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Hyperspectral Remote Sensing:

Review of Current Capabilities

Hyperspectral Remote Sensing: Review of Current Capabilities

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I. Purpose and Scope

1.1 Purpose

This study provides a technology assessment in the field of hyperspectral imaging techniques, sometimes called imaging spectroscopy. Four areas of technology are of interest: (1) hyperspectral remote sensing instruments (sensors); (2) spectral reflectance databases, and instruments (spectrometers) to measure spectral reflectance in the laboratory and field; (3) hyperspectral image processing systems and spectrum identification, search and retrieval capabilities; and (4) the benefits of using polarization and midwave infrared (to 12 μm) to aid in spectral signature identification. The purpose of the study is to provide a summary of the technology so that intelligent planning can be done for the eventual application of this technology to the identification and mapping of known and unknown materials from space.

1.2 Tasks

The specific tasks to be accomplished in this study are enumerated below in accordance with the contract work statement. The report is organized somewhat differently and (hopefully) more logically. The work statement tasks are cross-referenced to the report chapters in Table 1-1.

TASK 1: IMAGING SPECTROMETER STUDY

- a. Identify, research and document all existing and proposed imaging spectrometers that could be used for hyperspectral research in the spectral region of 0.2 to 12 μm .
- b. Review the principal hardware features of the instruments. Evaluate their performance and note their strengths and weaknesses. Compare their overall parameters, and present a comparative summary in tabular form.

TASK 2: SPECTRAL LIBRARY DATABASE STUDY

- a. Catalog existing spectral databases for the spectral region of 0.2 to 12 μm .
- b. Summarize parameters for each database.
- c. Survey and describe instrumentation available to generate reflectance and emittance spectra in the laboratory and field.

TASK 3: SPECTRAL RETRIEVAL STUDY

- a. Survey and describe current spectrum (search and) retrieval software packages available on image cube processing systems (e.g., SPAM, GARP). Compare their strengths and weaknesses. Specify what atmospheric backout procedures are used.
- b. Summarize the main spectral search techniques available from software packages used by spectroscopists for spectrum processing only (e.g., Sadtler, Mattson, Nicolet, IBM,

SPECPR).

- c. Survey and describe existing image cube processing systems.
- d. Address the possible application of the spectral search techniques available for spectrum processing only (as identified in subtask b.) to "imaging spectroscopy," i.e., image cube processing.
- e. Review the need for, approaches to, and effectiveness of spectrum identification and interpretation, and discuss the potential for using automated methods.
- f. Review the need for, approaches to, and effectiveness of removing the atmospheric effects on spectra.
- g. Recommend research areas that are critical to improving existing hyperspectral image processing capabilities (e.g., the artificial intelligence approach for algorithm development), including the capability for atmospheric compensation.

TASK 4: SPECTRUM RANGE AND MODE STUDY

- a. Compare the spectral information that can be obtained in the spectral regions of 0.2 to 0.8 μm , 0.8 to 2.4 μm , and 2.4 to 12 μm . Compare the advantages and disadvantages of working in each of these regions.
- b. Determine the effect of polarization on a material's spectral signature. Document the results of current studies performed to-date on polarization as applied to imaging spectroscopy.

1.3 Schedule

The schedule for this study is given in Figures 1-1 and 1-2.

TABLE 1-1
**RELATIONSHIP OF WORK STATEMENT TASKS
TO REPORT CHAPTERS**

<u>WORK STATEMENT TASK</u>	<u>REPORT CHAPTER</u>
1a,b -----	3
2a,b -----	5
2c -----	4
3a -----	7.2
3b -----	7.3
3c -----	6
3d -----	7.4
3e -----	7.1
3f -----	8
3g -----	9
4a -----	10
4b -----	11

