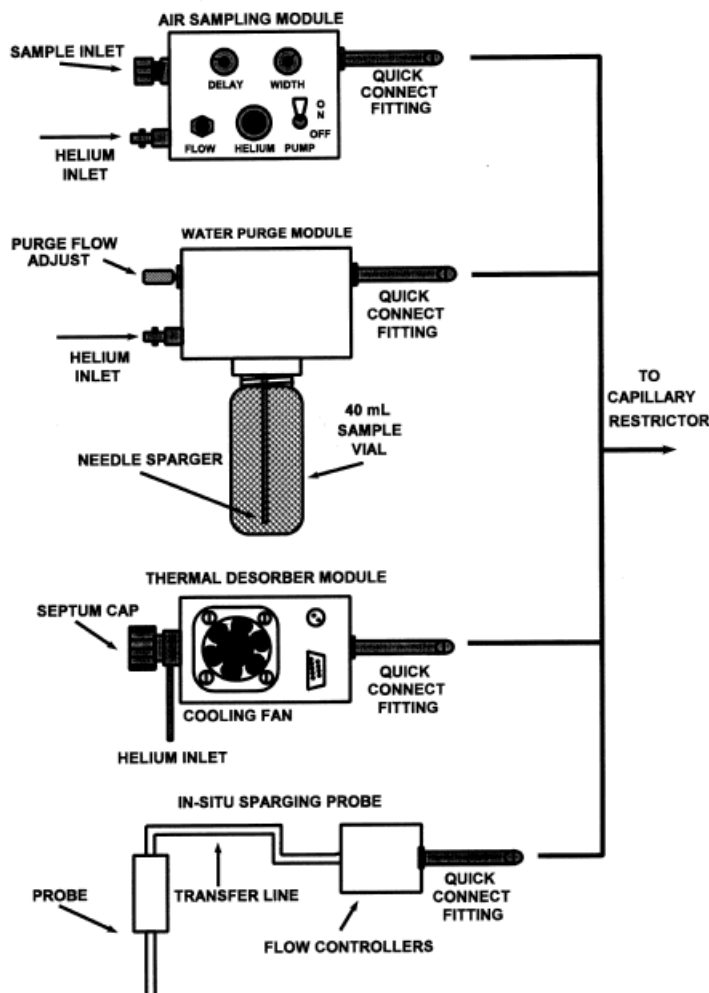


Figure 2.3. Some examples of sample introduction modules that can be attached to a capillary restrictor inlet by means of a quick-connect fitting. These modules permit the use of DSITMS for analysis of VOCs and some SVOCs in air, water, and soil (Wise et al. 1997).

The ion traps used for DSITMS applications are based on three-dimensional quadrupole ion trap mass analyzers; these have been commercially available for approximately fifteen years. As illustrated in Figure 2.4 (adapted from Yates et al. 1995), ion trap mass analyzers consist of a small, cylindrically-symmetric, stainless steel cell, comprised of a ring electrode and two hyperbolic end caps, an ion entrance end cap and an ion exit end cap. Each of the electrodes has accurately machined hyperbolic internal surfaces. Ions are created within the ion trap by the gated injection of electrons emitted from a filament, shown at the left of the Figure. Ions with a range of  $m/z$  (mass/charge) values are trapped (held in stable orbits) inside the cell by applying a 1.1 MHz rf (radio frequency) signal to the ring electrode. Mass analysis is accomplished by ramping the rf voltage from a few hundred volts to several thousand volts. As the rf voltage is increased, the motion of ions of increasing  $m/z$  become more and more energetic until their trajectories become unstable along the axis of cylindrical symmetry. As a result, the ions are ejected through holes in the right hand and are collected on the electron multiplier detector. The ejection of the ions occurs in the order of increasing  $m/z$ -value and the resulting signal represents the mass spectrum of the ions that were originally trapped. The assembled ion trap includes teflon or quartz spacers between the electrodes. The spacers ensure that the assembly is reasonably gas tight since the performance of the trap is improved by maintaining a pressure of about 0.1 Pa of helium gas during operation.

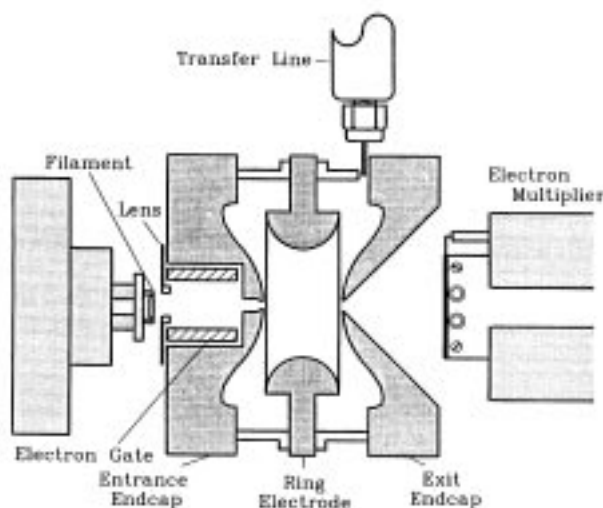


Figure 2.4. Schematic of an ion trap mass spectrometer using internal ionization. The helium-borne analytes enter the trap via the transfer line shown at the top. The pressure in the trap is ten times greater than the pressure in the surrounding vacuum system.

The high sensitivity of quadrupole ion traps largely results from their ability to continuously generate and store ions in the analyzer cell for several milliseconds prior to their ejection and detection. This allows a sufficiently large number of ions to accumulate so that a detectable signal is produced even for trace analytes. This ion storage capability also enables additional operating modes. For example, trapped ions can be subjected to chemical ionization reactions that enhance the response for specific analytes relative to others (potentially interfering analytes). It is also possible to probe the structure of specific ions using MS-MS techniques. In this mode of operation, the kinetic energy of selected ions is increased, causing them to fragment into smaller ions upon collision with neutral gas molecules added to the analyzer cell. The MS-MS

fragmentation patterns are often compound-specific and can be used to positively identify a targeted analyte in complex samples (Wise et al. 1993).

Other features of the DSITMS technology include the following:

- Full-scan mass spectra are generated every approximately 100 msec as the sample stream is being introduced.
- Ion signals characteristic of the analyte(s) of interest are plotted as a function of time to produce profiles whose areas are proportional to the amount(s) of analyte(s) present in the sample.
- The instrument is capable of ionization by both electron impact (EI) and chemical ionization (CI), and can automatically alternate between EI and CI every 0.5 seconds (multiplexed ionization). The CI spectra improve the detection limits for water-soluble compounds including aldehydes, ketones, and alcohols, and also improve the ability to differentiate compounds, which have similar EI fragmentation spectra, e.g., alkyl aromatics.
- Excess sample material can be collected on solid sorbent traps; for those cases in which interferences cannot be resolved directly, this trapped material can be analyzed later by conventional methods.

Limitations of the DSITMS technology include the following:

- Current instrumentation relies to a significant extent on off-line data processing.
- DSITMS methods have not been specifically “accepted” by regulatory agencies.
- Highly complex mixtures may contain chemical compounds that interfere with the accurate quantitative determination of some other chemicals of concern. Because there is no pre-separation of analytes, e. g., using a gas chromatograph, the system is limited to characterizing streams containing 5 analytes or less. In most cases, at DOE, DoD, and commercial sites, this is more than adequate. Nevertheless, especially for those applications where interferences are expected, the DSITMS results should be compared with those from standard accepted methods.
- At present, DSITMS instrumentation is not commercially available, off-the-shelf; DSITMS instrumentation can only be obtained by custom-modifying commercially available instruments.
- For non-routine applications, considerable experience is required to properly operate the instrument and interpret the data.

## Overall Process Definition

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As described in Wise and Guerin 1997, Direct Sampling Ion Trap Mass Spectrometry (DSITMS) refers to the introduction of analytes from a sample directly into an ion trap mass spectrometer using a simple interface with minimal or no sample preparation and no prior chromatographic separation. This translates into simplicity, real-time response, and high sample throughput capability. Multiple inlet configurations permit the screening of most types of environmental samples for volatile and semi-volatile organic compounds (VOCs and SVOCs) (Wise et al. 1993).

The Direct Sampling Ion Trap Mass Spectrometer (DSITMS) was developed at Oak Ridge National Laboratory. The system utilizes a commercially available ion trap mass spectrometer; modifications to the sample inlet on the spectrometer allow for direct injection of the sample material, eliminating the need for sample preparation, saving time and money. With some modifications, the mass spectrometer is made field transportable. As noted earlier in this section, several different probes have been developed for sampling of different media and sample types. Each is interchangeable on the DSITMS. They allow in-situ determination of volatile organic compounds (VOCs) in soil, groundwater, and flowing streams, and can be fitted to standard



sample collection vials for the analysis of collected samples. In all cases, the sample is sparged with helium to release the VOCs. This stream is directly injected into the DSITMS for analysis.

## System Operation

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### Instrumental Characteristics and Operating Requirements

- The total instrument volume is less than 8 cubic feet.
- The DSITMS instrumentation weighs approximately 120 pounds.
- The DSITMS power requirements are approximately 500 W (average) at 110 V AC. This can be supplied either by a small generator or by a DC to AC power inverter running off one or more deep-cycle storage batteries.
- With the exception of helium gas for purging samples, transporting VOCs from the samples into the DSITMS, and for operation of the ion trap mass spectrometer, the expendable items used in operation of the DSITMS are the same as those used in the baseline method. The costs of all those items are addressed in the Cost section of this report.

### Operational Parameters, Conditions, and Procedures

A complete description of the operational procedure, operational parameters, materials, energy requirements, and conditions for determination of VOCs in groundwater using the in situ sparge method with DSITMS is given in a recent article in *Current Protocols in Field Analytical Chemistry* (Davis, Furey, and Porter 1998).

### Operator skills and training requirements.

Experiences during demonstrations in the early 1990s suggested that the DSITMS instrumentation was relatively difficult to operate. At that time, a technician with approximately 10 years of analytical laboratory experience required two weeks of specialized training. Experiences during the last three years are different, however. ORNL and USAE personnel have successfully provided on-the-job field training in the application of the DSITMS for USAE Savannah and USAE Tulsa District personnel.

### Secondary waste considerations.

In general, the types and amounts of secondary waste generated as a result of DSITMS operation are similar but less than those generated by the baseline methods. When DSITMS is used with *in situ* air sparging, the amount of secondary waste is less because no groundwater is pumped and no samples are collected.



## SECTION 3

# PERFORMANCE

### Demonstration Plan

As noted earlier, the capabilities and performance of DSITMS have been tested, demonstrated, and employed on numerous occasions. A partial list of demonstrations/applications is given in Appendix C. The major objectives of the tests and demonstrations have been to establish, extend, and evaluate the performance capabilities of the technology, usually in comparison with the baseline technology, analysis at an off-site commercial laboratory using EPA Methods.

The key characteristics evaluated included the following:

- method detection limits
- dynamic range
- accuracy
- reproducibility
- the number and types of analytes that can be measured
- compatible sample matrices
- the rates of false positive and false negative results

DSITMS rates well in each of the above areas.

### Results

The ability of DSITMS to detect volatile organic compounds at very low concentrations is key to its usefulness for screening without false negatives. DSITMS meets EPA method detection limit requirements, one to five ng/ml (parts per billion by weight), for the 34 Target Compound List VOCs in water with a three minute purge time. The observed DSITMS method detection limits are given in Table 3.1 for some representative VOCs in water as determined by direct purge into an ion trap mass spectrometer.

