SPACE TECHNOLOGY FOR APPLICATION TO TERRESTRIAL HAZARDOUS MATERIALS ANALYSIS AND ACQUISITION

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ABSTRACT

In-situ and remote measurements of elemental, molecular and mineralogical composition of materials has been part of the space science program since its beginnings. There is a great deal of commonality between space science missions and terrestrial hazardous materials screening in the types of measurements, methods and instrumentation used. There are also strong parallels between the hostile environments of space and those of a hazardous material site.

This paper discusses the measurements, methods and instrumentation used on past, present and future space missions for in-situ and remote analysis of materials. Specific instrumentation discussed includes gas chromatographs, mass spectrometers, imaging spectrometers, X-ray and gamma-ray spectrometers. Work sponsored by the National Aeronautics and Space Administration's Sample Acquisition, Analysis and Preservation technology program is discussed, including concepts and hardware for multi-spectral remote sensing, instrument data analysis and interpretation, material acquisition and processing. Some new concepts for micro sensors for making various chemical measurements are also discussed. Possible applications of space technology to terrestrial hazardous materials field acquisition and analysis are presented.

INTRODUCTION

In-situ and remote measurements of elemental, molecular and mineralogical composition of materials has been part of the space science program since its beginnings. Two of the best known surface science missions were the Viking mission to the surface of Mars and the Soviet Venera series to Venus. The Galileo spacecraft is carrying a probe to sample Jupiter's atmosphere and the National Aeronautics and Space Administration (NASA) has just started a project to make a variety of in-situ measurements of the comet Kopff. NASA is currently working on technology to enable robotic and human missions to the Moon and Mars. Such missions will include a wide variety of in-situ and remote science and engineering measurements. There is a great deal of commonality between space science missions and terrestrial hazardous materials screening in the types of measurements, methods and instrumentation used as well as in the hostile nature of the environment in which these measurements are made. NASA is very active in the design, development and utilization of the instruments. Table 1 contains a listing of some science data requirements and associated instrument(s) that are used and/or under development within NASA for its past, present and future missions.

NASA has established a technology program called Sample Acquisition, Analysis and Preservation (SAAP) to address the specific needs of in-situ science and engineering measurements. SAAP is intended to develop critical and significantly enhancing technologies for remote identification, acquisition, processing, analysis and preservation of materials for in-situ science, engineering characterization and earth return. Although the technology being developed in the SAAP program is not currently being applied to specific missions, the SAAP program will broaden the base of technology available for future missions. Specifically, SAAP is developing concepts and hardware for multi-spectral remote sensing, instrument data analysis and interpretation, material acquisition and containment [1,2,3,4]. Some new concepts for microsensors for making various chemical measurements are also under development. There are many possible applications of space technology to terrestrial hazardous materials field acquisition and analysis.

SPACE INSTRUMENTS, MEASUREMENTS AND APPLICATIONS

There is very high scientific value to direct surface measurements, independent of whether a sample is returned to a laboratory. In particular, the analysis of volatiles is probably best done in-situ due to the potential for loss or chemical change after prolonged storage. For space applications, in-situ measurements may be a necessity because of the limitations on sample return.

Table 1. SCIENCE DATA REQUIREMENTS vs INSTRUMENT TYPES

Required Data	Example Instruments
Elemental Composition	Gamma-ray Spectrometer, a-p-x Spectrometer XRF, a-Backscatter
Mineralogical Composition	Visible-Infrared Spectrometer Mossbauer Spectrometer, DSC, XRD
Water Detection and Mapping	Neutron Spectrometer, Electromagnetic Sounder
Atmospheric Composition	GCMS, Laser Spectrometer
Subsurface Structure	Electromagnetic Sounder, Active Seismometer
Seismometry	Passive Seismometer
Volatiles	DSC-EGA, Visible-Infrared Spectrometer
Imaging	Camera, Imaging Sectrometer
Exobiology	Viking Biology Instrument
Magnetic Fields	Magnetometer

Although terrestrial applications do not face the same limitations, major advantages in speed and accuracy can be gained by employing field analysis prior to selecting samples for laboratory study.

Below are listed some of the characteristics of a few instruments that have been flown by NASA or are being proposed for NASA future missions. The constraints on mass and power, combined with the need to function in a hostile environment, place severe requirements on these instruments. The technology developed to meet these requirements could benefit the production of similar instruments for terrestrial applications.