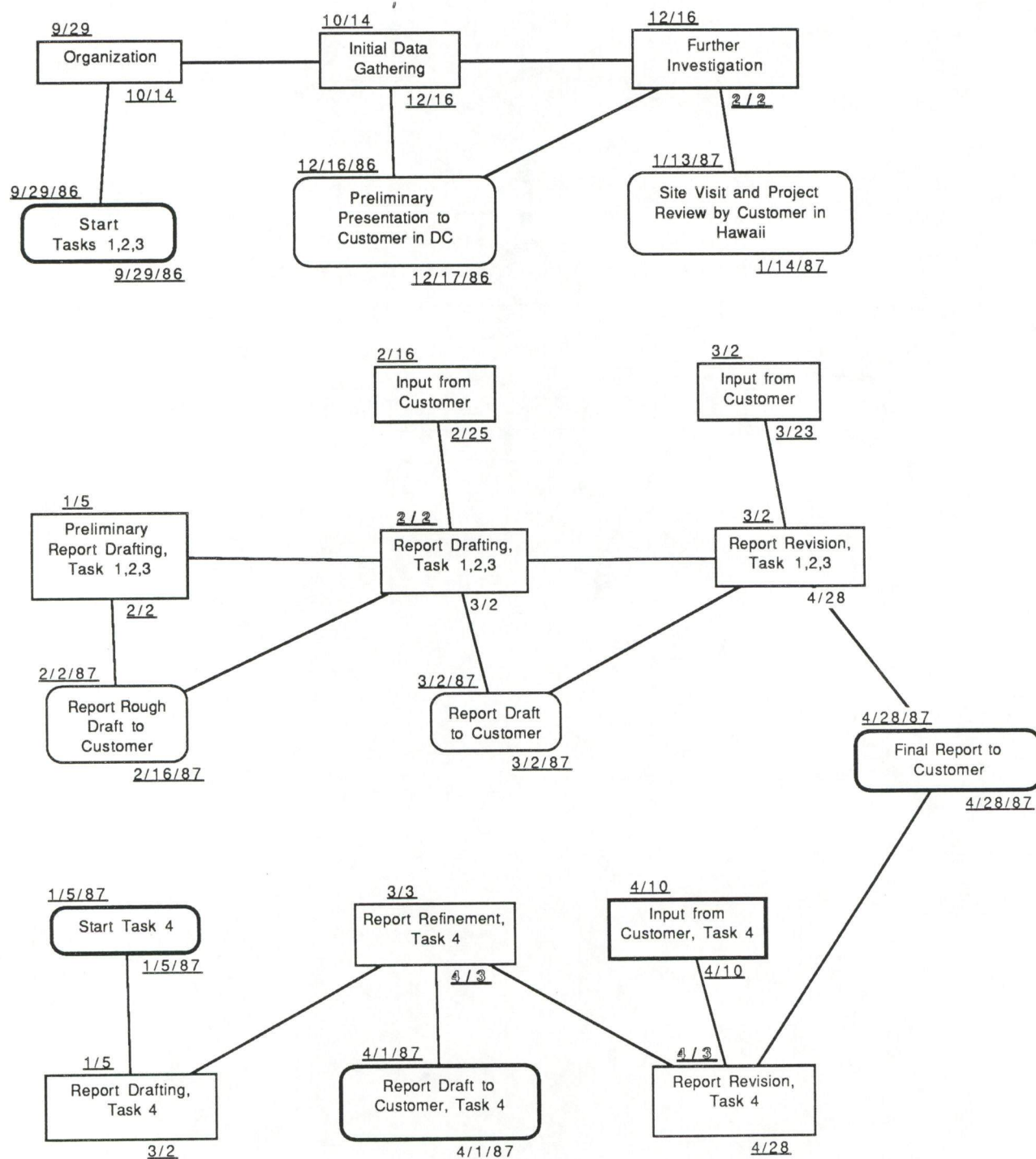
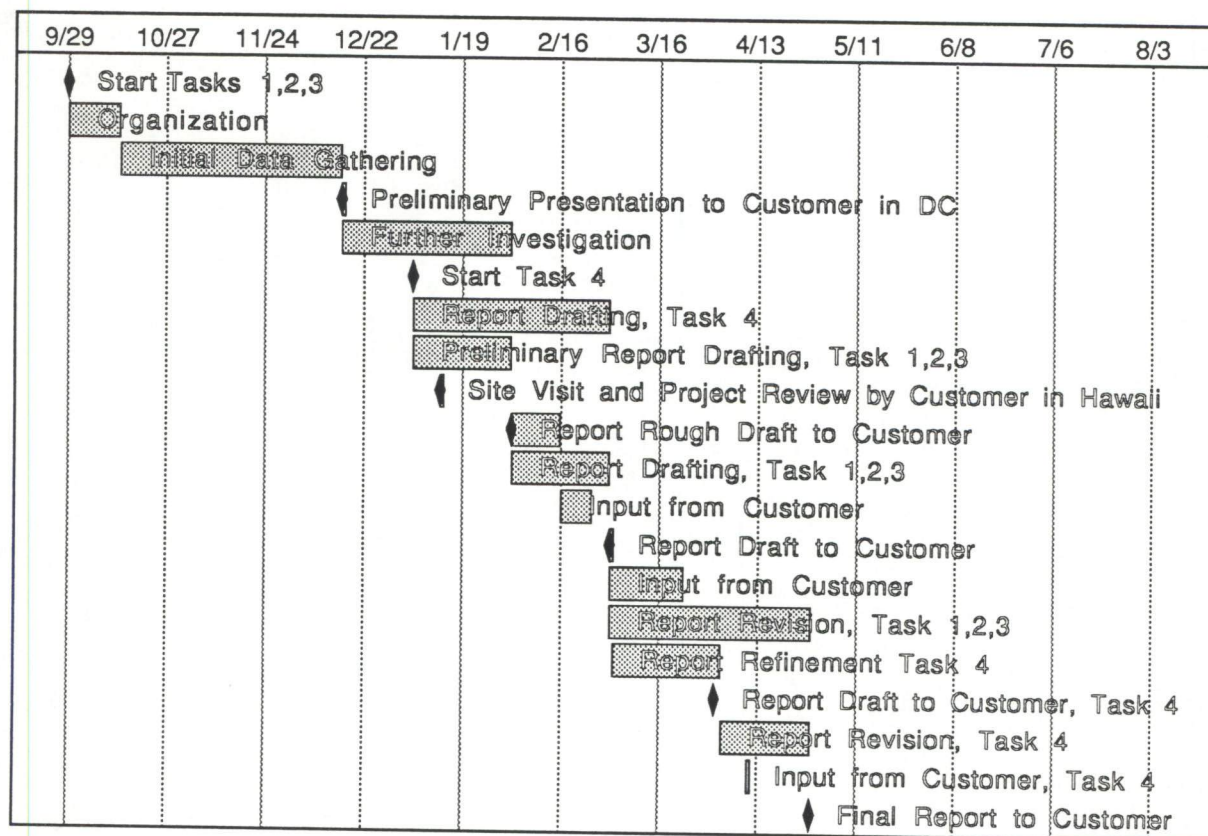


FIGURE 1-2
TASK TIMELINE



2. Summary and History of the Technique

2.1 History

Hyperspectral remote sensing, also called imaging spectroscopy, is the merging of two techniques developed earlier: (1) multispectral imaging and (2) spectroscopy. Digital multispectral imaging of the Earth and other planets has been practiced from air and space platforms for about 15 years. Current active space platforms with this capability include Landsat 4 and 5; NOAA 7, 8 and 9; and SPOT 1. This technique involves measuring the same scene in up to about 10 spectral bands and analyzing the spatially registered images for areas of common spectral properties. The technique works well for defining and mapping areas of common spectral properties, but it usually is not possible to identify the specific material(s) present without groundtruth.

Reflectance spectroscopy has been used extensively as a remote sensing technique for observing the Earth and planets only during the last 20 years or so because the radiation detector technology for measuring (with sufficient precision and spectral coverage) the reflectance spectrum of distant objects had not been available earlier. Even so, attempts were made to observe other planets using groundbased telescopes since nearly the beginning of this century. The development of the capability to effectively observe objects in the solar system resulted in a wealth of observational data, and was quickly followed by the theoretical and laboratory work necessary to interpret the observed spectra and to improve the technique.

The excitement of initial and continued discoveries using reflectance spectroscopy created an increase in the number of scientists developing and applying it, and in the funds made available to support the work. The NASA Solar System Exploration Program was one of the early supporters of this work and continues to be a major supporter.

Reflectance spectroscopy for remote sensing is an active and productive technique that is applied using groundbased telescopes as well as laboratory and theoretical investigations. Over 100 articles appear annually in professional journals from about 25 active workers in the field. Major discoveries have been made and much of the early reconnaissance of several objects or object systems (e.g., asteroids) has been carried out. Technique and instrument development has been driven by the telescopic observations. Essentially all existing reflectance spectra remote sensing data sets for solar system objects other than the Earth were acquired using groundbased telescopes; a few sets have resulted from Earth-orbital telescopes.

With the success of the techniques, nearly every planetary mission advisory committee in the past ten to fifteen years has recommended that a reflectance spectrometer be included on almost every proposed mission payload. The technique is now considered so important for flight missions that NASA has declared it a facility experiment to be provided by the flight projects (like the spacecraft itself and the television imaging experiments) rather than by the principal investigators.

But reflectance spectroscopy has not yet played a role in flight missions of the NASA Solar System Exploration Program because of: (1) the increasingly long lead time NASA requires for development and flight of spacecraft instruments; (2) the lack of initiative for new experiments caused by the great success of the imaging systems of the early lunar and planetary missions; and (3) the hiatus in planetary missions resulting from budget cuts and NASA priorities over the past 10 years or so. Nevertheless, a reflectance spectrometer was chosen for the later-cancelled Lunar Polar Orbiter Mission in

1975. A reflectance spectrometer was apparently intended to be an instrument on the Comet Halley Flyby - Temple 2 Rendezvous Mission, but instruments were never formally selected for this mission after an AO (Announcement of Opportunity) was circulated in 1976. The Near Infrared Mapping Spectrometer (NIMS) experiment was chosen in 1976 for the Galileo Project, and the instrument is now built and awaiting the eventual launch of the spacecraft (last scheduled for 1989). The Mars Observer Mission (MOM) has a Visible Infrared Mapping Spectrometer (VIMS), selected in April 1986. The Comet Rendezvous - Asteroid Flyby (CRAF) Mission has a facility reflectance spectroscopy instrument as part of its payload; Lunar Geoscience Orbiter and Cassini Mission science working groups have strongly recommended this investigation. Because of the impending mission involvement, the field has recently evolved as a subdivision of the planetary exploration program. As a consequence, the activities in this field have become tailored to accommodate specific mission capabilities.