**Table 3.1. Observed method detection limits for representative VOCs in water as determined by direct purge into an ion trap mass spectrometer (Wise et al. 1997).**

Compound	Ionization mode	Method detection limit (ng/ml)
Acetone	CI	2.3
Benzene	EI	1.7
Carbon tetrachloride	EI	1.8
Carbon disulfide	EI	2.1
Chloroform	EI	2.0
Dibromochloromethane	EI	5.8
Ethyl benzene	CI	1.8
Methyl ethyl ketone	CI	4.2
Perchloroethylene	EI	1.7
Toluene	CI	0.6
Trichloroethylene	EI	3.5
Vinyl acetate	CI	4.4
Vinyl chloride	EI	1.3



Figure 3.1 shows typical calibration results for measurement of VOCs in groundwater by the direct purge DSITMS technique. The data show a linear dynamic range of at least two orders of magnitude

Figure 3.2 shows the correlation of measurement results obtained for VOCs in groundwater by the Hydrosparge technique (*in situ* sparge plus DSITMS) and results obtained by U. S. EPA Method 8260 laboratory analysis of samples collected from the same points (Davis et al. 1998). Results are shown for more than 200 direct comparisons at seven different geographic sites. The results show a strong linear correlation ( $r^2 = 0.84$ , slope =1.2) and low false positive and false negative rates.

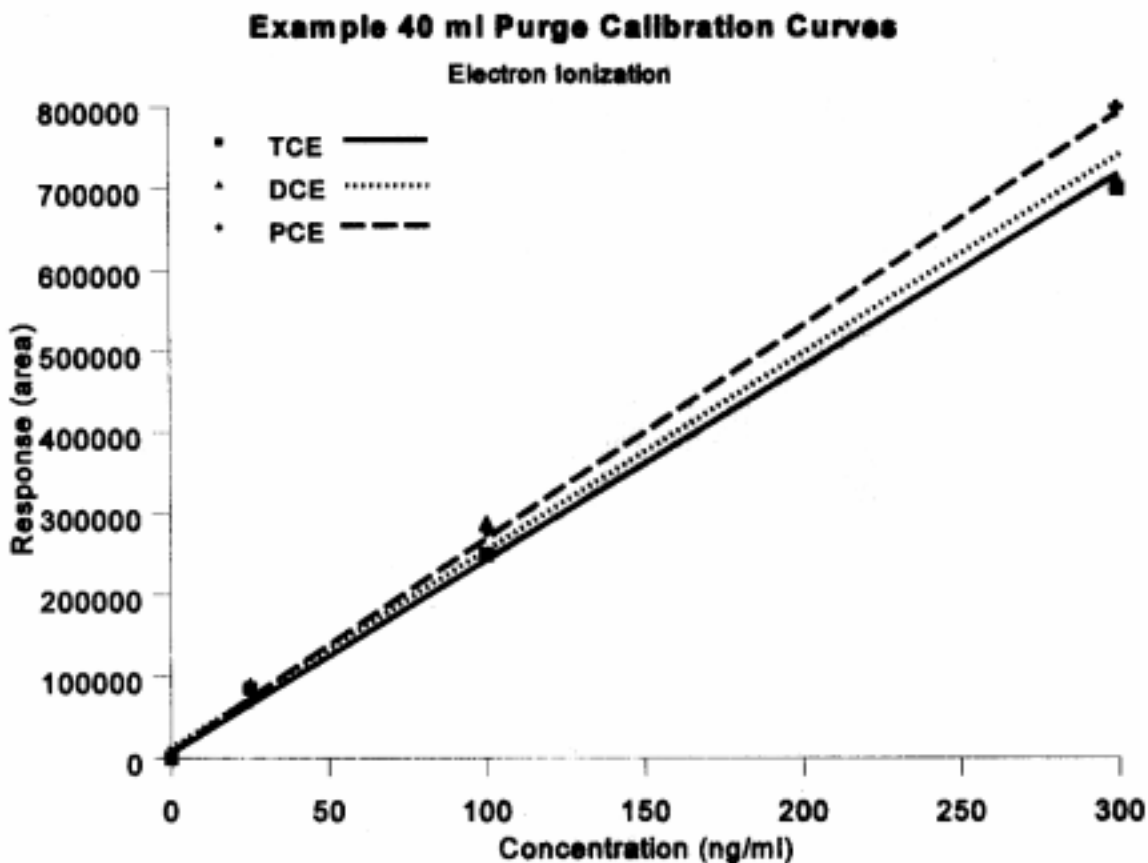


Figure 3.1. Typical instrument calibration data for measurement of some VOCs, trichloroethylene (TCE), dichloroethylene (DCE) and perchloroethylene (PCE), in groundwater by DSITMS.





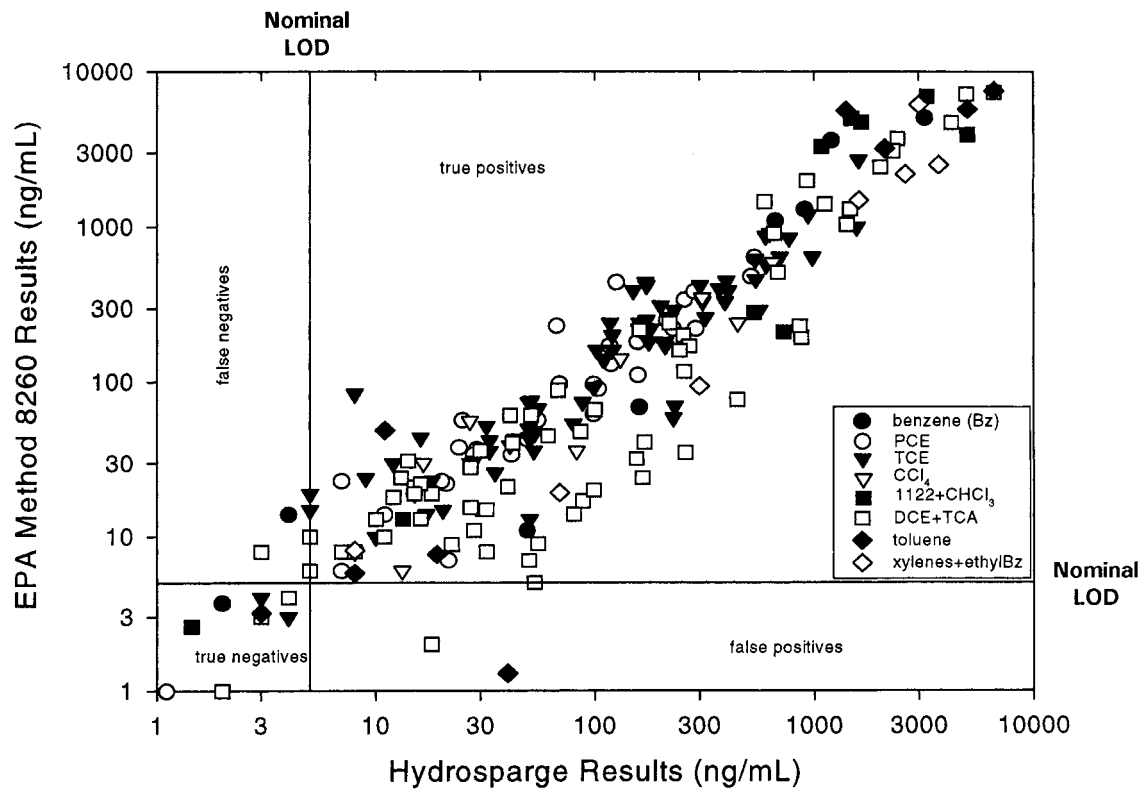


Figure 3.2. Correlation of Hydrosparge (*in situ* sparge plus DSITMS) results and U. S. EPA Method 8260 laboratory analysis results for > 200 direct comparisons at seven different geographic sites. The data showed a strong linear correlation ( $r^2 = 0.84$ , slope = 1.2).

## SECTION 4

# TECHNOLOGY APPLICABILITY AND ALTERNATIVES

The target problem for DSITMS is rapid, quantitative measurement of volatile organic compounds (VOCs), generally solvents, and semi-volatile organic compounds (SVOCs) in the groundwater, soil, soil-gas, air, and gaseous remediation process streams at hazardous waste sites.

- The technology is especially effective at waste sites where historical information is available on the identity of the expected contaminants and their concentrations.
- DSITMS can be used for site characterization and monitoring, and gaseous remediation waste stream (i.e., offgas) monitoring.
- DSITMS can also be used for other applications such as:
  - environmental monitoring of chemical processes, fugitive emissions and OSHA/CAA materials
  - industrial monitoring including continuous emissions monitoring (CEM) of stack emissions (Ghorishi et al. 1996), particle chemical processes, and other processes
  - detection of contraband, drugs, explosives, and lethal chemicals for law enforcement and the military
  - workplace monitoring for environmental health and safety.
- Environmental applications include:
  - Field screening, the most common environmental application of DSMS. Screening is a quick and economical means of guiding yes/no decisions regarding specific site activities, such as differentiating clean areas from contaminated areas, eliminating clean samples from those sent to a laboratory for analysis by EPA promulgated methods, and determining whether or not a remediation activity must continue at a given location. Appropriate use of field screening can promote more effective characterization and remediation by ensuring that the most time, money, and effort are focused on the most highly contaminated areas. Example field-screening applications include the following:
    - Expedited site characterization
    - Checking outfalls and seeps for contamination
    - Checking soil and solids for SVOCs such as pesticides, CW agents, or PCBs.
    - Detection of solvents and petroleum products from leaking underground storage tanks (LUSTs)
    - Screening of drilling muds and groundwater samples during well placement
  - Periodic monitoring of VOC contamination in groundwater monitoring wells at contaminated sites
  - Environmental remediation process monitoring
  - Continuous emissions monitoring for hazardous waste treatment facilities
  - Fugitive emissions monitoring
  - Vehicle exhaust monitoring
- Field screening with the DSITMS does not replace laboratory analysis, but it can be used to significantly reduce the number of samples sent off-site for more expensive laboratory analysis.
- Field screening with the DSITMS allows development of comprehensive data sets because of the relatively low cost of analyzing samples. In addition, collection of a large number of replicate measurements at a low cost allows for a more thorough statistical evaluation of the analytical results.



## Competing Technologies

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- **Baseline --**

The baseline approach is to collect groundwater and/or soil samples and/or gas samples and have them analyzed in a stationary analytical laboratory, often an off-site commercial laboratory, using RCRA protocols. This approach involves collection, packaging, and documentation of the samples according to EPA sample handling and chain-of-custody requirements, and shipping them to a laboratory for analysis. There, the analyses are performed using EPA methods (EPA 1995).

- **Other competing technologies --**

DSITMS competes with a number of person-portable and other field-transportable analytical instruments including FTIRs, GCs, and GC/MSs.

The EPA Consortium for Site Characterization Technologies has published evaluation reports on the commercially available Bruker-Franzen Analytical Systems, Inc. (EPA 1997) and Viking Instruments Corp. (EPA 1997b) field-transportable GC/MS instruments. Some of the key findings are described immediately below.