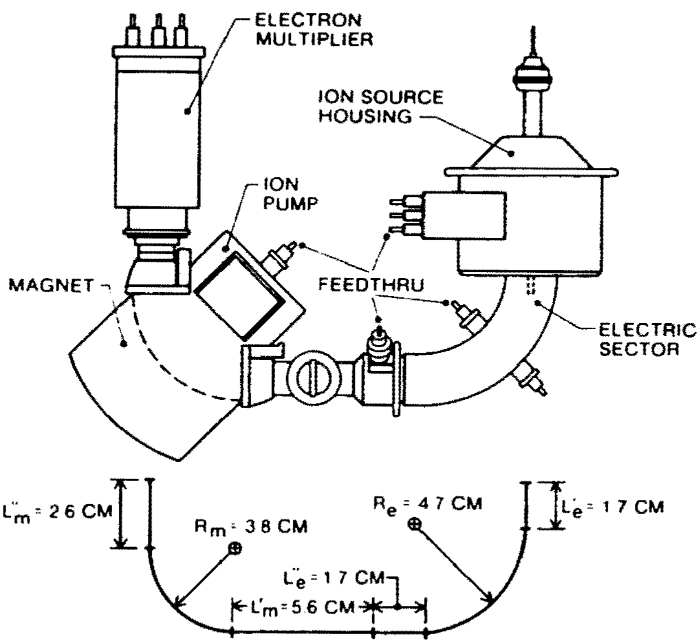

Figure 1. The mass spectrometer for the Viking Lander GCMS. The electric sector has a radius of 4.7 cm.

Chemical Analyzers

The prime example of a chemical analyzer is the Biology Experiment on the Viking Landers. The experiment included a GC-MS system for analysis of organic compounds in Martian soil [5]. The GC-MS part of the system had a mass of 16 kg, measured 28 cm x 38 cm x 27 cm and consumed 25 to 125 W when active. When the system was presented with a soil sample it could sift a soil sample into a pyrolysis tube, seal the tube to a GC inlet, perform a controlled heating on the sample, and perform a mass spectral analysis of the GC effluent with exceptionally high sensitivity. The mass spectrometer also had a direct inlet for analysis of the Martian atmosphere. Figure 1 shows a diagram of the mass spectrometer.

Currently under development for the Comet Rendezvous/Asteroid Flyby mission is the Cometary Ice and Dust Experiment (CIDEX) instrument that incorporates a 3-column GC system for evolved gas analysis over a sample temperature range of -90 to +1000 C. The instrument also includes an x-ray fluorescence experiment in a 15 kg package that uses an average of about 22 W. The system will analyze comet dust for organic materials and elemental composition.

New GC-MS systems have been proposed that combine the analytical speed of microbore GC columns with the exceptionally high sensitivity of a focal-plane mass spectrometer equipped with an integrating focal plane detector. Such a flight system would be comparable in size and mass to the Viking Lander GC-MS, but with analytical cycle times of a few minutes and the ability to analyze GC peaks separated by a few hundred milliseconds. Such a system could measure dynamic processes or determine planetary atmospheric composition while descending on a probe or parachute. The robust, portable nature of such an instrument would make it a good candidate for deployment in terrestrial field screening activities as well. A gas chromatogram from a laboratory prototype is provided in Figure 2.

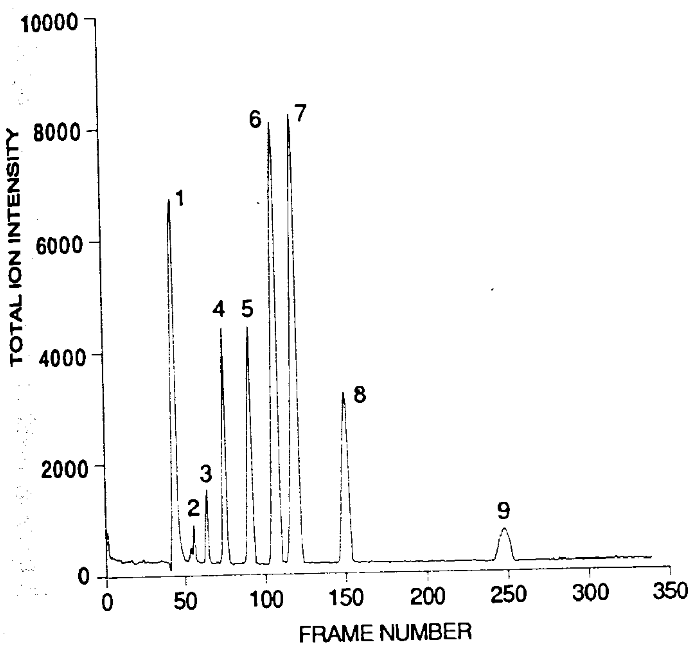

Figure 2. Chromatogram of a mixture of EPA priority pollutants. Each 50 mg frame contains a time-integrated mass spectrum from mass 25 to 500 amu. (Peak 1 is air and peak 9 is toluene.)