Reflectance spectroscopy has become increasingly important in the area of terrestrial remote sensing as well. The NASA Earth Sciences and Application Program was not as aggressive in this area at first. A point spectrometer was flown in the early Landsat Mission but it did not function well and no other investigations were flown. More recently, the developments in this area have in some ways led technique development and application in the planetary program. In the last year, a NASA airborne program has successfully flown the Airborne Imaging Spectrometer (AIS), developed at the Jet Propulsion Laboratory (JPL), and is planning to fly the Advanced Visible and Infrared Imaging Spectrometer (AVIRIS) in the summer of 1987.

A related area of remote sensing that was active 20 years ago and has again become active is emittance spectroscopy. This field continues the same general approach used in reflectance spectroscopy farther into the infrared spectral region where thermal emission becomes the dominant source of radiation from planetary surfaces and atmospheres. Much of the approach to reflectance spectroscopy measurement and analysis still applies, and the physics of the emission process becomes almost totally controlled by molecular processes. This area is much less developed but holds considerable potential for remote sensing identification and mapping of materials.

2.2 The Technique of Reflectance Spectroscopy

The primary reflectance spectroscopy data set results from the measurement of reflected sunlight from a surface and the calibration of the measurement instrument and the conditions so that the ratio of reflected to incident sunlight as a function of wavelength (spectral reflectance) can be calculated. The spectral reflectance of a particulate surface is dependent on many factors: material type, chemical composition, abundance, and particle size are the most important. Most minerals show diagnostic absorptions due to molecular vibrations, electron charge transfer, conduction bands, and electronic transitions. Second-order effects on absorption band presence and wavelength position arise from viewing geometry, particle packing, and temperature. Other effects such as weathering (which produces other minerals) and sputtering can be major or minor. The magnitude of these effects depends on the exposure time, intensity, and the exact nature (i.e., mechanism) of the weathering and sputtering processes.

The technique of reflectance spectroscopy involves the interpretation of the reflectance spectra in order to detect these absorptions, identify the mineral phases, metals and other materials present, and determine abundances and physical states through available (theoretical and empirical) models. Often, it can also work in the opposite sense, that is, determining what is not present on the surface.

The theoretical models and laboratory measurements of candidate materials from which the interpretation of the planetary data set can be derived are of primary importance. The fundamental data set used for interpreting the planetary spectra and determining the composition of planetary surfaces is the laboratory reflectance spectra of minerals, rocks, gases, and ices (which themselves are minerals) under simulated planetary conditions. The spectra of many hundreds of (planetary surface analog) materials

have been measured, allowing many of the discoveries cited in Chapter III. Theoretical models to calculate reflectance spectra from basic material optical properties, and examples from laboratory measurements are critical for efficient interpretation of the coming wave of new data. Laboratory measurement of all materials under all relevant conditions is time-consuming and expensive, and is virtually impossible.

The successful application of reflectance spectroscopy requires contributions from many areas (see Figure 2-1). Four distinct and equally important areas are:

- Development, operation and maintenance of laboratory, telescopic and flight instrumentation and related facilities, and development of required personnel;
- Measurement of spectra and supporting parameters for candidate materials in the laboratory, using telescopes, spacecraft and laboratory systems, and archival of spectra databases, in order to address well-formulated and significant questions or technique development needs;
- Development of reflectance spectroscopy theory, rigorously based on radiative transfer theory, along with interpretive calibrations and procedures, from which techniques can be developed for deriving chemically, physically and mineralogically significant properties from spectral data sets;
- Interpretation of the observational data set in order to determine the surface materials and atmosphere properties, and integration of those properties with other available information into an appropriate model that addresses the specific issue raised in the original statement of the problem that motivated the measurement.

Instrumentation, interpretive calibrations, laboratory data sets and theoretical modeling represent enabling technologies. They permit acquisition of spectral data and interpretation of those data sets in order to identify materials and their physical properties, and to derive certain atmospheric properties. Proper database management procedures must be followed to ensure that the data sets are useful to the community at large well into the future. All these activities are essential to the successful application of reflectance spectroscopy, and most must be carried out as an integrated activity with participating scientists ideally working in and familiar with several areas.

2.3 Measurement Considerations

The fundamental measurement is the ratio of reflected to incident sunlight on a given area. This is made using detectors and wavelength-discriminating devices that (ideally) yield a spectrum of light intensities as a function of wavelength, polarization state, location on the surface of the object, and the angular relations between the Sun and the object, and between the object and the observer at the time of measurement.

Reflectance spectroscopy depends on an illuminating source of light, which in most studies is the Sun. As a quasi-blackbody radiator at 6000°K, the Sun is a very efficient radiator of energy in the near ultraviolet, visible, and near infrared spectral regions. However, somewhere in the spectral region between roughly 1.6 and 5.0 μm for the terrestrial planets (depending on the distance of an object from the Sun), the body itself becomes a radiator and emits as much or more thermal energy from its surface than the energy of sunlight that it scatters back to space. When the emitted energy becomes the major fraction of the reflected energy at a given wavelength, the interpretation of the measured spectrum becomes difficult to impossible. At ultraviolet wavelengths shortward of about 0.4 μm , the solar flux decreases rapidly. Therefore, the region of most interest here covers the wavelength interval from about 0.3 μm through about 5.0 μm , where reflected incident solar light is usually the primary source flux from

surfaces and atmospheres of sufficient strength to be measured accurately.

The light scattered by a surface or atmosphere can be the result of a very complex interaction. Surface reflections and diffuse scattering from several materials of various grain sizes can be mixed in a single measurement for one resolution element. For many materials in the solar system, reflectance spectra can be considered to be primarily a function of the mineral or molecular species, and their abundance and composition. For solid surfaces, the measurement usually involves only the upper few millimeters of the surface material. These materials at ultraviolet, visible and near infrared wavelengths exhibit absorption features that are due to molecular vibrations and electronic energy transitions of several types. This first-order effect is modified by a number of second-order effects, such as geometry and particle size, which usually alter the spectral properties in a way that slowly varies with wavelength. There are materials which are important exceptions, such as various ices and oxide minerals, where particle sizes have a major first-order effect on the absorption band properties in the spectrum. Thus, the problems of complex scattering and mixtures below the spatial resolution element are sometimes very important, even to the point of making it impossible to separate atmospheric and surface effects.