□ “The [Bruker-Franzen] EM640™ is a commercially available GC/MS system that provides laboratory-grade performance in a field transportable package. The instrument is ruggedized and may be operated during transport. It weighs about 140 pounds and can be transported and operated in a small van. The EM640™ used in the demonstration used a Spray-and-Trap Water Sampler, direct injection for soil gas, and heated headspace analysis for soil samples. The minimum detection limit is 1 ppb for soil gas, 1g/L for water, and 50 g/kg for soil. The instrument requires a skilled operator; recommended training is one week for a chemist with GC/MS experience. At the time of testing, the baseline cost of the EM640™ was \$170,000 plus the cost of the inlet system.

“The throughput was approximately 5 samples per hour for all media when the instrument was operated in the rapid analysis mode. Throughput would decrease if the instrument were operated in the analytical mode.

□ “The Viking SpectraTrak™ 672 is a commercially available GC/MS system that provides laboratory-grade performance in a field transportable package. The instrument, including the on-board computer, is ruggedized and encapsulated in a shock-mounted transport case. It weighs about 145 pounds. And can be transported and operated in a small van. The instrument used in the demonstration used a purge and trap device for water and soil analysis and direct injection for soil gas samples. The minimum detection limit is 5 ppb for soil gas, 5 g/kg for soil, and 5 g/L for water. The instrument requires a skilled operator. Recommended training is one week for a chemist with GC/MS experience. At the time of the demonstration, the baseline cost of the SpectraTrak™ 672 was \$145,000.

“Sample throughput was approximately 30 minutes for soil extracts and water samples using purge and trap. The direct injection soil gas samples required 15 minutes each for analysis.

- **DSITMS advantages and disadvantages as compared to baseline --**



- Analytical results from DSITMS field screening are available in the field, in near real time, as opposed to typical turnaround times of weeks for results from an analytical laboratory. Thus, DSITMS supports expedited site characterization, using a dynamic work plan and in-field decision making. This provides faster, better, cheaper characterization and enables better decision-making and better design of remediation activities.
  - Field-screening and laboratory analyses by DSITMS are less expensive per sample than analyses by a commercial laboratory using EPA methods.
  - Field analysis of samples minimizes problems associated with potential loss of VOCs during sample handling, transport, and holding.
  - Field analysis eliminates problems associated with sample holding time requirements.
  - DSITMS can complete more analyses per day than a commercial laboratory using EPA methods.
  - Analysis by DSITMS requires little or no sample preparation as compared to that required for analysis by EPA methods.
  - Analytical laboratory analyses typically address all VOCs, whereas DSITMS, because it does not employ a gas chromatograph for pre-separation, typically addresses no more than five VOCs. For most sites this is not an important difference because the compounds of concern are generally known and are co-contaminants.
  - Application of DSITMS with *in situ* sparging of for field measurement of VOCs in groundwater minimizes investigation-derived waste as compared to the baseline approach.
- **DSITMS advantages and disadvantages as compared to other competing technologies --**  
As noted above, DSITMS competes with a number of person-portable and other field-transportable analytical instruments including GCs and GC/MSs.
    - The performance of the person-portable GCs and the portable and transportable GC/MS instruments is comparable to that of the DSITMS but their sample analysis times are longer, reducing analytical productivity and increasing analysis cost per sample.
    - Many other field instruments are commercially available but most are not comparable because either they do not adequately speciate contaminants or they do not have adequate sensitivity (e.g., FTIR, fluorescence, Raman, surface acoustic wave detectors, solid state sensors on a chip, photoionization detectors, electron capture detectors, flame ionization detectors, and immunoassay test kits).

## Technology Applicability

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- **Technology Selection Considerations.** The technical and economic benefits DSITMS can provide more clearly outweigh the additional responsibilities associated with use of an innovative analysis methodology (demonstration and documentation of performance; gaining regulator acceptance) when the number of required analyses is large. The break-even number will depend on the specific regulator and on the proficiency and track record of the DSITMS analyst.
- **Other Potential Applications.** DSITMS is potentially applicable as a continuous emissions monitor (CEM) for continuous monitoring of VOC emissions from incinerators or hazardous waste combustors (Ghorishi et al 1996). Because exceptional sensitivity is needed for that application, an approach that collected contaminants on a sorbent and then used thermal desorption to introduce them rapidly into the DSITMS would likely be required.



## Patents/Commercialization/Sponsor

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- **Patents.** Finnegan MAT, Inc. and Teledyne Electronic Technologies, Inc. hold licenses to an ORNL patent on the direct sampling interface and sampling modules (Patent No. 4,989,678, February 1991).
- **Commercial Involvement.** Commercialization has been pursued under an ARPA - Technology Reinvestment Program project lead by Teledyne Electronic Technologies. However, that effort stalled when Teledyne was acquired by a large steel company that had no interest in the DSITMS technology. According to Mike Guerin, another instrument company has expressed interest in assuming leadership of the commercialization effort, but that company requires additional funding that, so far, has not been secured (Haas 1998).
- **Sponsors.** Development of DSITMS has been supported by the DOE EM Office of Science and Technology and by the U.S. Army Environmental Center.
- **Potential Privatization.** Recent applications of DSITMS under the auspices of the U.S. Army Engineers have included participation and report preparation by commercial environmental restoration/consulting companies. Such companies are considered crucial to the privatization of new technology use.



## SECTION 5

### COST

#### Introduction

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The information in this section was prepared from data contained in documentation provided by M. R. Guerin, Oak Ridge National Laboratory (Guerin et al. 1998). The cost analysis based on that data was performed by J. R. Gunderson of the Energy and Environment Research Center, University of North Dakota. Details concerning the analysis methods and various assumptions made in conducting that analysis are described in the complete cost savings analysis report, *Cost Savings Analysis: Direct Sampling Ion Trap Mass Spectrometer* (Gunderson 1998).

The EERC cost analyses are not intended to be comprehensive cost estimates. They were performed only to compare the costs of the DSITMS technology to those of the baseline technology.

#### Methodology

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The cost savings analysis reported here compares the cost of the Direct Sampling Ion Trap Mass Spectrometer (DSITMS) technology to the cost of the baseline technology for determination of volatile organic compounds (VOCs) in groundwater. Three different scenarios are considered:

1. Laboratory screening of water samples for characterization of VOC contamination in groundwater at the Oak Ridge K-25 site;
2. Field-screening of VOC contamination in groundwater at the Lake City Army Ammunition Plant, and
3. Laboratory screening of water samples for periodic groundwater quality monitoring at the Savannah River Site.

The baseline technology for each of these scenarios sends all samples to an off-site commercial laboratory for analysis using EPA Methods.

Scenarios 1 and 2 are examples of actual DSITMS applications, and the cost data were collected from those applications. Scenario 3 is a proposed new DSITMS application. The baseline technology for Scenario 3 is described in *The Savannah River Site's Groundwater Monitoring Program - First Quarter 1998* (WSRC 1998).

In each scenario, the costs of DSITMS analysis were compared to the cost of analysis by the baseline method for a life-cycle period of five years. Assumptions were made concerning the number of applications, number of analyses required, fraction of samples sent for analysis by the baseline method to satisfy QA/QC concerns, etc.) in these cost analysis periods. The effect of the most important of those assumptions (parameters) was then documented by performing sensitivity analyses based on those parameters.

#### Cost Analysis for Scenario 1

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**Description:** Laboratory screening of water samples for site characterization (groundwater contamination) investigations. Water samples are collected and sent to an on-site laboratory for fast screening analysis by DSITMS. Only samples that exhibit contamination equal to or greater than a pre-established action level are sent to an off-site commercial laboratory for analysis by EPA Methods.

#### Basis for Cost Comparison:

Groundwater samples for VOCs from drive points at Oak Ridge K-25 site, May-June 1997, overnight results. 249 samples, 292 person-hours (at \$100/person-hour) plus supplies, total actual cost was approximately \$33,000.

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**Characteristics/Advantages:**

Sampling team mobilizations are limited (all sampling completed in less than one week).

**Baseline:**

The conventional approach sends all samples to an off-site commercial laboratory for analysis by EPA Methods. To minimize costs, the sampling/ analysis plan is conservative and usually involves several mobilizations of the sampling team, and later sampling depends on the analytical results obtained from the preceding mobilization(s). The additional mobilizations increase the cost of sampling.

**Assumptions:**

- **Baseline characterization**

- Requires 4 mobilizations to complete
- Requires fewer overall samples
- 10% of samples also submitted to second analytical laboratory for QA/QC
- Average cost of off-site commercial laboratory analysis = \$254/sample
- Time value of analytical results not considered

**Cost Conclusions for Scenario 1** 

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As indicated in Table 5.1, comparison of actual costs incurred at the Oak Ridge K-25 Site and off-site commercial laboratory analysis costs indicate a cost savings of 37% when only DSITMS is used to measure VOC contamination levels in groundwater samples. This is the case in which none of the samples is found to contain sufficient contamination to require verification analysis by a commercial analytical laboratory. Expected savings are less when a fraction of the samples is found to be sufficiently contaminated to require verification analysis. The DSITMS approach has a cost advantage when up to 39 percent of the samples are found to require analysis by the off-site commercial analytical laboratory. For cases, where more than 39 percent require such analysis, the DSITMS approach retains its advantage in completion time (schedule), but ceases to have a cost advantage over the baseline.



**Table 5.1. Cost Savings Analysis for Scenario 1 at Oak Ridge K-25 Site.**

<u>DSITMS</u>				<u>CLP</u>			
Mobilizations			1	Mobilizations			4
Cost per mobilization			\$8,463	Cost per mobilization			\$2,554
Breakdown:				Breakdown:			
Personnel	2@\$35/hr per day		\$7,840	Personnel	2@\$35/hr per day		\$2,240
Duration	7 days			Duration	2 days		
Supplies:				Supplies:			
vials	\$2.50 per sample		\$623	vials	\$2.50 per sample		\$138
	249 samples				55 samples		
				Shipping	\$96 per 30 sample		\$176
Total Cost of mobilizations			\$8,463	Total Cost of mobilizations			\$10,214
Analytical Costs:	@\$132.53/sample			Analytical Costs:	@\$254/sample		
	249 samples		\$33,000		220 samples		\$55,880
<b>Subtotal</b>			\$41,463	<b>Total Cost</b>			\$66,094
<u>Samples sent to lab</u>		<u>CLP Cost</u>	<u>Total Cost</u>	<u>Cost Savings</u>			
0%	0	\$0	\$41,463	\$24,632			
10%	24.9	\$6,325	\$47,787	\$18,307			
20%	49.8	\$12,649	\$54,112	\$11,982			
30%	74.7	\$18,974	\$60,436	\$5,658			
40%	99.6	\$25,298	\$66,761		Breakeven		38.95%
50%	124.5	\$31,623	\$73,086				
60%	149.4	\$37,948	\$79,410				
70%	174.3	\$44,272	\$85,735				
80%	199.2	\$50,597	\$92,059				
90%	224.1	\$56,921	\$98,384				
100%	249	\$63,246	\$104,709				





## Cost Analysis for Scenario 2

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**Description:** Field screening of groundwater to rapidly characterize the location, nature, and extent of VOC contamination and/or to characterize migration of contaminated groundwater.

1. Water samples are collected and analyzed in the field by DSITMS. Samples can be from existing conventional wells or mini-wells installed using direct-push techniques.
2. The VOC content of the water in existing conventional wells and/or in mini-wells installed using direct-push techniques is determined by *in situ* sparging and field analysis by DSITMS.