Elemental Analyzers

Gamma-ray spectrometers have been used in orbiting spacecraft to obtain elemental maps of atmosphere-free bodies such as the moon. The Mars Observer spacecraft will contain a gamma-ray spectrometer for elemental mapping of the Martian surface through its thin atmosphere. The recently built and proposed gamma-ray systems for elemental analysis have tended to follow commercial technology by use of cooled germanium detectors. These detectors use radiators aimed into cold space to achieve the required temperatures. The detected elements are those with naturally radioactive isotopes or which are excited by cosmic rays. Long counting times are needed. Related instruments may be useful in the remote determination of radioactive isotope composition at terrestrial sites.

New, high efficiency x-ray fluorescence analyzer systems have been proposed for lunar and Martian landers that use new toroidal focussing crystals to achieve many orders of magnitude increase in x-ray flux from microfocus x-ray tube sources to achieve rapid and high sensitivity analyses [6]. With the use of uncooled mercuric iodide x-ray detectors, such an x-ray fluorescence system might have mass of 4 kg, consume 10 W, and occupy a volume of about 35 cm x 25 cm x 25 cm. The same microfocus x-ray source could be used in a high-efficiency, toroidal-focussing powder x-ray diffractometer for identification of minerals. Both instruments can work in an atmosphere of low x-ray absorption density, such as that on Mars, or in vacuum.

VISIBLE AND NEAR INFRARED REMOTE SENSING

Imaging spectrometers play a major role in both Earth observation and planetary exploration. The Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) images with 20 m x 20 m spatial resolution in 224 spectral channels from 400 to 2450 nm wavelengths [7,8]. The data, obtained from NASA ER-2 aircraft at 20 km altitude, is spectrally and radiometrically calibrated to provide information for disciplines such as ecology, geology, oceanography, inland waters, snow hydrology and atmospheric science. An AVIRIS type instrument might be used for aircraft tracking of ocean oil spills, smoke plumes, or other indicators of chemical contamination.

In addition to visible and near infrared imaging spectrometers, NASA has developed a portable backpack point spectrometer (Portable Instantaneous Display and Analysis Spectrometer - PIDAS). At a mass of about 30 kg, PIDAS obtains and records with integrating detectors, reflectance spectra in 830 bands from 400 to 2450 nm. The instrument, developed at JPL, has been used to support geological and ecological disciplines, and can be calibrated for identification of a wide range of materials. The instrument field of view is 10 to 30 cm when hand held. NASA is currently, working to develop an adaptive, reliable and compact imaging spectrometer system for autonomous site and sample selection and analysis of materials. This system will provide wide area as well as close-up identification of minerals which is enabling for surface science and engineering missions.

The key element of the SAAP remote sensing subsystem is a multi-spectral imager based on the solid-state acousto-optic tuneable filter (AOTF). This device operates on the principle of acousto-optic interaction in an anisotropic medium and acts as a controllable narrow band filter. The current breadboard version can collect spectral images at 4 nm spectral resolution in the visible range (0.5 and 0.8 microns). It has been implemented with a 1000x1000 fiber optic bundle between the foreoptics and the AOTF. The fiber optic cable enables the mounting and articulation of the foreoptics, remote from the main spectrometer body. Figure 3 shows the current breadboard hardware.

By altering the pass band sequentially, only the desired spectral bands are collected. Each pixel has a spectral signature associated with it and classification is accomplished on the basis of elemental content and spatial location. Figure 4 shows a set of spectrometer images of a rock containing the rare earth mineral neodymium taken in the range of 783-710 nanometers. The absorption characteristics of this mineral at around 750 nanometers is evident in the dark spot in the right-center of the second row of images. Figure 5 shows the complete spectral signature of neodymium as taken by the AOTF spectrometer.

Although the current instrument operates in the visible region, the AOTF technology will also allow construction of tunable filters for the infrared and ultraviolet regions of the spectrum, with a total range between 0.35 and 25 microns. This may provide a new class of tunable spectral analyzers for a variety of space and earth applications.