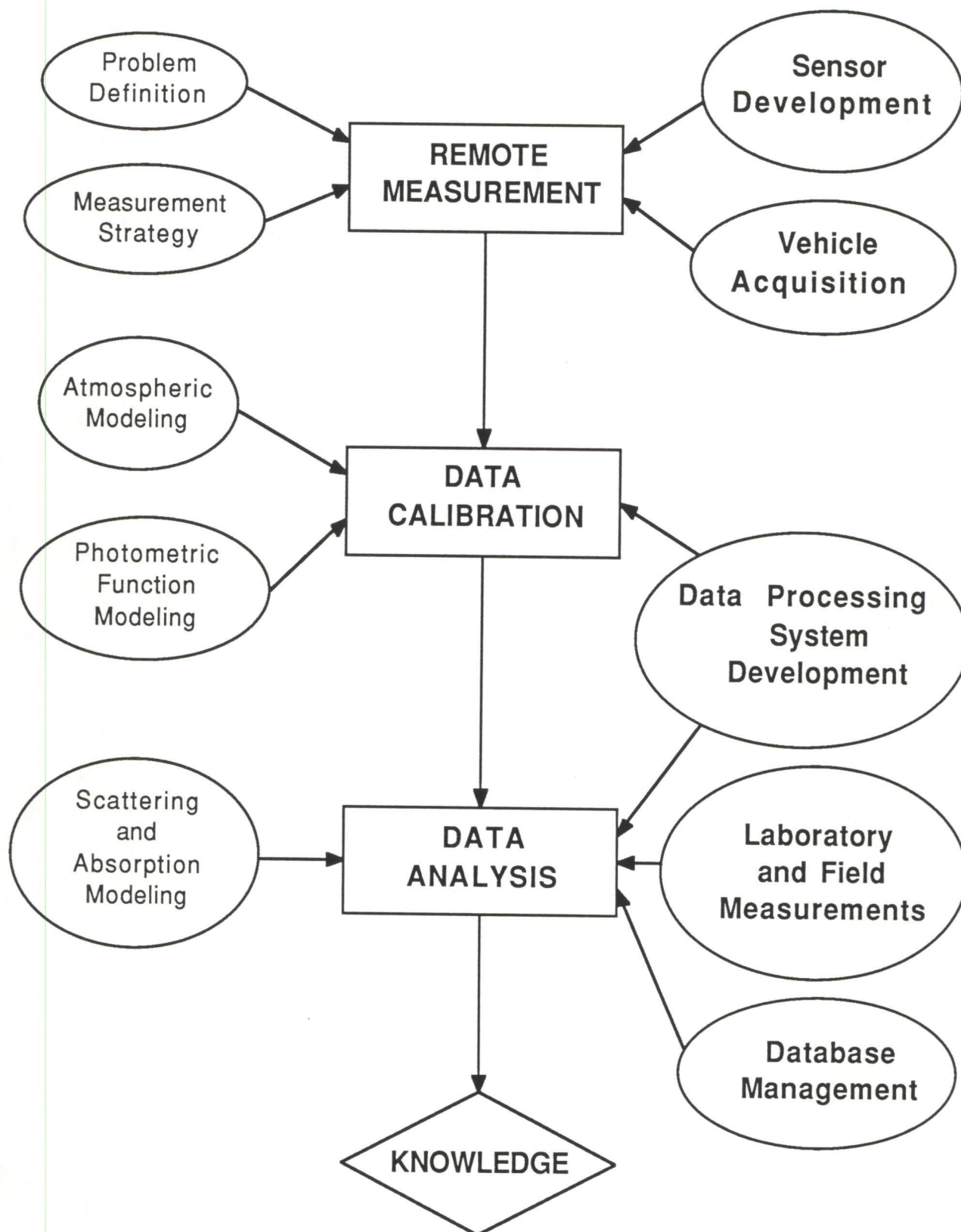
2.4 Physical Basis

There is a direct link between the phenomenological aspects producing reflectance (or absorption) spectra and the regions of the electromagnetic spectrum where features are observed. In the wavelength range of 0.2 to 5.0 μm , spectral features have origins involving electronic, vibrational and rotational energy levels. These transitions are further subdivided into: anion $\rightarrow$ cation electron transfers (e.g., $\text{O}^{2-} \rightarrow \text{Fe}^{2+}$) in the near ultraviolet; metal $\rightarrow$ metal intervalence electron transitions (e.g., $\text{Fe}^{2+} \rightarrow \text{Fe}^{3+}$ or $\text{Ti}^{3+} \rightarrow \text{Ti}^{4+}$ in pyroxenes) in the visible infrared; intraelectronic or crystal-field transitions (e.g., $t_{2g} \rightarrow e_g$ energy levels of 3d orbitals of Fe^{2+} in olivines) in the visible to near infrared; and vibrational and rotational transitions of specific functional groups of molecules or anions that are observed in the near infrared as combination and overtone bands (e.g., H-O-H or CO_2), or anions (e.g., O-H^- or CO_3^{--}) in, for example, clay silicates and carbonates.

In general, wavelengths (energies) of these transitions are diagnostic of cations and their crystalline environments, or of functional molecular or anionic groups in minerals. However, additional theoretical analyses of spectra and energy levels, utilizing crystal chemistry, bonding models, quantum theory and selection rules, are often required to facilitate the assignment of features in reflectance spectra. On the other hand, laboratory spectral measurements of correlative mineral assemblages or rock-types believed to be models of surfaces of planets have had to be made under physical conditions simulating their regoliths. An ongoing research area is to measure spectra at different temperatures, confining (atmospheric) pressures, particle sizes, grain-size packings, and modal mineral proportions. Thus, laboratory and theoretical calibration studies are prerequisites to detailed interpretations of remote-sensed reflectance spectra.

FIGURE 2-1

AREAS RELATED TO REFLECTANCE SPECTROSCOPY



3. Imaging Spectrometers for Remote Sensing

3.1 Summary and Conclusions

This section reviews and evaluates the existing or proposed instrument systems known to us, that are capable of measurement from air or space and are able to obtain hyperspectral data sets. The sensors described here are those intended for scientific research applications; they do in all probability reflect the state of the art in hyperspectral sensors, partly because detector capabilities provide the ultimate limits on sensor performance. Many of the unclassified sensors presently in use employ detectors that are at the limit of theoretical sensitivity. There are continuing efforts to enhance both sensor and detector technologies, but this is no longer possible in some areas.

The sensors to be reviewed are listed in Table 3-1. The review consists of a compilation of technical data describing the sensors, summarized in Table 3-2a, and a description and discussion of each instrument. For those sensors that have successfully obtained data, the quality of the data collected will be discussed. Of the sensors evaluated, the TIMS and the AVIRIS are the only ones available for use in data collection from an Earth-oriented platform. Both sensors are far from space qualification; the data collected with these two systems leave large portions of the near infrared (2.4 to 5.0 μm) unsampled and have very low spectral resolution in the thermal infrared. The NIMS is flight-ready but is intended for deep space application.

This study describes four approaches in sensor development that cover the near and thermal infrared. It is not possible to recommend any one particular design without knowing the specific application and the resource trade-offs (mass, power, logistics, space) for the particular situation.

1. The VIMS/NIMS approach sacrifices sensitivity to utilize a single focal plane.
2. The MRS/SISEX/HRIS approach uses dichroic beamsplitters to maximize sensitivity and to assure strict simultaneous acquisition of spectral data and relatively easy implementation of two-dimensional detector arrays.
3. The AVIRIS approach achieves a broad spectral range while sacrificing strict simultaneity. It relies on sampling several spectral regions serially and approximates simultaneity through very rapid sampling. This approach is easily extensible to any wavelength region where efficient optical fiber technology exists. It could be extended to area array detectors if optical fiber ribbon cables were constructed to carry the spatial dimension from the focal plane to the spectrometers.
4. ATOF technology can currently be used in the visible and near infrared spectral regions. There are some other dispersive techniques which might be used in the thermal infrared region.
5. Imaging interferometry is a proposed technology for the Hubble Space Telescope second-phase instrument complement.