### Example:

Lake City Army Ammunition Plant, Independence, Missouri – SCAPS and *in situ* sparging of groundwater

Area 03, Area 12, along Eastern Plant Boundary, Area 17, and inside the plant. Similar work has been performed at Aberdeen Proving Ground, Aberdeen, MD. The latter work included SCAPS, HydroPunch, PowerPunch, and *in situ* sparging of groundwater, August 13-20, 1995, and June 9-19, August 11-14, and August 20-23, 1996.

### Characteristics / Advantages:

- When the DSITMS is deployed with direct push sampling techniques, field measurement results are almost immediately available to help guide subsequent pushes and/or other characterization activities.
- Sample chain-of-custody, transportation, and holding costs are avoided.
- When DSITMS is employed with *in situ* sparging, sample collection and packaging costs are also avoided.
- This rapid screening-level characterization enables appropriate design and implementation of lower cost, EPA-compliant, monitoring arrangements (i. e., fewer, but more appropriately placed, conventional monitoring wells).

### Baseline:

The conventional approach sends all samples to an off-site commercial laboratory for analysis. To minimize costs, the sampling/analysis plan is conservative and usually involves several mobilizations of the sampling team, where later sampling depends on the analytical results obtained from the preceding mobilization(s).

### Discussion:

Work performed at the Lake City Army Ammunition Plant is used as the basis for this analysis. Work performed during 1997 used the DSITMS for site characterization activities. Site characterization involves using SCAPS (Site Characterization and Analysis Penetrometer System) in conjunction with DSITMS to access and analyze groundwater. The real-time characterization rate is limited by the number of pushes that can be performed in a given time period. For this reason, real-time site characterization does not utilize the full potential of the DSITMS analytical throughput capability. The five-year life-cycle analysis assumes that 8 pushes (samples) can be accomplished in a single day. This is slightly higher than reported sampling rates at the Lake City Army Ammunition Plant. Sampling rates are highly dependent upon local soil conditions and the required depth of SCAPS penetrations.



Over a one-year period, a total of 643 pushes were accomplished at the Lake City Army Ammunition Plant. Analysis for VOCs was accomplished in the field with DSITMS. This level of effort, for what has been characterized as a production characterization activity, is assumed to represent a common level of utilization of the DSITMS for site characterization activities. It is further assumed that characterization activities at similar sites would utilize the DSITMS at similar levels over the 5-year life cycle considered here. In the Lake City case, the purpose of the characterization was to establish a technically sound basis, in partnership with regulatory agency personnel, for the installation of wells for effective and efficient groundwater monitoring. Analysis by EPA methods was not required for that characterization. Nevertheless, for quality control purposes, replicates from 10% of all samples were sent to an off-site commercial laboratory for analysis using EPA Methods. The estimated sampling schedule for the 5-year, life-cycle analysis is provided in Table 5.2.1.

**Table 5.2.1. Estimated Sampling Schedule**

	Year				
	1	2	3	4	5
Lake City Characterization	643				
Other Sites		643	643	643	643
Replicates (10% of Total)	64	64	64	64	64
<b>Total Samples</b>	<b>707</b>	<b>707</b>	<b>707</b>	<b>707</b>	<b>707</b>

**Assumptions**

1. The 5-year, life-cycle analysis assumes a constant level of activity for all years, i.e., 643 samples per year.
2. For QA/QC purposes, replicate samples are collected for 10% of the total number of analyses and are analyzed at an off-site commercial laboratory using standard EPA Methods.
3. Commercial laboratory costs were assumed to be \$254/sample, based on previously reported cost averages.
4. The discount rate used in the analysis was assumed to be 3.30%.
5. Two technicians are required to perform the field measurements.
6. Penetrations using SCAPS can be accomplished at the rate of 8 per day, resulting in a sampling rate of 8 per day.
7. Travel costs are assumed at \$600/person for round trip air travel to the field site, \$50/night per person for overnight accommodations, and \$40/day per person for meals.

**5-Year Life-Cycle Cost Analysis:**

On-site analysis for VOCs using the DSITMS requires capital expenditures in year 1 and operating/maintenance expenditures in years 1 through 5 of the cost analysis. Estimated capital and operating costs for the DSITMS are provided in Tables 5.2.2 and 5.2.3. These costs are compared with those expected using the baseline technology, GC/MS analysis at a commercial laboratory using EPA Method 8260, provided in Table 5.2.4. Although sampling costs are similar for each, there are some minor differences. A breakdown of these costs is shown in Table 5.2.3.



One common method for assessing the least cost alternative for analysis of VOCs is to determine the present value cost over the 5-year analysis period for each option. Because there is always a time value to money, a discount rate is used to determine the present value of a future expenditure. In addition, inflationary pressures depress the future value of an investment growing at a fixed rate. The discount rate used is subjective and should be adjusted for inflation. In this analysis, it is assumed that dollars spent today could achieve a minimum 5% return annually. When adjusted for inflation, current estimates are approximately 1.7% per year; the discount rate is approximately 3.3%.

When compared with the baseline costs, the DSITMS provides an excellent return on investment (165%, Table 5.2.5), with payback of initial capital costs in 7 months. Comparison of the total cost associated with each option indicates that, over the 5-year period, savings of approximately \$684,000 (present value of \$636,000) may be realized. Since cost savings are directly related to the number of samples required to characterize a given site, a sensitivity analysis is also provided in Table 5.2.5. The annual cost savings are reported for sampling rates between 100 samples per year (IRR = -5%, payback = 71 months) and 1500 samples per year (IRR = 402%, payback = 3 months). Payback period and internal rate of return as a function of annual sampling rate is provided in Figure 5.2.1. The DSITMS will pay for itself over a 5-year period at an annual sampling rate of 112.

Additional cost savings were realized as a result of the characterization completed at the Lake City Army Ammunition Plant. Because of the information collected, the regulatory agency accepted a groundwater monitoring plan based on three judiciously placed groundwater monitoring wells in place of the initially proposed plan, which would have required 10 monitoring wells. The reduction in monitoring wells also decreases the number of samples required to complete quarterly monitoring activities for each of the new wells. An estimate of the additional cost saving resulting from the DSITMS simplification of groundwater monitoring activities at the Lake City Army Ammunition Plant is summarized in Table 5.2.6. That estimate indicates a cost saving of approximately \$27,500 in the first year and \$10,000 per year in the succeeding years.

### **Table 5.2.2. 5-Year Life-Cycle Cost Analysis, Lake City Army Ammunition Plant**



	<b>Year</b>				
	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>
<b>Capital Costs:</b>					
Ion Trap Mass Spectrometer	\$60,000				
Modifications to inlet for sampling	\$26,500				
Rugged Support Base (shock absorbing)	\$1,000				
Portable computer system	\$4,000				
Printer	\$400				
Generator/portable power supply	\$500				
4 lead-acid batteries and dc>ac inverter system	\$1,200				
<b>Total Capital Cost</b>	<b>\$93,600</b>				
<b>Operating Costs:</b>					
Number of Field Samples	643	643	643	643	643
Mobilization Costs	\$115,840	\$115,840	\$115,840	\$115,840	\$115,840
(See Table 2-3 for Breakdown)					
Number of Replicate Samples	64	64	64	64	64
Cost of Commercial Analysis	\$16,640	\$16,640	\$16,640	\$16,640	\$16,640
Consumable parts: pumps, electron impact filament, electron multiplier detector, etc.	\$5,000	\$5,000	\$5,000	\$5,000	\$5,000
Maintenance contract for ion trap mass spec.	<u>\$5,000</u>	<u>\$5,000</u>	<u>\$5,000</u>	<u>\$5,000</u>	<u>\$5,000</u>
<b>Total Annual Operating Cost</b>	<b><u>\$142,480</u></b>	<b><u>\$142,480</u></b>	<b><u>\$142,480</u></b>	<b><u>\$142,480</u></b>	<b><u>\$142,480</u></b>
<b>Annual Capital and Operating Cost</b>	<b>\$236,080</b>	<b>\$142,480</b>	<b>\$142,480</b>	<b>\$142,480</b>	<b>\$142,480</b>
<b>Cumulative Life-Cycle Cost</b>	<b>\$236,080</b>	<b>\$378,560</b>	<b>\$521,040</b>	<b>\$663,520</b>	<b>\$806,000</b>
t value for discount calculations	0	1	2	3	4
Discount Rate: 3.30%					
<b>Present Value of Total Annual Costs</b>	<b>\$236,080</b>	<b>\$137,928</b>	<b>\$133,522</b>	<b>\$129,257</b>	<b>\$125,127</b>
<b>Cumulative Life-Cycle Cost Present Value</b>	<b>\$236,080</b>	<b>\$374,008</b>	<b>\$507,530</b>	<b>\$636,787</b>	<b>\$761,915</b>



**Table 5.2.3. Breakdown of Sampling Mobilization Costs**

		<u>DSITMS</u>	<u>Baseline</u>
<b>Breakdown of Costs:</b>			
Personnel	2@\$70/hr	\$22,400	\$22,400
Duration	20 days 161 samples		
Supplies:			
vials	\$2.50 per sample		\$403
Off-gas Treatment	\$5 per day	\$100	
Reagent H2O	\$4 per day	\$80	
He for purge	\$4 per day	\$80	
Shipping	\$96 per 30 samples		\$515
Travel Costs:			
Vehicle	\$80 per day	\$1,600	\$1,600
Air Travel	\$600 per person	\$1,200	\$1,200
Hotel	\$50 per night	\$1,900	\$1,900
Per Diem	\$40 per person	\$1,600	\$1,600
Cost per mobilization		<u>\$28,960</u>	<u>\$29,618</u>
<b>Number of Mobilizations:</b>		4	4
<b>Annual Mobilization Costs:</b>		\$115,840	\$118,472

**Table 5.2.4. 5-Year Life-Cycle Analysis – Baseline (Commercial Analysis)**

	<u>Year</u>				
	1	2	3	4	5
Number of Samples	643	643	643	643	643
Replicates (10%)	64	64	64	64	64
Total Number of Samples for Analysis	707	707	707	707	707
Mobilization Costs	\$118,472	\$118,472	\$118,472	\$118,472	\$118,472
(See Table 2-3 for Breakdown)					
Laboratory Cost \$254 /sample	<u>\$179,578</u>	<u>\$179,578</u>	<u>\$179,578</u>	<u>\$179,578</u>	<u>\$179,578</u>
<b>Total Annual Cost</b>	\$298,050	\$298,050	\$298,050	\$298,050	\$298,050
Cumulative Life-Cycle Cost	\$298,050	\$596,100	\$894,150	\$1,192,200	\$1,490,250
t value for discount calculations	0	1	2	3	4
Discount Rate: 3.30%					
<b>Present Value of Total Annual Costs</b>	\$298,050	\$288,529	\$279,311	\$270,388	\$261,751
<b>Cumulative Life-Cycle Cost Present Value</b>	<u>\$298,050</u>	<u>\$586,579</u>	<u>\$865,890</u>	<u>\$1,136,278</u>	<u>\$1,398,029</u>