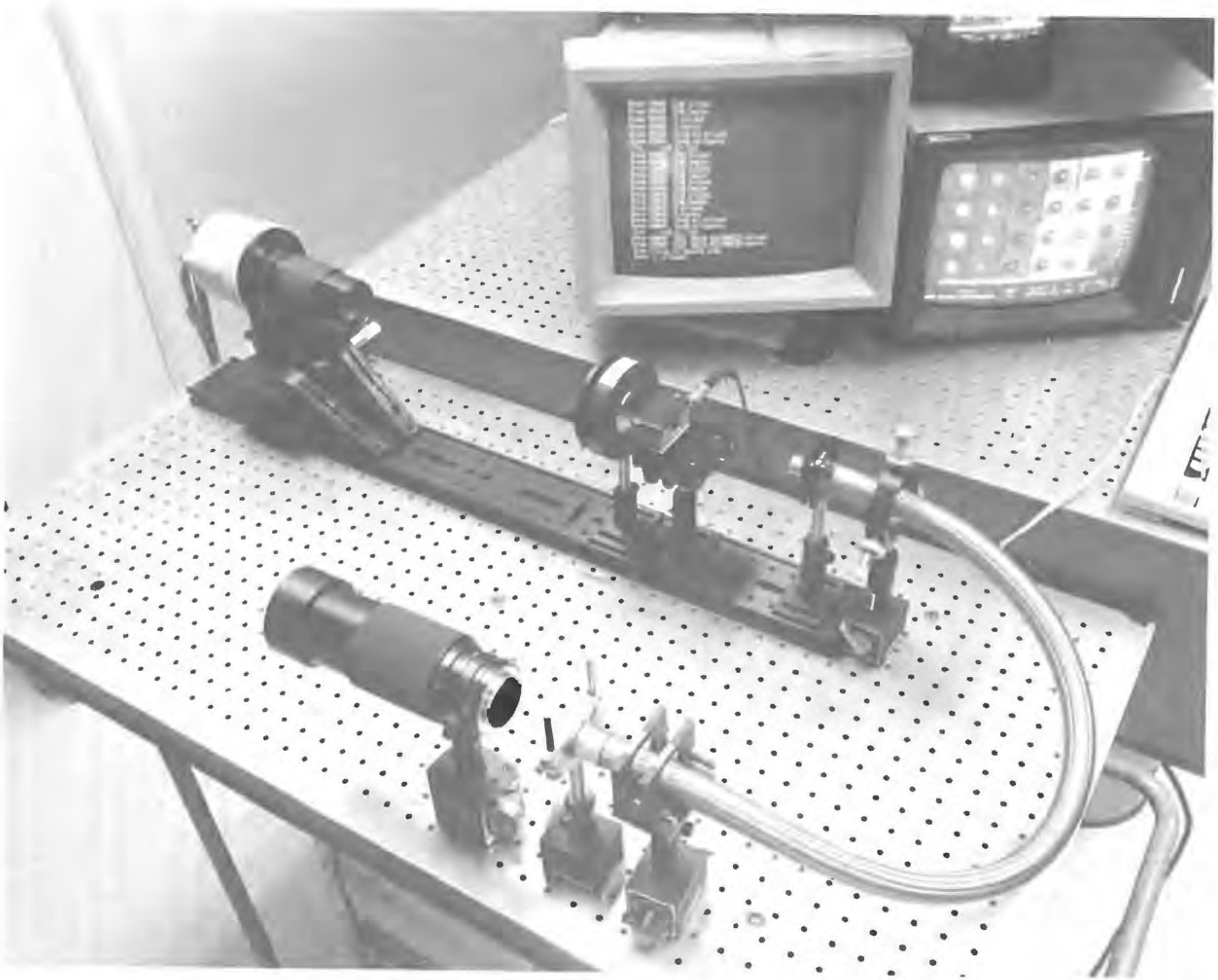

Figure 3. AOTF Spectrometer Breadboard

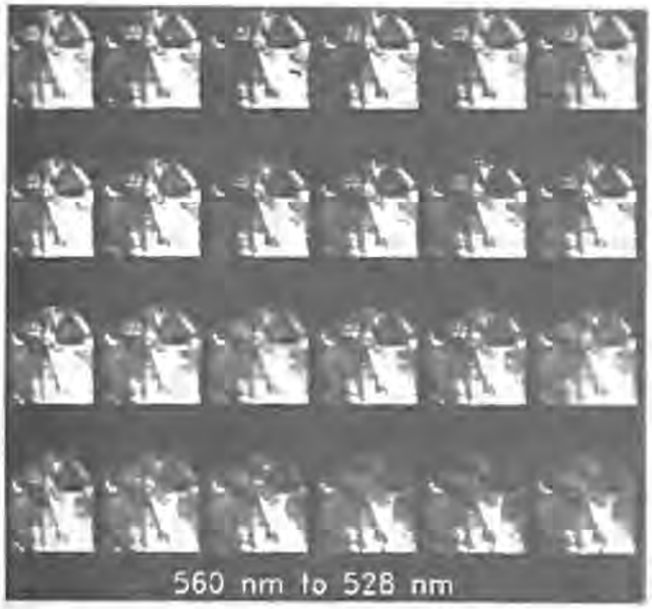

Figure 4. AOTF Spectrometer Output in 710-783 nm

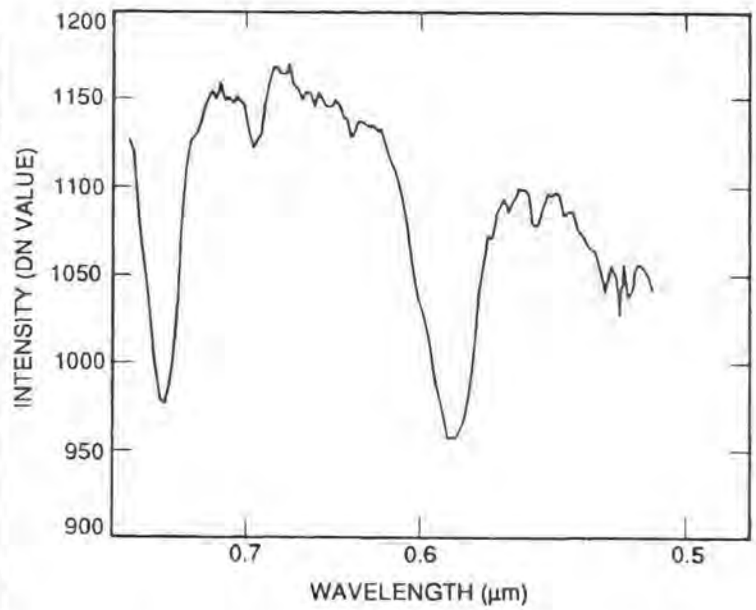

Figure 5. Neodynium Absorption Spectrum from AOTF Spectrometer

The completed imaging spectrometer will be capable of collecting high resolution images at hundreds of discrete wavelengths. Processing of such a large amount of information (>1 gigabit per scene) will strain computational systems without some means of data reduction. Hierarchical analysis schemes, in combination with neural nets, have been shown to produce several orders of magnitude reductions in total computation time and are discussed below.

INTELLIGENT DATA ANALYSIS

Spectral data from a variety of instruments is used in many areas of chemical analysis. The proceedings of the First International Symposium on Field Screening Methods for Hazardous Waste Site Investigation [9] report on the use of fieldable instruments for mass spectroscopy, x-ray fluorescence spectroscopy, infrared spectroscopy and Raman spectrosopy. For any of these instruments, the spectral data produced is complex, requires a highly trained chemist to assist in the interpretation process, and often requires extensive computer work for proper analysis. In many cases the data analysis and interpretation step presents a significant bottleneck which prevents the most efficient utilization of the instruments.