A decision as to which options would be most appropriate should be based on available detector technology (line or area arrays), the need for strict simultaneity (dichroic vs. fiber/ATOF), and the willingness to support the development of immature technologies (ATOF, two-dimensional detector arrays).

in the thermal infrared, fiber ribbons, etc.). A most conservative approach would be to use dichroic dissection of the input beam, line arrays and grating spectrometers in the visible and near infrared, and a grating spectrometer or interferometer in the thermal infrared, together with fiber connections to spectrometers. Such a modular design would greatly speed up sensor implementation.

3.2 Discussion

Hyperspectral sensors have the basic subsystems shown in Figure 3-1. These sensors can be divided into two types based upon the axis along which a two-dimensional focal plane is scanned in order to produce the three-dimensional image cube. The first, and most commonly conceived, is the "imaging spectrometer" or "mapping spectrometer." In this type of sensor the focal plane of the instrument is composed of a spectral vs. spatial image. All spectral bands for a line of spatial elements are present on the focal plane for measurement by an appropriate detector array. If implemented with continuous array detectors, this scheme has the principal advantage of preserving the spectral purity of each spatial element. No postacquisition processing (such as coregistration) is necessary in order to extract raw spectral information for any point in the scene observed. This feature is particularly important for data calibrations under conditions where the spectral properties of the atmosphere between the light source and the object, and between the object and the observer change rapidly. There are three principal disadvantages to this scheme. First, spatial relationships can be compromised during the third-axis scan, making geometric corrections necessary. Second, if fewer than all bands designed into the instrument are utilized, the information is discarded and the portions of the detector array assigned to those wavelengths are not utilized. Third, the scheme taxes the dynamic range of detectors because of large variations in input flux. This last disadvantage can be partially compensated for by appropriate, wavelength-dependent filtering of the input radiation. In practice, imaging spectrometers have been subdivided into two categories: (1) sensors of about 1% spectral resolution that cover a broad spectral range, i.e., most of the visible and near infrared spectral region; and (2) sensors designed to cover narrow spectral ranges for specific applications.

The second type of sensor is the "multispectral imager" with a spatial vs. spatial focal plane. In this sensor, an image of an entire scene is obtained for each wavelength band (or portion of the power spectrum in imaging interferometers), and scanning is performed along the spectral axis, one band at a time. There are several advantages to this scheme. For example, it preserves the spatial integrity of the scene. A second advantage (in non-interferometers) is that integration times in each band can be appropriately adjusted for the available flux in that band, thereby improving the signal-to-noise ratio. A third advantage is that if less than full spectral coverage is desired, unwanted bands can be passed over, allowing full utilization of the array detector (not true for interferometers). A fourth advantage, limited to electronically tunable filters or interferometers, is variable resolution. For all multispectral imagers, postprocessing may be required to register the image planes, particularly if there is platform motion during data acquisition. Furthermore, if atmospheric properties are changing faster than the time required to produce an entire spectrum, accurate calibrations are made very difficult or impossible.

Particular attention will be paid to the spectrometer portion of the sensor for two reasons:

1. The detector is the heart of the sensor and its properties provide the ultimate limits to sensor performance. However, as the detector technology develops, detector performance is constantly improved and is largely out of the control of sensor designers. Two approaches have been applied to this problem. The first is to meet measurement goals by utilizing mature, proven detector technology. This approach assures success, though perhaps limiting data collection and sensor systems. A variety of scanners, including the AVIRIS instrument, are based on this philosophy. The second approach is to develop a design using experimental, but potentially much more capable, detectors. The MRS, AIS, and SISEX utilize this approach. The SISEX also includes sensor development as an essential part of its overall development program.

2. Data rates and volumes are dependent upon the digitization scheme and the data acquisition and handling system. Data acquisition variables which limit sensor performance are often specified for reasons other than ultimate performance, such as platform considerations, money available for hardware, time, and externally imposed limits on data volume or data rate. These limits result in a loss of data which could otherwise be successfully obtained.

Given a fixed detector technology and a data collection system that makes full use of the output of the detector, the spectrometer design and implementation are crucial limitations on overall sensor performance. For this reason, the sensor will be discussed as a system in terms of the effectiveness of the spectrometer.

3.3 Evaluation of Hyperspectral Sensors

3.3.1 Spectrometers with 1% spectral resolution and broad spectral range

The following sensors are designed to cover wide portions of the visible and near infrared. These sensors employ or are intended for a wide variety of platforms: aircraft, Earth-orbiting spacecraft, interplanetary spacecraft, and groundbased telescopes.

MRS--Mapping Reflectance Spectrometer: This instrument was designed and built by the Planetary Geosciences Division of the University of Hawaii (PGD/UH) and the Massachusetts Institute of Technology. It was designed as a prototype for spacecraft use and is to be used on groundbased telescopes.

The instrument covers a broad spectral range while maximizing efficient use of the input beam. It is primarily intended for use with area array detectors. However, line arrays have been used in this instrument. Because Earth-based telescopes have the foreoptic aperture fixed and observation time is at a premium, the light falling on the focal plane of the telescope has to be used as efficiently as possible. Efficiency is accomplished through the use of dichroic beamsplitters which subdivide input energy into wavelength bands one spectral octave in width. Conceptually, the MRS contains four separate spectrometers which efficiently share a single input beam. After dispersion by gratings, the beam from each spectrometer is directed through a dedicated transmission camera optics onto the detector in the focal plane. The optical layout is shown in Figure 3-2. The current implementation utilizes a single cold surface for all focal planes but this can be modified to use multiple cold surfaces of temperatures specific to individual detectors. This design enables detectors of widely differing technologies to be applied to specific wavelength regions in order to maximize sensitivity. The subdivision of input light into octaves allows the use of transmission optics, which can provide compactness and superior image quality.

The primary disadvantages of this instrument are: (a) electronic complexity is increased with multiple detector technologies; (b) cooling is more difficult as different technologies require different operating temperatures; and (c) multiple spectrometers increase the number of calibrations and alignments needed.

The primary advantages of this instrument are: (a) its capability for simultaneous

acquisition of spectral information; (b) efficient use of the input beam; and (c) ability to use a two-dimensional array detector.

NIMS--Near Infrared Mapping Spectrometer: This was the first imaging spectrometer to be completed. It was built by the Jet Propulsion Laboratory (JPL) for use on the Galileo mission to Jupiter.

Instrument design was driven by weight, size and power consumption constraints. The capability to cover a broad spectral range utilizing a single detector focal plane array was met through the use of a dual-blazed grating and order-separating filters fastened directly over the appropriate detector elements. The optical layout is shown in Figure 3-3. The NIMS design uses an array of 17 discrete detectors in the focal plane. While each detector in this array is quite sensitive, the overall sensitivity is low because the array intercepts a small portion of the spatial-spectral image at any one time. Sampling the entire spatial-spectral image requires scanning of the grating to fill in the spectral axis, and scanning of the telescope secondary mirror to obtain the spatial axis. It requires $4 \frac{2}{3}$ seconds to acquire the full spectrum for a spatial line 20 pixels long.