**Table 5.2.5. Calculated Return on Investment**

Samples/yr	IRR	Payback	Capital Cost	Annual Cost Savings				
				1	2	3	4	5
100	-5%	71	-\$93,600	\$15,756	\$15,756	\$15,756	\$15,756	\$15,756
200	34%	27	-\$93,600	\$41,508	\$41,508	\$41,508	\$41,508	\$41,508
300	66%	17	-\$93,600	\$67,264	\$67,264	\$67,264	\$67,264	\$67,264
400	96%	12	-\$93,600	\$92,964	\$92,964	\$92,964	\$92,964	\$92,964
500	125%	9	-\$93,600	\$118,720	\$118,720	\$118,720	\$118,720	\$118,720
600	153%	8	-\$93,600	\$144,472	\$144,472	\$144,472	\$144,472	\$144,472
<b>643</b>	<b>165%</b>	<b>7</b>	<b>-\$93,600</b>	<b>\$155,570</b>	<b>\$155,570</b>	<b>\$155,570</b>	<b>\$155,570</b>	<b>\$155,570</b>
700	181%	7	-\$93,600	\$170,228	\$170,228	\$170,228	\$170,228	\$170,228
800	209%	6	-\$93,600	\$195,980	\$195,980	\$195,980	\$195,980	\$195,980
1000	264%	5	-\$93,600	\$247,488	\$247,488	\$247,488	\$247,488	\$247,488
1500	402%	3	-\$93,600	\$376,208	\$376,208	\$376,208	\$376,208	\$376,208

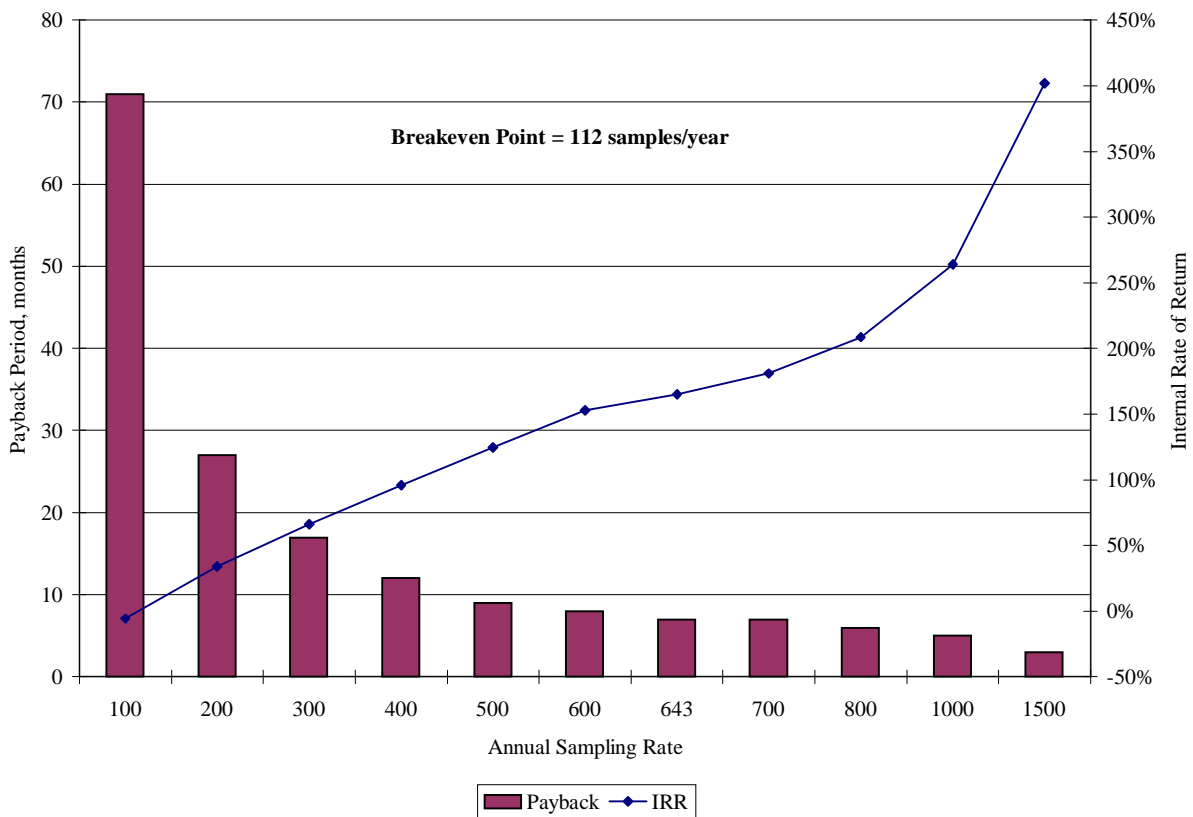


Figure 5.2.1. Sensitivity analysis for Scenario 2: Payback period and internal rate of return as a function of annual sampling rate.



**Table 5.2.6. Additional Cost Savings at Lake City Army Ammunition Plant**

	<u>Proposed</u>	<u>Actual</u>
<b>Number of Wells</b>	10	3
<b>Cost of Wells</b>	\$25,000	\$7,500
<b>Samples for Monitoring:</b>		
<b>1 sample /qtr per well</b>	40	12
<b>Replicates (10%)</b>	4	1
<b>Total Samples</b>	44	13
<b>Sampling Labor @ \$70/hr</b>	\$2,800	\$840
<b>Commercial Lab Cost:</b>		
<b>\$259 per sample</b>	<u>\$11,396</u>	<u>\$3,367</u>
<b>Total Cost</b>	\$39,196	\$11,707
<b>Savings</b>	<b>\$27,489</b>	

## Cost Conclusions for Scenario 2

Field screening performed at the Lake City Army Ammunition Plant, Independence, Missouri, resulted in significant cost savings over the baseline alternative. Over a one-year period, 643 samples were analyzed using DSITMS, resulting in savings of more than \$155,000 when compared with expected costs for off-site commercial analysis. With a capital cost expected at \$93,600, the DSITMS pays for itself in just over 7 months. If the DSITMS were used at similar levels over a 5-year period, the total cost savings would result in a rate of return approaching 165% annually. Since cost savings are highly dependent upon the number of samples analyzed, a sensitivity analysis was also performed for sampling rates as low as 100 per year and as high as 1500 per year. The breakeven point is 112 samples per year.

The characterization activity using DSITMS also generated additional cost savings at the Lake City Army Ammunition Plant. Because of the information collected, the regulatory agency accepted a groundwater monitoring plan based on three judiciously placed groundwater monitoring wells in place of the initially proposed plan, which would have required 10 monitoring wells. This reduction resulted in a cost savings of approximately \$17,500 in the first year (cost avoidance for seven wells not drilled) and of approximately \$50,000 (\$10,000 per year) for groundwater monitoring samples not collected and not analyzed in the five year cost analysis period.



## Cost Analysis for Scenario 3

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**Description:** Laboratory screening of water samples for periodic groundwater quality monitoring at the DOE Savannah River Site. Water samples are periodically collected from wells that must be monitored and are sent to an on-site laboratory for fast screening analysis by DSITMS. Only samples that exhibit contamination (or contamination level change) equal to or greater than a pre-established action level are sent to an off-site commercial laboratory for analysis by EPA Methods.

**Example:**

Groundwater samples from quarterly (or annual) monitoring of 350 wells at SRS as required under RCRA permit.

**Characteristics / Advantages:**

Analysis costs are minimized but complete historical database is maintained.

**Baseline:**

The conventional approach sends all samples to an off-site commercial laboratory for analysis by EPA Method.

**Discussion:**

During the first quarter of 1998, as part of the Savannah River groundwater monitoring program, analyses were performed for determination of VOCs in samples taken from 350 wells at that site. For quality control, the work included both replicate samples and duplicates. Thus, a total of 815 VOC analyses were performed. To perform the life-cycle cost analysis, an estimated sampling schedule was developed (see Table 5.3.1) based on results from first quarter analyses and sample scheduling criteria provided in Appendix B of *The Savannah River Site's Groundwater Monitoring Program, First Quarter 1998*. Included in the scheduling criteria are the following:

1. New Wells – Once each quarter during year 0.
2. Well samples once every 3 years for wells included in the site's environmental screening program.
3. Screening based on flagging levels:
  - a. Flag 0 – Once every 3 years or by request.
  - b. Flag 1 and 2 – Once every year until level drops to Flag 0 for 3 consecutive sampling periods.

The schedule in Table 5.3.1 shows 32 new wells were monitored during the first quarter (year 0), requiring additional sampling in each quarter. Based on the number of wells at the site and the number of analyses performed, it was assumed that a minimum of 2 samples would be collected from each of the new wells for a total of 192 additional samples in year 0 of the cost analysis. Sampling in subsequent years is based on estimates of the site's environmental screening program and flagging levels determined during the first quarter in year 0. During years 1 and 2 of the cost analysis, all wells with Flag 1 and 2 levels will be re-sampled as required. For the cost analysis it is assumed that 20% of all Flag 0 samples will be included in the site's environmental screening program or as an additional sampling request. Of the new wells sampled in year 0, it is further assumed (based on rough percentages of year 0 first quarter data) that 33% of all new well samples will fall under either Flag 1 or Flag 2 criteria, requiring annual analysis. In year 3 of the





analysis, all wells must be sampled similarly to year 0, with the exception of Flag 0 samples analyzed in years 1 and 2 that require only triennial sampling. Year 4 estimates mirror the requirements in years 1 and 2. The sampling schedule assumes that no new wells will be established in years 1 through 4 of the cost analysis.

**Table 5.3.1. Estimated Sampling Schedule**

	Year				
	0	1	2	3	4
Flag 0 samples	482	96	96	290	96
Flag 1 samples	24	24	24	24	24
Flag 2 samples	232	232	232	232	232
New Well samples	192	21	21	192	21
Total Primary Samples	930	373	373	738	373
Replicates and others (10% of total)	93	37	37	74	37
<b>Total Samples</b>	<b>1023</b>	<b>410</b>	<b>410</b>	<b>812</b>	<b>410</b>

Sampling data taken from "The SRS's Groundwater Monitoring Program, 1st quarter, 1998."

Assumes that 20% of Flag 0 samples will be part of site's environmental screening program.

Assumes that 33% of all new well samples will fall under Flag 1 or Flag 2 criteria.

**5-Year Life-Cycle Cost Analysis:**

On-site analysis for VOCs using the Direct Sampling Ion Trap Mass Spectrometer requires capital expenditures in year 0 and operating/maintenance expenditures in years 0 through 4 of the cost analysis. Estimated capital and operating costs for the DSITMS are provided in Table 5.3.2. These costs are then compared with those expected for use of the baseline technology, GC/MS analysis at a commercial laboratory using EPA Method 8260, et al. The costs of the baseline approach are provided in Table 5.3.3. In the current analysis, sampling costs are assumed to be identical for the DSITMS and baseline approaches and are not included in either breakdown.

Life-cycle cost analysis results indicate that over the 5-year period, the DSITMS could be used for on-site determination of VOCs at a total present value cost of approximately \$198,000. Included in this cost is an estimate of personnel time to perform the analyses at an assumed rate of 6 analyses per hour. The total cost is considerably less than the cost of the baseline alternative, which has a present value of approximately \$753,000, yielding cost savings of approximately \$555,000.

However, it is reasonable to assume that some percentage of samples will require verification by commercial laboratory analysis. 5.3.4 provides the cumulative present value cost of the total annual costs for analysis using the DSITMS as a function of the percent of total analyses



submitted for verification. A graphical comparison between the cost of DSITMS analysis and the cost of analyses by an off-site commercial laboratory is provided in Figure 5.3.1. These considerations indicate that over the 5-year period, the DSITMS provides a cheaper alternative even when more than 70% of all samples analyzed require verification using the current standard laboratory technique. The results also indicate that the DSITMS would have a payback period of less than one year even with 60% of all samples requiring verification.