Work done within the SAAP program has concentrated on the the analysis of visible and near infrared spectra for mineral determination [10]. The developing system incorporates a number of data analysis methods and algorithms which will transfer readily to use with other types of spectral data. Application of these approaches to the instrumental analysis required for field screening of toxic waste will improve the speed and efficiency of the analysis step. Table 2 shows a comparison for speed and accuracy of four classification methods. The first matched filter is a brute force approach using full dimensionality of all patterns, and requiring the most computation. By reducing the dimensions used for matching, or performing the matching in several steps (e.g. a grouping step and a finer classification step), the computation is reduced. The hierarchy of neural network pattern classifiers combines these approaches. Images consist of 32-band spectra for all pixels, and are classified as one of 28 known minerals in each case.

Neural networks are trained to recognize spectra or classes of spectra by presenting many examples of each spectrum, complete with noise and normal variation in features. Following training, new variants of the spectra contained in the training set may be identified with a high degree of accuracy. During the training procedure, the network extracts the common features among the training examples representative of each type of spectrum, and learns to recognize these as important identifying factors, while the noise is discarded. Thus new spectra are classified based on the presence of the diagnostic features specific to a type of compound, without significant interference due to normal variation, noise, and background contamination. The major components in mixture spectra may also be identified, if the mixing process does not obscure the critical features.