The primary disadvantages of this instrument are its limited sensitivity, inefficiency, and mechanical complexity.

The primary advantage of this instrument is that it was able to meet spacecraft resource limits with the technology available at the time it was designed (about 10 years ago).

VIMS--Visible and Infrared Mapping Spectrometer: This instrument built by JPL is intended to be the successor to NIMS and will fly on the Mars Orbiter Mission and the Comet Rendezvous - Asteroid Flyby Mission.

The design (Figure 3-4) utilizes an optical design similar to the NIMS (Figure 3-3) and shares the attenuation of input radiation inherent in that design. A continuous linear array obviates the need for spectral scanning. Spatial scanning is still required. VIMS should be at least an order of magnitude more sensitive than the NIMS.

The primary disadvantages of this instrument are its mechanical complexity and optical inefficiency.

The primary advantages of this instrument are: (a) it simultaneously acquires spectral data, and (b) it meets the spacecraft resource limits.

AVIRIS--Advanced Visible and Infrared Imaging Spectrometer: This instrument built by JPL is intended for use as an airborne instrument for terrestrial remote sensing.

The design includes capabilities to measure the full wavelength range with four spectrometers and is similar in concept to the MRS. In this instrument, however, the spectrometers do not share the same input beam. Rather, each entirely separate spectrometer obtains its input from an optical fiber linking the focal plane of the foreoptic to the focus of the collimating mirror of each spectrometer (Figure 3-5). The four fibers are arranged in a line on the foreoptic focal plane. Each spectrometer measures a different but adjacent spot on the ground. Correction is made by scanning the image along the fiber

optic array axis, which causes a spot on the ground to be measured by each spectrometer after four scan steps. The AVIRIS is currently undergoing flight testing.

The primary disadvantages of this instrument are: (a) the instrument cannot be upgraded to area array detectors; (b) it cannot be used for point sources; and (c) spectral data are not acquired simultaneously.

The primary advantages of this instrument are its high optical efficiency and modularity of design.

SISEX--Shuttle Imaging Spectrometer Experiment: The SISEX was being built by JPL and was intended for terrestrial observations from the Space Shuttle. The temporary loss of launch capability following the Shuttle explosion led to the recent cancellation of the SISEX. Nevertheless, its design should be studied by those interested in the general field of imaging spectrometer design.

The design employs two area arrays to collect the spectral-spatial information. As such, it should be one to two orders of magnitude more sensitive than an instrument that relies on line arrays. The SISEX design achieves a broad spectral range through the use of a dichroic beamsplitter with a $1.0\text{ }\mu\text{m}$ cutoff and two prism spectrometers (Figure 3-6). The field of view of the SISEX is rather narrow (2.8 degrees), and so a cross-track scanning mirror is provided to enlarge the coverage. An along-track scan mirror is also provided to allow two degrees of freedom in off-nadir pointing.

The primary disadvantages of this instrument are its large size and weight.

The primary advantages of this instrument are its high sensitivity and capability for simultaneous spectral data acquisition.

HIRIS--High-resolution Infrared Imaging Spectrometer: The HIRIS is being designed by JPL to be flown on the Eos (one of the planned Earth observation system satellites) and is intended as a follow-on device to the AIS and the SISEX. Shuttle delays have led to the cancellation of the SISEX and development will proceed directly to the HIRIS.

Its design closely follows that of the SISEX. The HIRIS is to be flown on the NASA Eos satellite planned for launch in 1996. It is to have an instantaneous field-of-view (IFOV) of 30 m and a swath width of 30 km. The spectral coverage is to be 0.4 to $2.5\text{ }\mu\text{m}$ with a spectral resolution of 1% or better.

3.3.2 Narrow spectral range sensors

The following instruments cover less than a single octave in the spectral domain, thereby avoiding the compromises attendant with acquiring broad coverage:

AIS--Airborne Imaging Spectrometer: This sensor built by JPL is intended to measure the reflectance of terrestrial surface materials at a spectral resolution high enough to distinguish a variety of clay minerals and salts between 1.2 and $2.4\text{ }\mu\text{m}$.

The design employs a 32×32 IR array that is stepped four times to acquire 128

spectral channels. The optical train, shown schematically in Figure 3-7, has the potential for scattered light leaks, which are difficult to correct due to the intricate folded design. This problem is borne out by empirical tests of the data and has hindered efforts to correct the data for atmospheric transmission. Tests for scattered light, as well as throughput, instrumental spectral response and other tests, have not yet been performed. One feature of this instrument is the separation of the detector focal plane assembly and the instrument, allowing separate testing of the detector and the spectrometer with a high degree of confidence in predicting integrated performance. This concept is also found in the AVIRIS.

The primary disadvantages of this instrument are poor-quality area array detectors, and spectral contamination due to grating-order overlap, which was resolved through the addition of order-separating filters. The photometric accuracy of the instrument is as yet unknown but is probably poor due to uncompensated scattered light, nonrepeatable positioning of the grating after scanning, and inadequate testing and inflight calibration.

The primary advantage of this instrument is that it is a compact hyperspectral sensor which has produced considerable data of quality sufficient to identify the positions of narrow absorption bands. AIS has also demonstrated that hyperspectral data of some utility can be obtained from an airborne platform with existing technology.

TIMS--Thermal Infrared Multispectral Scanner: This instrument was built by Daedalus to acquire broadband spectra in the 8 to 14 μm region.

This grating spectrometer design utilizes an off-axis paraboloid and transmission camera optics. The instrument uses a linear HgCdTe array and thus requires a second axis of scan to build the image. While the spectrometer is of 1% resolution, a custom-built HgCdTe continuous linear array with six detectors of variable length is used to define broad bandpasses. Constraints on image quality are therefore relaxed. Daedalus found changes in the dimension of the transmission lens (with cooling) to be a source of difficulty in early calibration, but this was eventually corrected with iterative testing and adjustment. This instrument (Figure 3-8) has produced much data for technique demonstration and scientific analysis.

The primary disadvantage of this instrument is the noise problem associated with operating the sensor in the electrically noisy aircraft environment.

The primary advantages of this instrument are its capability for simultaneous acquisition of spectral data and its flight-proven status.

3.3.3 Scanners

Scanners have long been used for acquisition of multispectral data in wavelength regions where detector technology is limited to single-element detectors. While scanners are inherently less efficient than instruments utilizing arrays, there is considerably more experience in their design and operation. In its most basic implementation, a scanner is neither an imaging spectrometer nor a multispectral imager because it senses only a single point of the image cube at a time.

GEOSCAN Scanner: This instrument was built by the GEOSCAN company for obtaining

data in the visible, near infrared (IR) and mid IR.

The design employs three detectors--one silicon, one InSb, and one HgCdTe--to acquire 24 bands of data in the visible, near IR and mid IR, using circular variable filters. The sensor is primarily application-oriented and provides onboard processing. A degree of calibration is done in real time.

The primary disadvantage of this instrument is its limited spectral coverage.

The primary advantages of this instrument are that: (a) GEOSCAN thermal data have ten times the signal-to-noise ratio of the TIMS, despite the line array used in the latter; and (b) this instrument, or one like it, is suited to applications where the spectral data to be acquired is well known and can be limited to a few tens of bands.