**Table 5.3.2. 5-Year Life-Cycle Cost Analysis, Savannah River Site DSITMS Analysis**

	Year				
	0	1	2	3	4
<b>Capital Costs:</b>					
Ion Trap Mass Spectrometer	\$60,000				
Modifications to inlet for sampling	\$26,500				
Rugged Support Base (shock absorbing)	\$1,000				
Portable computer system	\$4,000				
Printer	\$400				
Generator/portable power supply	\$500				
4 lead-acid batteries and dc>ac inverter system	\$1,200				
<b>Total Capital Cost</b>	<b>\$93,600</b>				
<b>Operating Costs:</b>					
Number of Samples for Analysis	1023	410	410	812	410
One technician @ \$70 /hr	\$11,935	\$4,783	\$4,783	\$9,473	\$4,783
Consumable parts: pumps, electron impact filament, electron multiplier detector, etc.	\$5,000	\$5,000	\$5,000	\$5,000	\$5,000
Consumable Supplies: He purge gas, 99.9995% pure Calibration standards Reagent grade water VOC off-gas treatment	\$5,000	\$5,000	\$5,000	\$5,000	\$5,000
Maintenance contract for ion trap mass spec.	<u>\$5,000</u>	<u>\$5,000</u>	<u>\$5,000</u>	<u>\$5,000</u>	<u>\$5,000</u>
<b>Total Annual Operating Cost</b>	<b><u>\$26,935</u></b>	<b><u>\$19,783</u></b>	<b><u>\$19,783</u></b>	<b><u>\$24,473</u></b>	<b><u>\$19,783</u></b>
<b>Annual Capital and Operating Cost</b>	<b>\$120,535</b>	<b>\$19,783</b>	<b>\$19,783</b>	<b>\$24,473</b>	<b>\$19,783</b>
<b>Cumulative Life-Cycle Cost</b>	<b>\$120,535</b>	<b>\$140,318</b>	<b>\$160,102</b>	<b>\$184,575</b>	<b>\$204,358</b>
t value for discount calculations	0	1	2	3	4
Discount Rate: 3.30%					
<b>Present Value of Total Annual Costs</b>	<b>\$120,535</b>	<b>\$19,151</b>	<b>\$18,540</b>	<b>\$22,202</b>	<b>\$17,374</b>
<b>Cumulative Life-Cycle Cost Present Value</b>	<b>\$120,535</b>	<b>\$139,686</b>	<b>\$158,226</b>	<b>\$180,428</b>	<b>\$197,802</b>



**Table 5.3.3. 5-Year Life-Cycle Cost Analysis, Savannah River Site Commercial Laboratory Analysis**

	<b>Year</b>				
	0	1	2	3	4
Number of Samples for Analysis	1023	410	410	812	410
EPA approved vials     \$165 /72	\$2,344	\$940	\$940	\$1,861	\$940
Shipping                     \$96 /cooler of 30	\$3,274	\$1,312	\$1,312	\$2,598	\$1,312
Laboratory Cost             \$254 /sample	<u>\$259,842</u>	<u>\$104,140</u>	<u>\$104,140</u>	<u>\$206,248</u>	<u>\$104,140</u>
<b>Total Annual Cost</b>	\$265,460	\$106,392	\$106,392	\$210,707	\$106,392
Cumulative Life-Cycle Cost	\$265,460	\$371,852	\$478,243	\$688,950	\$795,342
t value for discount calculations	0	1	2	3	4
Discount Rate:             3.30%					
<b>Present Value of Total Annual Costs</b>	\$265,460	\$102,993	\$99,703	\$191,152	\$93,434
<b>Cumulative Life-Cycle Cost Present Value</b>	<u>\$265,460</u>	<u>\$368,453</u>	<u>\$468,155</u>	<u>\$659,307</u>	<u>\$752,741</u>

**Table 5.3.4. Cumulative Present Value Cost of DSITMS Analysis of Monitoring Samples with Commercial Laboratory Verification of a Percentage of Those Samples.**

Percent Verified	<b>Year</b>				
	0	1	2	3	4
10%	\$147,081	\$176,532	\$205,041	\$246,359	\$273,076
20%	\$173,627	\$213,377	\$251,857	\$312,289	\$348,350
30%	\$200,173	\$250,222	\$298,673	\$378,220	\$423,624
40%	\$226,719	\$287,067	\$345,488	\$444,151	\$498,898
50%	\$253,265	\$323,913	\$392,304	\$510,082	\$574,173
60%	\$279,811	\$360,758	\$439,119	\$576,012	\$649,447
70%	\$306,357	\$397,603	\$485,935	\$641,943	\$724,721
80%	\$332,903	\$434,449	\$532,750	\$707,874	\$799,995
90%	\$359,449	\$471,294	\$579,566	\$773,804	\$875,269
100%	\$385,995	\$508,139	\$626,381	\$839,735	\$950,543
<b>Baseline Cost</b>	<u>\$265,460</u>	<u>\$368,453</u>	<u>\$468,155</u>	<u>\$659,307</u>	<u>\$752,741</u>



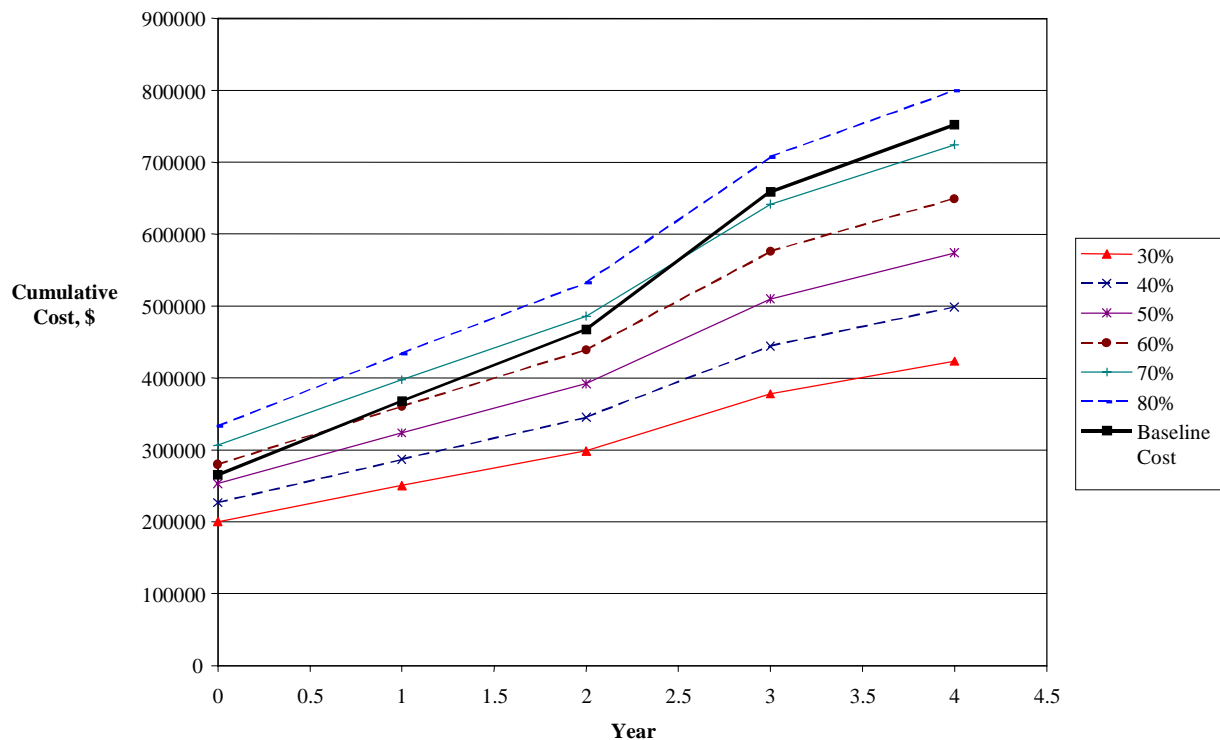


Figure 5.3.1. Cumulative present value life-cycle cost as a function of the percentage of samples sent for commercial analysis, showing 5-year DSITMS cost is less than 5-year baseline cost for percentages somewhat greater than 70 percent.

### Cost Conclusions for Scenario 3

Cost savings analysis of groundwater monitoring activities at the Savannah River Site suggest DSITMS would be an extremely cost-effective method for screening samples for VOCs. Based on the expected sampling schedule and using an off-site commercial laboratory for verification of 10% of all samples, the total savings over a 5-year period is expected to be more than \$600,000, with payback of initial capital expenditures (\$93,600) in just over 5 months. As indicated in Figure 5.3.1, sensitivity analysis indicates that more than 70% of all samples analyzed by DSITMS could be sent to an off-site laboratory for verification at the same cost as the baseline technology.

### Other Conclusions

- In addition to the cost savings that can be documented relative to traditional laboratory analysis, DSITMS can provide further economic benefits by reducing sample handling costs, permitting high-resolution characterization of a site and providing immediate results to sampling and remediation crews. For example, DSITMS instruments that are equipped with in situ probes for measuring VOCs in groundwater can virtually eliminate the cost of sample collection and handling. Instruments that are equipped with real-time monitoring probes for VOCs in air or aqueous process streams can enable remediation processes to be quickly optimized. Finally, the coupling of DSITMS probes with cone penetrometer or other drive-point sampling techniques can provide a means of accurately profiling the vertical and horizontal distribution of contamination at a site without the cost and time associated with drilling wells, discrete sample collection, and laboratory analysis (Wise et al. 1997).
- The results of the cost analysis and performance evaluation conducted here, based on actual deployment data for two of the three scenarios, compare favorably with the findings of the cost and performance evaluations performed earlier by Los Alamos National Laboratory (Henricksen and



Booth 1992, Henricksen and Grant 1993). The results of those earlier studies are summarized in Appendix B of this report.

- DSITMS is expected to see additional application, in place of the baseline, as site managers and regulators respond to:
  - Public demand for more efficient and effective remediation action,
  - Renewed EPA emphasis on performance-based analysis, and
  - Increased budget pressure.



## SECTION 6

# REGULATORY AND POLICY ISSUES

### Regulatory Considerations

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The regulatory requirements pertinent to the use and regulatory acceptability of an innovative sampling and testing methodology are often overstated, even by apparently knowledgeable analysts and environmental managers. In fact, in a recent memorandum (EPA 1998), the EPA Office of Solid Waste set forth additional guidance regarding certain methods in Update III to *Test Methods for Evaluating Solid Waste, Physical/Chemical Methods* (SW-846) and the use of SW-846 methods in general, in order to assure appropriate use by the laboratories and the regulated community. The memorandum set forth the additional guidance as a clarification to SW-846 for reference and distribution to the States and to other interested parties, including laboratories and the regulated community. The key paragraph of the memorandum states:

“SW-846 contains the analytical and test methods that EPA has evaluated and found to be among those acceptable for testing under subtitle C of the Resource Conservation and Recovery Act (RCRA). In most situations, SW-846 functions as a guidance document setting forth acceptable, although not required, methods to be implemented by the user, as appropriate, in responding to RCRA-related sampling and analysis requirements. The methods are intended to be used and modified, as needed, to promote unbiased, sensitive, precise, comparable, and specific analyses and test results. In addition, with the exception of method-defined parameters (e.g., Method 1311, the Toxicity Characteristic Leaching Procedure), SW-846 methods need not be applied in a prescriptive manner. The Agency strongly recommends that the regulated entity develop a project-specific sampling and analysis plan in conjunction with other professionals (e.g., laboratories) and the regulating authority, to address both sample collection and method application and to assure the generation of data of the appropriate quality. The Disclaimer and Chapter Two of SW-846 provide additional guidance regarding the appropriate use of SW-846 methods, and Chapter One provides guidance regarding the development of a project-specific sampling and analysis plan.