The neural network spectrum classifiers currently used within the SAAP system work hierarchically, placing spectra into progressively more detailed classes. This approach allows either a rough estimate of mineral composition, or a very detailed analysis and identification. The final analysis step includes an assessment of the classification accuracy. This allows the system to identify those spectra which were poorly classified, and which may represent mixtures or other unexpected spectra. Since the

Table 2. COMPARISON OF 4 SPECTRAL CLASSIFICATION METHODS			
METHOD	DATASET	TOTAL OPERATIONS	ACCURACY
Single Matched Filter	Mars	16,226,560	80%
	AISA	5,017,600	
Reduced Dimension Matched Filter	Mars	8,113,280	80%
	AISA	2,508,800	
Two Step Matched Filter	Mars	6,374,720	69%
	AISA	1,971,712	
Hierarchy	Mars	4,858,284	89%
	AISA	1,006,099	

Note: Mars dataset is a simulated multispectral image derived from a Viking Lander image. AISA dataset is a real multispectral image taken by the Airborne Imaging Spectrometer.

final application of this spectral analysis system requires almost complete automation of the analysis process, the results of the spectral analysis are integrated into an automated decision making procedure. The decision making is goal-driven: specific classes of minerals may be searched for and analyzed in great detail, while other less important compounds are discarded at an early step in the analysis procedure.

The goals of the existing (planetary) spectral analysis and decision making system include identifying interesting and uninteresting areas on the basis of spectral information, and identifying samples which should be acquired for more detailed analysis. Similar goal driven systems could be designed with the objectives of finding specific types of chemical compounds or determining which samples will prove most informative regarding chemical distribution in an area. The hierarchical goal driven architecture allows the system to analyze many samples rapidly, and to provide the user with information regarding which samples are most important for further examination.

Application to field screening for hazardous waste:

Two aspects of the work done for spectral data analysis in planetary exploration will be of interest for the field screening of hazardous waste. The neural network based spectral analysis approach will be useful for the analysis of IR, XRF, Raman, and mass spectra, if networks are trained with real spectra gathered under the anticipated field conditions. The hierarchical analysis architecture that incorporates goal driven decision making may be adapted to assist field workers in making rapid decisions regarding the areas requiring special attention during a field screening operation.

Although special neural network pattern recognition systems will be required for each type of instrument data, the basic algorithms developed for the analysis of visible/near IR mineral spectra should transfer readily to the analysis of other spectra. A hierarchical, neural network based spectral identification system will have several applications:

1. Unknown identification.

A network based hierarchy can replace a library search procedure with favorable results for the identification of unknown spectra. Progress is being made in the implementation of hardware network pattern matchers which will allow the equivalent of very large library search procedure to occur in microseconds.

2. Searching for specific compounds.

A hierarchy of networks is particularly well suited to the search for specific compounds. A spectrum is presented to the hierarchy, and is progressively classified until it becomes apparent that the spectrum does not represent the desired compound (or until the desired compound is found). A negative result is usually determined fairly quickly, since at each step of the hierarchy, a large group of spectra may be eliminated since they are not potential matches.

3. Searching for classes of compounds based on specific features.

This is a variant of the hierarchical search for a specific compound, with the difference that a positive result may occur when a given branch point of the hierarchy is reached, rather than only at the end of the search. The hierarchy is designed so that the groups of spectra that represent important classes are together within a branch of the hierarchy. The selection of critical spectral features for identifying a class is ensured by using specific spectral bands for training the networks. Extensive knowledge of the chemistry is required at the training step for optimal results.

4. Extracting major components from mixtures.

Identification of spectra of mixtures presents problems for traditional library search and match techniques. Since mineral spectra generally derive from mixtures of pure minerals, this problem is being addressed in the work within the SAAP program. The neural network approach has the advantage of basing results on important features which are extracted from the anticipated data in advance, rather than on complete spectral matching. This allows identification of major components in many mixtures. Situations where mixing causes masking or shifting of critical spectral features require special treatment.

SYSTEM CONCEPTS

In-situ analysis systems can range from single instruments placed on the surface to multi-purpose, mobile units looking for specific materials or unique materials units. An autonomous space exploration system will require the functions of planning, analysis, execution control, reflex action, data processing and interpretation, in order to operate in real time in a hostile environment.

For an in-situ analysis subsystem, the spectrum of possible architectures can be characterized by two extremes. At one end is a set of disjoint, self-contained elements working more or less independently to perform the required functions. At the other extreme is a fully integrated system with many interdependent relations between the elements. The former case is probably more comparable to the terrestrial applications, where several independent instruments are operated by humans. This system design causes some problems for space systems since it is not efficient in terms of mass or power and compromises science due to uncoordinated measurements. Multi-instrument data fusion and corroboration is an important consideration in this system design.

An extreme example of the latter case is a multi-purpose, factory-like system, implementing a set of processes that may vary significantly depending on the desired outcome or product. Physical material, not just data, must move between the elements. Current requirements and desires for coordinated measurements as well as mass, power and volume limitations make an integrated design approach the logical basis for technology requirements, but this approach clearly pushes technology. Technology developed for such an integrated system could be applicable to the automation of sample gathering and analysis in extremely hostile earth environments, in cases where human interaction must be remote and limited for safety reasons.