3.3.4 Multispectral imagers

The last two sensors to be discussed here are multispectral imagers of radically different concepts. Neither of these sensor concepts has been thoroughly tested at this time.

ATOF--Acoustically Tuned Optical Filter: This is a concept for an infrared multispectral imager that would utilize an electronically tunable filter placed over a two-dimensional infrared array detector. This concept has been successfully applied to the visible portion of the spectrum using charge-coupled devices (CCDs) as detectors. This filter technology allows random access to the entire 1 to 5 μm band at variable resolutions, with bandpass changes accomplished in fractions of a millisecond. A sensor of this type would build a complete image cube one plane at a time.

The primary advantages of this instrument are that: (a) it is useful in situations where variable resolution is desired or incomplete spectral coverage is possible; and (b) the entire detector array is constantly accumulating useful data.

The primary disadvantages of this instrument are that: (a) spectral data are not acquired simultaneously, giving rise to problems with calibration if atmospheric changes occur more rapidly than spectral acquisition; and (b) image plane registration may be required, although if platform motion is well known or motion compensation is employed, this problem can be reduced.

HIMS--Hubble Imaging Michelson Interferometer Spectrometer: This instrument is intended for the Hubble Space Telescope and is intended to acquire 1% and 0.1% spectral resolution data from 1 to 2.5 μm using a two-dimensional HgCdTe array.

The interferometer design acquires a three-dimensional data set which has two spatial axes and one axis which is the Fourier transform of the spectral information at each spatial element. Spatial information is acquired by the detector and the scanning is performed along the interferogram axis.

The primary disadvantage of this instrument is that for downward-looking applications, this instrument has very little applicability because the entire image cube must be obtained before inversion into spectral space is possible.

Thus, the data are acquired nonsimultaneously, and no random or noncontinuous access to wavelengths is possible.

The primary advantage of this instrument is its variable resolution.

3.4 References

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- Vane, G., M. Chrisp, H. Enmark, S. Macenka, and J. Solomon (1984), Visible/Infrared Imaging Spectrometer (AVIRIS): An advanced tool for earth remote sensing, *Proceedings of the 1984 International Geoscience and Remote Sensing Symposium*, Strasbourg, 27-30 August, 751-757.
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TABLE 3-1
HYPERSPECTRAL SENSORS REVIEWED

- **AIS** **Airborne Imaging Spectrometer**
- **TIMS** **Thermal Infrared Multispectral Scanner**
- **NIMS** **Near Infrared Mapping Spectrometer**
- **AVIRIS** **Advanced Visible and Infrared Imaging Spectrometer**
- **SISEX** **Shuttle Imaging Spectrometer Experiment**
- **HIRIS** **High-resolution Infrared Imaging Spectrometer**
- **VIMS** **Visible and Infrared Mapping Spectrometer**
- **MRS** **Mapping Reflectance Spectrometer**
- **GEOSCAN**
- **HIMS** **Hubble Imaging Michelson Interferometer Spectrometer for Hubble Space Telescope**
- **ATOF** **Acoustically Tuned Optical Filter-based Multispectral Imager**

TABLE 3-2a

SUMMARY CHARACTERISTICS OF IMAGING SPECTROMETERS

<u>SENSOR</u>	<u>BUILDER</u>	<u>CUBE DIMENSIONS</u>	<u>WAVELENGTH RANGE</u>	<u>STATUS</u>
AIS	JPL	32 x n x 128	1.2-2.4	operational
TIMS	Daedalus	638 x n x 6	8.2-12.2	operational
NIMS	JPL	20 x n x 204	0.7-5.2	awaiting launch
AVIRIS	JPL	550 x n x 220	0.4-2.4	under testing
SISEX	JPL	256 x n x 256	0.4-2.5	cancelled
HIRIS	JPL	1000 x n x ~200	0.4-2.5	in design
VIMS	JPL	70 x n x 320	0.3-4.3	design/construction
MRS	UH/MIT	70 x n x 280	0.25-4.0	under testing
GEOSCAN	GEOSCAN	~500 x n x 24	VISNIR-TIR	operational
Daedalus	Daedalus	various	VISNIR-TIR	operational
HIMS	UH/JPL	61 x 61 x ~200	0.5-2.5	under development
ATOF	TBD	TBD	0.25-5.0	concept

TABLE 3-2b

DETAILED CHARACTERISTICS OF IMAGING SPECTROMETERS

	A	B	C	D	E	F
3	PARAMETERS	NIMS	AIS	TIMS	AVIRIS	SISEX
5	SYSTEM					
6	Sensor type	Imaging spectrometer	Imaging spectrometer	Imaging spectrometer	Imaging spectrometer	Imaging spectrometer
7	Spectral range	0.7-5.2 μm	1.2-2.4 μm	8.2-12.2 μm	0.4-2.5 μm	0.4-2.5 μm
8	Resolution	0.6%	0.5%	5-10%	1.0%	1.0%
9	No. of spectral channels	204	128	36	224	128
10	Angular resolution (IFOV)	30.5-0.5 mrad	1.9 mrad	2.5 mrad	1 mrad	10 mrad
11	No. of spatial channels	20 x n	32 x n	638 x n	550 x n	400 x n
12						
13	Platform	Spacecraft	Airborne	Airborne	Airborne	Spacecraft
14	Cooling scheme	Passive	LN2	LN2	LN2	TBD
15	Mass	18 kg				
16	Volume					
17	Power	12 W				
18	Data rate	11.52 kbs	394 kbs	40-50 kbs	19 mbs	50 mbs
19	Data precision	10 bits			11 bits	
20	Etendue	1.1 E-4 $\text{cm}^2 \text{sr}$				
21						
22	SUBSYSTEMS					
23	Foreoptics					
24	Type	Ritchey-Chretien	Schwartzchild		Kennedy scanner	Schmidt
25	Aperture	23 cm	2.4 cm	19 cm	12 cm	11 cm
26	Focal length	380 mm	170 mm	33 cm	14.4 cm	41.6 cm
27	Focal ratio	f/3.3	f/3.5	f/3	f/1.9	f/3.8
28						
29	Spectrometer					
30	Dispersion technique	Grating, dual-blazed	Grating	Grating	Grating	Prism
31	Input focal ratio	f/3.5		f/1.9	f/0.44	
32	Provision for additional scan	2 axis internal	1 axis internal	2 axis internal	1 axis	2 axis
33	Spectral responsivity					
34	Size of resolution element	0.2 mm		0.38 mm	0.2 mm x 0.2 mm	
35						
36	Detector					
37	Focal plane assembly					
38	Material	2 Si, 12 InSb	HgCdTe	HgCdTe	1-32 Si/3-64 InSb	64x404, Si 64x404 HgCdTe
39	Array dimensions	1 x 17	32 x 32	1 x 6		TBD
40	Cell dimensions	0.2 mm	0.05 mm	0.43 mm		0.05 mm
41	QE	~80%	50%	50%	80% cMax	50%
42	Temperature requirements	InSb-80K	77K		InSb80K, Si150K	120K
43	Low background effectiveness	Yes				
44	Power dissipation	5 MW				
45						
46	Electronics					
47	Mass					
48	Power					
49	Detector system NEP	10E4 Watts		NE T 6.1°C		
50	Precision	10 bits		8 bits	11 bits	
51						
52	Data Acquisition and Control					
53	Control system	RCA 1802				
54	Data storage	Platform				
55	Type					
56	Data volume					
57						
58	Onboard Processing					
59	Corrections					
60	Dark	Chopped				
61	Sensitivity					
62	Radiometric					
63	Atmospheric					