According to the SW-846 Disclaimer, the Agency

“compiled this methods manual in order to provide comprehensive guidance to analysts, data users, and other interested parties regarding test methods that may be employed for the evaluation of solid waste and other testing specified in regulations issued under the Resource Conservation and Recovery Act (RCRA).”

The same disclaimer then goes on immediately to say,

“Except where explicitly specified in a regulation, the use of SW-846 methods is not mandatory in response to Federal testing requirements.”

Along the same lines, the disclaimer concludes as follows:

“EPA emphasizes that the ultimate responsibility for producing reliable analytical results lies with the entity subject to the Federal, State, or local regulation. Thus, members of the regulated community are advised to refer to the information in Chapter Two and to consult with knowledgeable laboratory personnel when choosing the most appropriate suite of analytical methods. The regulated community is further advised that the



methods here or from other sources need only be used for those specific analytes of concern that are subject to regulation or other monitoring requirements.

“Many of the methods include performance data that are intended as guidance on the performance that may be achieved in typical matrices and may be used by the analyst to select the appropriate method for the intended application. These performance data are not intended to be used as absolute QC acceptance criteria. Rather, each laboratory should develop performance criteria as described in Chapter Two and elsewhere in the manual.

“In summary, the methods included here provide guidance to the analyst and the regulated community in making judgements necessary to generate data that meet the data quality objectives for the intended use of the results.

In Chapter Two of SW-846, the Agency goes on to say:

“... if an alternative analytical procedure is employed, the EPA expects the laboratory to demonstrate and document that the procedure is capable of providing appropriate performance for its intended application. This demonstration must not be performed after the fact, but as part of the laboratory’s initial demonstration of proficiency with the method. The documentation should be in writing, maintained by the laboratory, and available for inspection upon request by authorized representatives of the appropriate regulatory authorities. The documentation should include the performance data as well as a detailed description of the procedural steps as performed (i.e., a written standard operating procedure).

Thus, it seems clear that depending on (1) the intended purpose of the analysis and the corresponding data quality objectives and (2) demonstration and documentation that the procedures used are capable of providing the required performance, DSITMS technology, although not specifically “accepted” by regulatory agencies or included in any SW-846 method, can indeed be acceptable. As noted immediately above, the site regulator will ordinarily expect demonstration and documentation that the DSITMS procedure provides appropriate performance for the intended application. In many previous applications, satisfactory agreement of analytical results from DSITMS application and from commercial analytical laboratory application of an SW-846 method for some fraction (typically ten percent) of the samples has been sufficient to satisfy the demonstration and documentation requirement. As more and more experience is gained, the fraction of samples required for this demonstration of performance is expected to decrease.

## **Evaluation of DSITMS With Respect to CERCLA Criteria**

1. Overall protection of human health and the environment. The improved and more economical characterization enabled by use of DSITMS is expected to facilitate risk reduction through source removal, treatment, and controls.
2. Compliance with ARARs. Not applicable.
3. Long-term effectiveness and permanence. The improved and more economical characterization and monitoring enabled by use of DSITMS is expected to provide better knowledge of the magnitude of residual risk and the adequacy and reliability of controls over time.
4. Reduction of toxicity, mobility, or volume through treatment. See item 3, above.



5. Short-term effectiveness. The improved and more economical characterization enabled by use of DSITMS is expected to reduce the time (and impacts on human health and the environment) until response objectives are met and until protection is achieved.
6. Implementability. The numerous demonstrations and applications of DSITMS show there is no particular technical difficulty or uncertainty associated with the use of DSITMS. In some cases, there may be difficulty and administrative uncertainty associated with establishing the regulatory acceptability of the results.
7. Cost. Cost considerations for DSITMS application are addressed in Section 5 of this report.
8. State (support agency) acceptance. Technical and administrative issues and concerns the State (support agency) may have are addressed in the preceding subsection of this report.
9. Community acceptance. Positive community reaction is expected because DSITMS provides faster, better, and more economical characterization, this enabling faster and better response actions.

## Safety, Risks, Benefits, and Community Reaction ---

### Worker and Community Safety Issues

- DSITMS is well suited to application with the cone penetrometer and *in situ* sparging for determination of VOCs in groundwater. Compared to the baseline, such applications provide improved worker safety because no wells are drilled or purged, no samples are collected, and little or no secondary waste is generated.

### Socioeconomic Impacts and Community Reaction

- Community reaction is expected to be positive because application of DSITMS, particularly with use of a cone penetrometer for subsurface access, generally provides faster, better, and cheaper characterization than the conventional well-drilling, sample collection, and off-site analytical laboratory methods.





## SECTION 7

### LESSONS LEARNED

#### Implementation Considerations

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- The technology implementer must work with the site customer to understand the characterization goals, schedule requirements, implementation and operational limitations or restrictions, and data quality objectives.
- The site manager and DSITMS operator must work with the regulator to ensure the acceptability of the data to be generated.
- The feasibility and economic attractiveness of using DSITMS as a replacement for quantitative GC or GC/MS will be heavily influenced by the number and types of contaminants known to be present at a site and by the probability of finding additional, unexpected or unusual, contaminants. The primary criterion is that DSITMS must be able to detect, distinguish, and quantify all of the contaminants with the same performance as an EPA method.
- Certain broad types of sites are generally good candidates for DSITMS because common types of work occurred there and more or less the same types of organic compounds (generally solvents) were generally used for that work. Examples include:
  - DOE and DoD sites: halogenated hydrocarbon solvents for cleaning and degreasing
  - DoD sites: petroleum fuel products, also petroleum, oil and lubricants
  - Other industrial sites, such as automobile service stations, dry-cleaners, furniture strippers, precision machine shops, etc., where only a limited number of compounds were used, produced, or disposed of.
- The speed and field applicability of DSITMS makes it useful for real-time monitoring and optimization of characterization and remediation activities.

#### Technology Limitations and Needs for Future Development

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- DSITMS methods have not been specifically “accepted” by regulatory agencies.
- User friendly software that automates most aspects of the DSITMS data acquisition and results reporting is lacking.

#### Technology Selection Considerations

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- Specific job requirements and site conditions will dictate the selection of the best technology for characterization of a particular site.
- The DSITMS should be considered as one tool within a toolbox of groundwater monitoring technologies. The DSITMS can provide rapid, minimum cost information concerning the location, extent, and migration of VOC and SVOC contamination at a site.
- The cost savings realized from application of DSITMS will be greatest for large sites and for sites that have complicated geology or several sources of contamination.



## APPENDIX A

### REFERENCES

- Davis, W. M., E. R. Cespedes, L. T. Lee, J. F. Powell, and R. A. Goodson. 1997. Rapid Delineation of Subsurface Petroleum Contamination Using the Site Characterization and Analysis Penetrometer System. *Environmental Geology* 29: 228-237.
- Davis, W. M., M. B. Wise, J. S. Furey, and C. V. Thompson. 1998. Rapid Detection of Volatile Organic Compounds in Groundwater by *In Situ* Purge and Direct-Sampling Ion-Trap Mass Spectrometry. *Field Analytical Chemistry and Technology* 2(2):89-96.
- Davis, W. M., J. S. Furey, and B. Porter. 1998. Field Screening of VOCs in Ground Water Using the Hydrosparge VOC Sensor. In *Current Protocols in Field Analytical Chemistry*, 1C4.1-1C4.10. New York: John Wiley & Sons.
- EPA (U. S. Environmental Protection Agency). 1995. *Test Methods for Evaluating Solid Waste: Physical/Chemical Methods, SW-846 Update III*. U. S. EPA, Washington, DC.
- EPA (U. S. Environmental Protection Agency). 1995b. Method 8260, In *Test Methods for Evaluating Solid Waste: Physical/Chemical Methods, SW-846 Update III*. U. S. EPA, Washington, DC.
- EPA (U. S. Environmental Protection Agency). 1997. *Environmental Technology Verification Report: Field Portable Gas Chromatograph/Mass Spectrometer. Bruker-Franzen Analytical Systems, Inc. EM640™*. EPA/600/R-97/149. Washington, DC.
- EPA (U. S. Environmental Protection Agency). 1997b. *Environmental Technology Verification Report: Field Portable Gas Chromatograph/Mass Spectrometer. Viking Instruments Corporation SpectraTrak™ 672*. EPA/600/R-97/148. Washington, DC.
- EPA (U. S. Environmental Protection Agency). 1998. Clarification Regarding Use of SW-846 Methods. August 7 memorandum from Elizabeth Cotsworth to RCRA Senior Policy Analysts, Regions I – X. Washington, DC.
- Guerin, M. R., M. B. Wise, C. V. Thompson, K. J. Hart, A. B. Dindal, R. Merriweather, and R. R. Smith. 1998. *Draft Update, Field Demonstration and Deployments, Direct Sampling Ion Trap Mass Spectrometry*. (unpublished). Chemical and Analytical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN. April 16, 1998.
- Ghorishi, S. B., W. E. Whitworth, Jr., C. G. Goldman, and L. R. Waterland. 1996. [Testing the Performance of Real-Time Incinerator Emission Monitors,] National Risk Management Research Laboratory, Office of Research and Development, U. S. Environmental Protection Agency, Cincinnati, Ohio, June 1996.
- Gunderson, J. R. 1998. *Cost Savings Analysis: Direct Sampling Ion Trap Mass Spectrometer* (Draft document in review). Grand Forks, ND. November 1998.



- Haas, W. J. 1998. Notes from telephone conversation with Mike Guerin, Oak Ridge National Laboratory, Oak Ridge TN, June 1, 1998.
- Haas, W. J. 1998b. Notes from telephone conversation with Bill Davis, USAE Waterways Experiment Station, Vicksburg, MS, September 22, 1998
- Henricksen, A. D., and S. R. Booth. 1992. *Cost effectiveness of an innovative technology for VOC detection: The direct sampling ion trap mass spectrometer*. Los Alamos National Laboratory LA-UR 92-3527.
- Henricksen, A. D. and D. E. Grant. 1993. *The Cost Effectiveness of Field Screening for VOCs*. Los Alamos National Laboratory LA-UR-93-2405.
- March, R. E. 1992. Ion Trap Mass Spectrometry. *International Journal of Mass Spectrometry and Ion Processes*. 118/119 (1992) 71-135.
- Sigmon, B. 1998. *DNAPLs Remediation Market Assessment (pre-publication draft, September 1, 1998)*. The Global Environmental Technology Enterprise, Oak Ridge, TN.
- Silva, E. M., and S. R. Booth. 1995. *Cost Effectiveness Studies of Environmental Technologies Volume I*. Los Alamos National Laboratory LA-UR-95-692.
- Todd, J. F. J. 1995. Ion Trap Theory, Design, and Operation, in *Practical Aspects of Ion Trap Mass Spectrometry Volume III*, pp. 3-26, R. E. March and J. F. J. Todd, eds., CRC Press, New York.
- WSRC (Westinghouse Savannah River Company). 1998. *The Savannah River Site's Groundwater Monitoring Program - First Quarter 1998*. ESH-EMS-9980568.
- Wise, M. B. and M. B. Guerin. 1997. Direct Sampling MS for Environmental Screening. *Analytical Chemistry* 69: 26A-32A.
- Wise, M. B., C. V. Thompson, M. V. Buchanan, R. Merriweather, and M. R. Guerin. 1993. Direct Sampling Ion Trap Mass Spectrometry. *Spectroscopy*, June 1993, 8(5)14-22.
- Wise, M. B., C. V. Thompson, R. Merriweather, and M. R. Guerin. 1997. Review of Direct MS Analysis of Environmental Samples. *Field Analytical Chemistry and Technology*, 1(5):251-276.
- Yates, N. A., M. M. Booth, J. L. Stephenson Jr., and R. A. Yost. 1995. Practical Ion Trap Technology: GC/MS and GC/MS/MS, in *Practical Aspects of Ion Trap Mass Spectrometry Volume III*, pp. 121-185, R. E. March and J. F. J. Todd, eds., CRC Press, New York.