Technology will be validated in the laboratory and then integrated into the series of evolving SAAP testbeds. The representative environment provided by the testbed will be used to verify technologies and demonstrate overall SAAP operational capability. By the end of September 1992 an initial laboratory testbed will be constructed to demonstrate sample identification and acquisition. By the end of 1995 a fully functional system testbed will be in operation which will transition into a complete self-contained transportable testbed for end-to-end "field" operations. A preliminary system conceptual design of a SAAP platform with a full complement of subsystem components except for a regolith deep core drill is shown in Figure 6. This configuration can be considered a preliminary model for the full-up system testbed; no final payload or mission configuration has been selected.

SAMPLE ACQUISITION

The capability to acquire physical samples robotically, without human intervention, would be significantly beneficifial in many hazardous waste screening applications. The principal requirement driving sample acquisition for planetary exploration is to obtain samples of weathered and unweathered materials from accessible rocks or outcrops. These samples must not be significantly altered either mechanically or thermally during acquisition. Conceptual designs and early experimental work have been completed to help understand the mechanical, controls and automation issues for sample acquisition in the hostile environment of a planetary surface. Effort has focused on mechanical designs to achieve functional capability and is now proceeding to include testing of control and automation methodologies. Laboratory validation at the component level will be followed by further development and verification at the system level in a series of SAAP testbeds.

Various techniques have been studied for sample acquisition including sawing, coring and chipping. Of these, core drilling represents an efficient way of obtaining surface and subsurface samples that are easy to handle by a preparation or storage subsystem. Terrestrial coring processes, however, require direct human supervision and utilize high power and introduce large volumes of fluid to aid the cutting process by cooling the bit and removing cuttings of rock and/or soil.

SAAP has developed the means for core drilling low porosity, high compressive strength rocks without the use of coolant. High velocity diamond matrix core barrels are used under the control of robotic manipulators. Under study are various control approaches and a variety of sensors modalities including, position, force, vision, spectral, temperature and vibration. Progress in this area should improve the prospects for remote robotic acquisition of solid samples from hazardous areas on earth as well.

In addition to tools, work is underway to identify and develop end effector and manipulator technologies necessary for the sample acquisition operations. Preliminary studies of end effector and manipulator dexterity versus reliability, mass, power and performance have been made for some mission scenarios. The current