## APPENDIX B

### PREVIOUS COST AND PERFORMANCE COMPARISON

In 1992, Los Alamos National Laboratory (LANL) described the cost and performance characteristics of the DSITMS compared to that of conventional (baseline) sample analysis methodology for site characterization and for remediation process monitoring (Henricksen and Booth 1992). Also in 1992, LANL compared the cost of analysis for VOCs in soil, water and gas samples by a commercial laboratory and by six different field instruments (Henricksen and Grant 1993). That study concluded field sampling and analysis of VOCs offers substantial savings above a certain threshold number of samples per year (approximately 100 samples per year). The LANL cost analysis group documented a factor of five reduction in cost per sample using field-screening methods over the conventional methodology (commercial laboratory analysis).

The LANL group compared six field-screening instruments, one of which was DSITMS. Table B-1 summarizes the LANL capital and operating cost estimates for the six instruments.

Table B-1. LANL estimates of capital and operating costs for six methods of VOC analysis in the field.

INSTRUMENT	CAPITAL COST 1992 dollars	OPERATING COST 1992 dollars	OPERATING COST 1997 dollars <sup>1</sup>
ORNL Direct Sampling Ion Trap Mass Spectrometer	\$111,525	\$148,674	\$172,460
LANL GC/MS with ion trap mass spectrometer	\$142,725	\$149,571	\$173,500
Hewlett Packard 5890 GC with Model 5971A mass selective detector	\$78,947	\$151,170	\$175,357
Viking SpectraTrak 620	\$165,575	\$158,541	\$183,910
Photovac GC with photoionization detector	\$42,010	\$146,823	\$170,315
Sentex GC with AID/Electron Capture Detector	\$42,645	\$147,862	\$171,520

<sup>1</sup> Assumes 3.1% per year escalation rate 1992-1997. The LANL reports were written in 1992 and the costs reported there were given in 1992 dollars. Although it is reasonable to escalate operating costs to 1997 dollars, it is not reasonable to escalate hardware prices since they typically do not increase. Typically the equipment manufacturer releases a new version of the instrument with improved capabilities, but not necessarily a higher price.



The operational scenario for the LANL analysis was rather conservative. It included the cost of two technicians and a vehicle to implement use of the instrument. In most DOE applications, personnel and vehicles are available and can be assigned to sampling and analysis tasks. The cost of implementation in those cases is much less than LANL estimate. This scenario was chosen so that the operating costs could be compared with those of the other instruments in the LANL reports. In fact, the annual operating expenses for the selected field-screening instruments were very similar. Consequently, the cost decision for selection of the field-screening devices was driven by capital cost of the instrument and supporting equipment.

A detailed discussion of the performance characteristics of the instruments is contained in the LANL reports. In summary, the DSITMS, the GC/MS, and the Amerasia Model 4100 Surface Acoustic Wave Gas Chromatograph (SAW/GC) can detect most compounds of interest at the low ppb level in real time. The Sentex instrument requires preconcentration to routinely detect at the ppb level and in real time can only detect at the ppm level. The Photvac can detect from ppm to low ppb for some compounds but in real time only at the ppm level.



## APPENDIX C

### DSITMS APPLICATIONS AND/OR DEMONSTRATIONS

DSITMS has been applied on numerous occasions to do real work. It has also been involved in numerous field demonstrations and field tests. A non-exhaustive tabulation of some key information concerning these applications and demonstrations is given below.

Application / Demonstration Site	Purpose	Date(s)
1. DOE Hanford Site, Richland, Washington	Compare real-time analytical performance of five different sensors for measurement of VOCs in soil gas.	April 19-21, 1993
2. Camp Forest Water Treatment facility, Arnold Engineering Development Center, Tullahoma, Tennessee	Soil and groundwater analysis for well siting	Apr. 6-7, Apr. 11-12, 1995
3. Dover Air Force Base, Dover, Delaware	Interagency cooperative demonstration of innovative field analytical technologies	Apr. 30, May 7, May 22-24, Jun. 18-23, 1995
4. DOE Oak Ridge National Laboratory, Waste Area Group 6 Site, Oak Ridge, Tennessee	Determine analytical impact of EPA regulatory requirement for purging water from groundwater wells before taking samples (sponsored by ORNL EM-40)	May 15-17, 1995
5. DOE Oak Ridge K-25 Site,	Perform real-time and collected process gas analysis for in situ soil heating demonstration by ITT Research Institute. Test feasibility of vapor extraction of VOCs from soil by resistive heating of the soil.	Jun. 30, Jul. 7, 1995
6. DOE Savannah River Site, Aiken, South Carolina	EPA-directed Consortium for Site Characterization Technology evaluated performance of three commercially available field mass spectrometers for on-site screening and analysis (Phase 1).	Jul. 17-21, 1995
7. EPA Incineration Research Facility, Jefferson, Arkansas	Test, validate performance of DSITMS for continuous emissions monitoring of VOCs.	Jul. 31 – Aug. 4, 1995
8. Aberdeen Proving Ground, Aberdeen, Maryland	Apply DSITMS with cone penetrometer and hydropunch to assist in rapid characterization of a VOC plume.	Aug. 13-20, 1995
9. DOE Oak Ridge K-25 Site, Oak Ridge, Tennessee	Provide real-time data to maximize efficiency of photocatalytic oxidation of VOCs in groundwater	Aug. 25 through Sep. 5, 1995
10. Wurtsmith Air Force Base, Oscoda, Michigan	EPA-directed Consortium for Site Characterization Technology evaluated	Sep. 9-14, 1995



	performance of three commercially available field mass spectrometers for on-site screening and analysis (Phase 2).	
11. Elgin Air Force Base, Fort Walton Beach, Florida	Assist U. S. Army Engineers, Waterways Experiment Station, in testing an in situ soil-heating sampler and interfaces to the DSITMS.	May 19-23, 1996
12. DOE Oak Ridge Y-12 Site, Oak Ridge, Tennessee	Collect information on the variations in the concentrations of VOCs as a function of depth in a well.	Jul. 12, 1996
13. Aberdeen Proving Ground (Bush River Study Area), Aberdeen, Maryland	Assist U. S. Army Engineers, Waterways Experiment Station, in characterizing VOC plumes and provide training on use of new technologies.	Jun. 9-19, Aug. 11-14, Aug. 20-23, 1996



<b>Application / Demonstration Site</b>	<b>Purpose</b>	<b>Date(s)</b>
14. Cape Canaveral Air Station, Cape Canaveral, Florida	Assist U. S. Army Engineers, Kansas City District, and Parsons Engineering Science in characterizing a plume of chlorinated hydrocarbon solvents in the groundwater.	Sep. 19-21, 1996 Apr. 9-11, 1997
15. Naval Air Station Fort Worth Joint Reserve Base, Fort Worth, Texas	Assist U. S. Army Engineers, Kansas City District, and CH2M Hill in characterizing a plume of chlorinated hydrocarbon solvents in the groundwater.	Oct. 30 through Nov. 6, 1996
16. McClellan Air Force Base and Davis Telecommunications Site, Davis, California	With U. S. Army Engineers, Waterways Experiment Station, demonstrate, test, and evaluate DSITMS instruments from two manufacturers, new thermal desorption sampler, and a triple-sorbent trap.	Nov. 11-22, 1996 Dec. 6-10, 1996 Feb. 12-17, 1997
17. Lake City Army Ammunition Plant, Blue Springs, Missouri	Assist U. S. Army Engineers, Kansas City District, in characterizing plumes of chlorinated hydrocarbons in the groundwater at the Plant boundary and at Plant Areas 05, 07, 14, 17, 29, and 30. The results support remediation design.	Jan. 21-23, Jan. 26 through Feb. 5, Feb. 23 through Mar. 5, Mar. 17-26, 1997
18. Lake City Army Ammunition Plant, Blue Springs, Missouri	Assist U. S. Army Engineers, Kansas City District, in characterizing plumes of chlorinated hydrocarbons in the groundwater at the Plant boundary and at Plant Areas 03,12,and 17.	May 13-23, May 27-31, Jun. 3-6, Jul. 9-16, Aug. 25-29, 1997
19. U. S. Army Engineers Cold Regions Research and Engineering Laboratory, Lebanon, New Hampshire	Assist U. S. Army Engineers, Waterways Experiment Station, in testing and evaluation of their new soil gas thermal desorption probe.	Jun. 1-2, 1997
20. F. E. Warren Air Force Base, Cheyenne, Wyoming	Assist U. S. Army Engineers, Kansas City District, in characterizing a plume of trichloroethylene (TCE) in the groundwater.	Sep. 5-6, 1997
21. Missouri National Guard, Camp Crowder, Missouri	Provide field analysis of VOCs in soil samples to assist U. S. Army Engineers, Kansas City District, in characterizing TCE and kerosene contamination at the site.	Sep. 17-19, 1997
22. Naval Air Station Fort Worth Joint Reserve Base, Fort Worth, Texas	Assist U. S. Army Engineers, Kansas City District, and CH2M Hill in characterizing a plume of chlorinated hydrocarbon solvents in the groundwater.	Oct. 28 through Nov. 3, 1997

Additional applications / tests / demonstrations were also conducted at the following sites: DOE Savannah River Site Integrated Demonstration Site, September 1991.





DOE Portsmouth Gaseous Diffusion Plant site  
Massachusetts Military Reservation  
Rock Mountain Arsenal



## APPENDIX D

### ACRONYMNS AND ABBREVIATIONS

ARARs	Applicable or relevant and appropriate requirements
ARPA	Advanced Research Projects Agency (DoD)
CW	Chemical warfare
DoD	U. S. Department of Defense
DOE	U. S. Department of Energy
DSITMS	Direct sampling ion trap mass spectrometry or direct sampling mass spectrometer
DSMS	Direct sampling mass spectrometry or direct sampling mass spectrometer
EPA	U. S. Environmental Protection Agency
GC	Gas chromatograph or gas chromatography
GC/MS	Gas chromatography / mass spectrometry
ID	internal diameter
LANL	Los Alamos National Laboratory
LUSTs	Leaking underground storage tanks
MDL	Method detection limit
ml	Milliliter
ng	Nanogram
ORNL	Oak Ridge National Laboratory
OST	Office of Science and Technology
OTD	Office of Technology Development
PCBs	polychlorinated biphenyls
ppb	parts per billion
PV	present value
SCAPS	Site characterization and analysis (cone) penetrometer system
SVOCs	Semi-volatile organic compounds
USAE	U. S. Army Engineers
VOCs	Volatile organic compounds