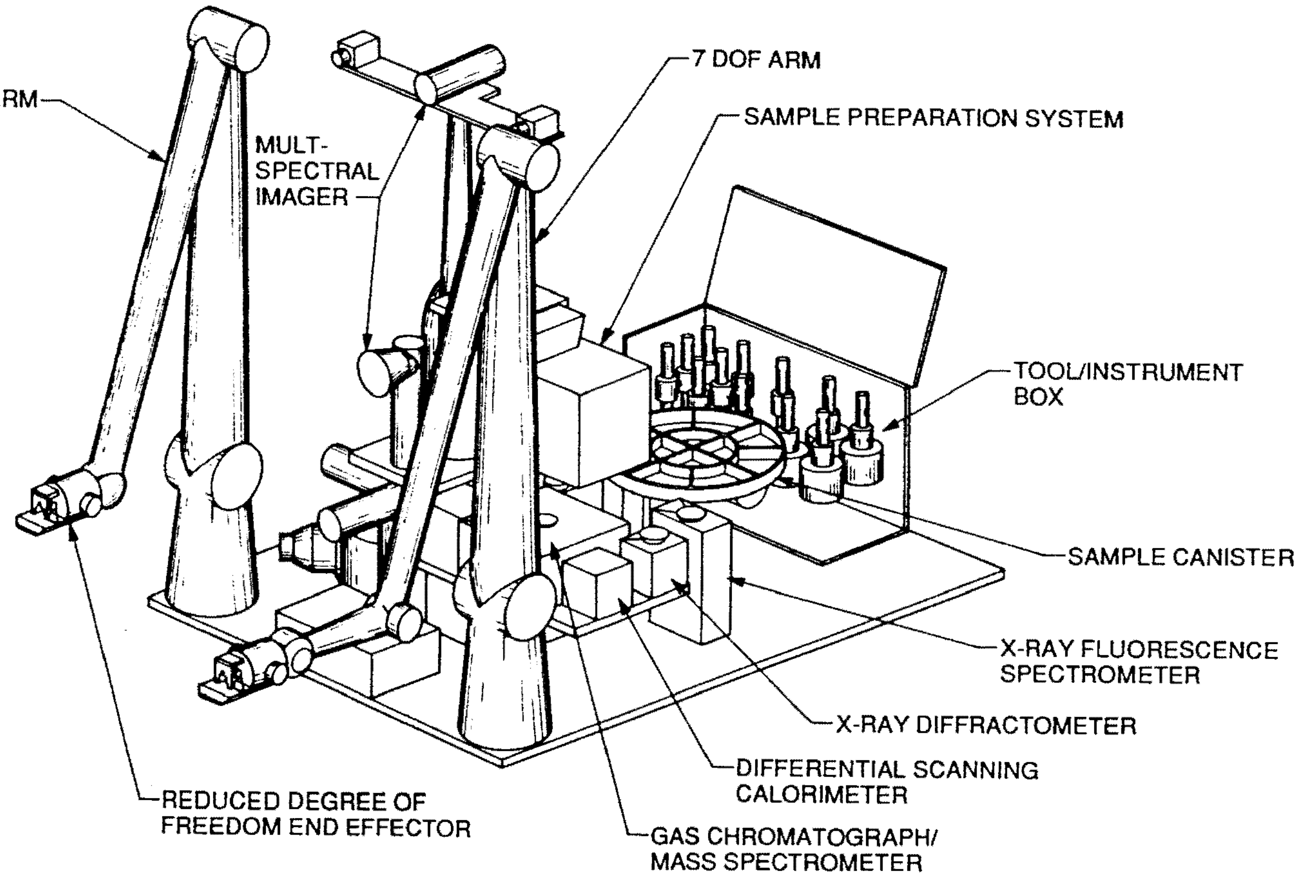

Figure 6. SAAP Preliminary System Conceptual Design

state-of-the-art in end effectors consists of either very limited capability industrial vise-type grippers, or extremely complex anthropomorphic designs being studied in research laboratories. In general, the fewer degrees of freedom the better for simplicity. However, to achieve high inherent reliability, mechanical redundancy at each degree of freedom will be required. Concepts that provide adaptability or flexibility and involve trade-off's of degrees of freedom with redundancy will be studied further.

ADVANCED CONCEPTS

NASA is interested in developing new sensing device technology for in-situ science investigations. Currently available instruments for in-situ science investigations are often incompatible with mission requirements due to their excessive mass, volume and power consumption. Science capabilities may be significantly extended by the development of sensing device systems which represent smaller payloads. The sensing device development is directed to enable compact, low-mass, low-power consumption instruments for a variety of mission requirements. The advanced technology of silicon micromachining for device fabrication will be employed to implement highly capable, sensitive, and robust instruments while retaining compact structure and low mass attributes.

The development of silicon micromachined gas sensors will be based on the compact gas chromatography (GC) instruments recently demonstrated in silicon micromachined structures. The key components of the compact GC systems include a silicon micromachined gas dispersion column, integral gas metering valves, and silicon thermistor gas detectors, fabricated entirely on a single silicon wafer. The successful operation of this prototype time-of-flight GC system indicates the range of opportunities for unique instruments of this type. In this task, specific gas detector applications will be identified and instrument requirements will be formulated. Gas sensors and instruments will fabricated and tested for operation in the Martian atmospheric environment. Finally, with results of device testing, complete instruments will be designed for specific mission applications.

CONCLUSION

This paper has discussed some of the measurements, methods and instrumentation used on past, present and future space missions for in-situ and remote analysis of materials. Work sponsored by NASA's Sample Acquisition, Analysis and Preservation technology program included concepts and hardware for multi-spectral remote sensing, instrument data analysis and interpretation, and material acquisition, and new concepts for micro sensors for making various chemical measurements. Much of the technology under development in the SAAP program has application to terrestrial hazardous waste materials acquistion and analysis.

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DISCUSSION

BRIAN PIERCE: My question concerns the fiber optic bundle. You said infrared. Do you mean the near infrared or closer to the mid I.R.?

SUSAN EBERLEIN: Right now the fiber optic bundle that we've actually worked with has only been in the visible range. We're looking this year in the near infrared of 1.2 to 2.5 microns. In the long-term maybe more, but I gather that as you go further into the infrared you get more trouble with your fibers.

BRIAN PIERCE: Yes, that's right. You also mentioned very intriguing hardware neural networks. What do you mean by that?

SUSAN EBERLEIN: What I mean by hardware neural networks is micro silicon chips where the connection weights for the neural network matrices are actually in the resistances in the chips. JPL is fabricating some of these. They are still in the early stages, and not as precise as we need them. Some other companies are working on making them commercially as well. If in fact they turn out to be a viable technology that can be space qualified, they offer very, very rapid processing for specific problems.

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