[illegible]

FIGURE 3-1

MAJOR SUBSYSTEMS OF IMAGING SPECTROMETERS

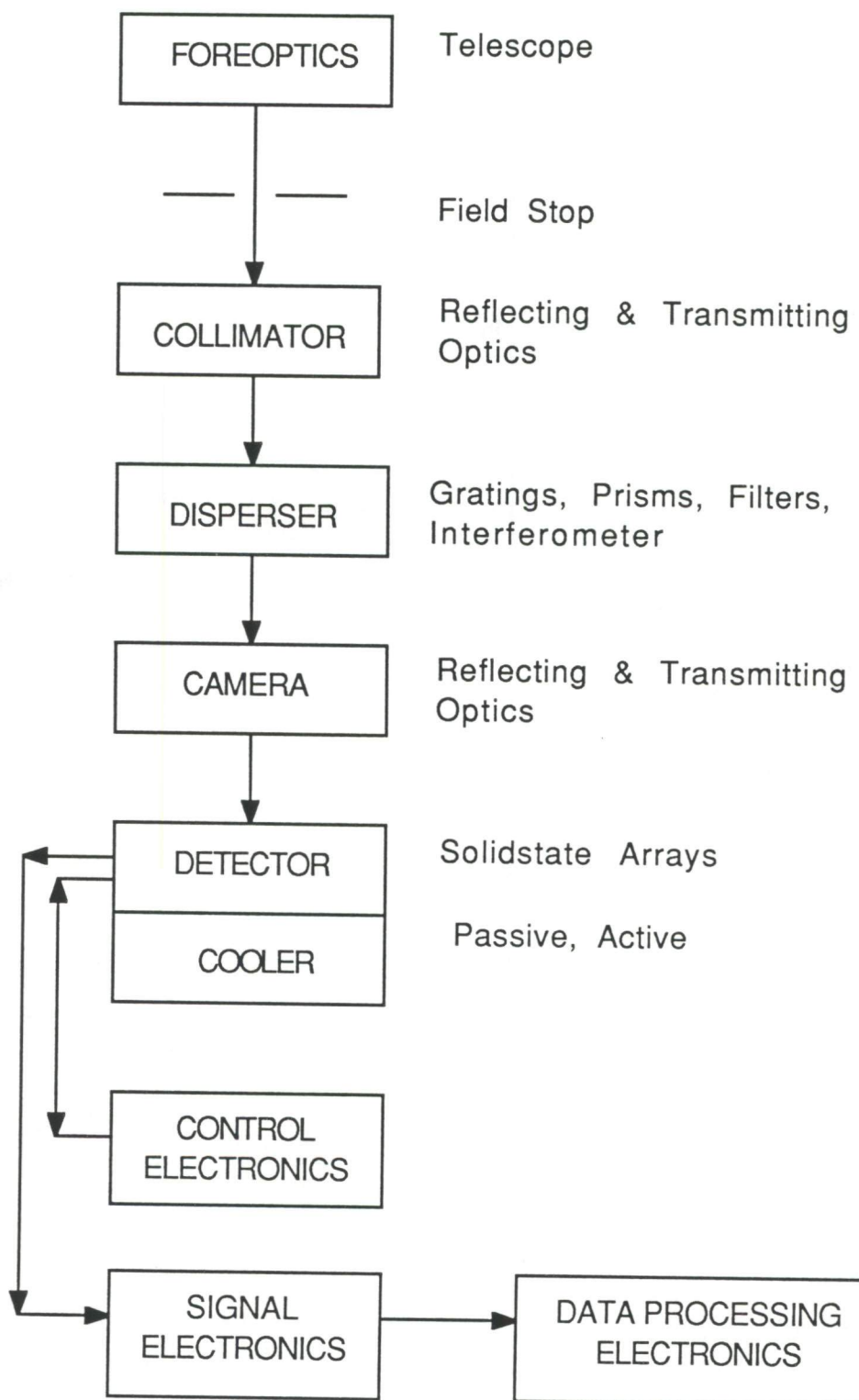


FIGURE 3-2

MRS OPTICAL LAYOUT

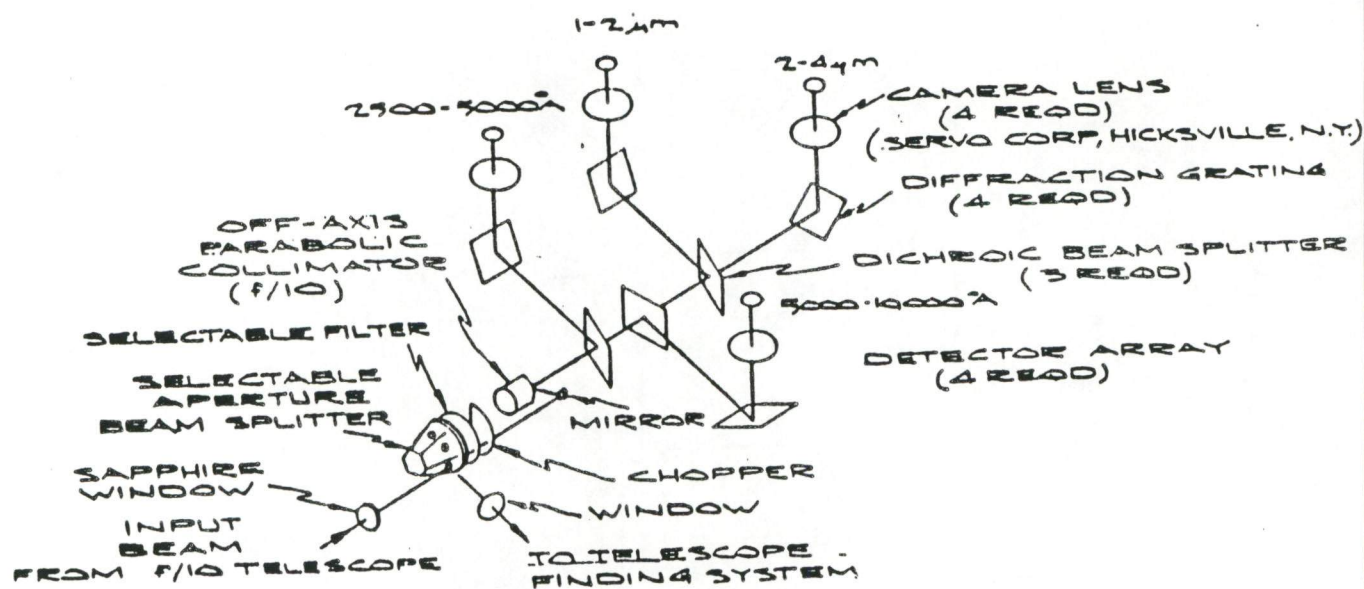


FIGURE 3-3
NIMS OPTICAL LAYOUT

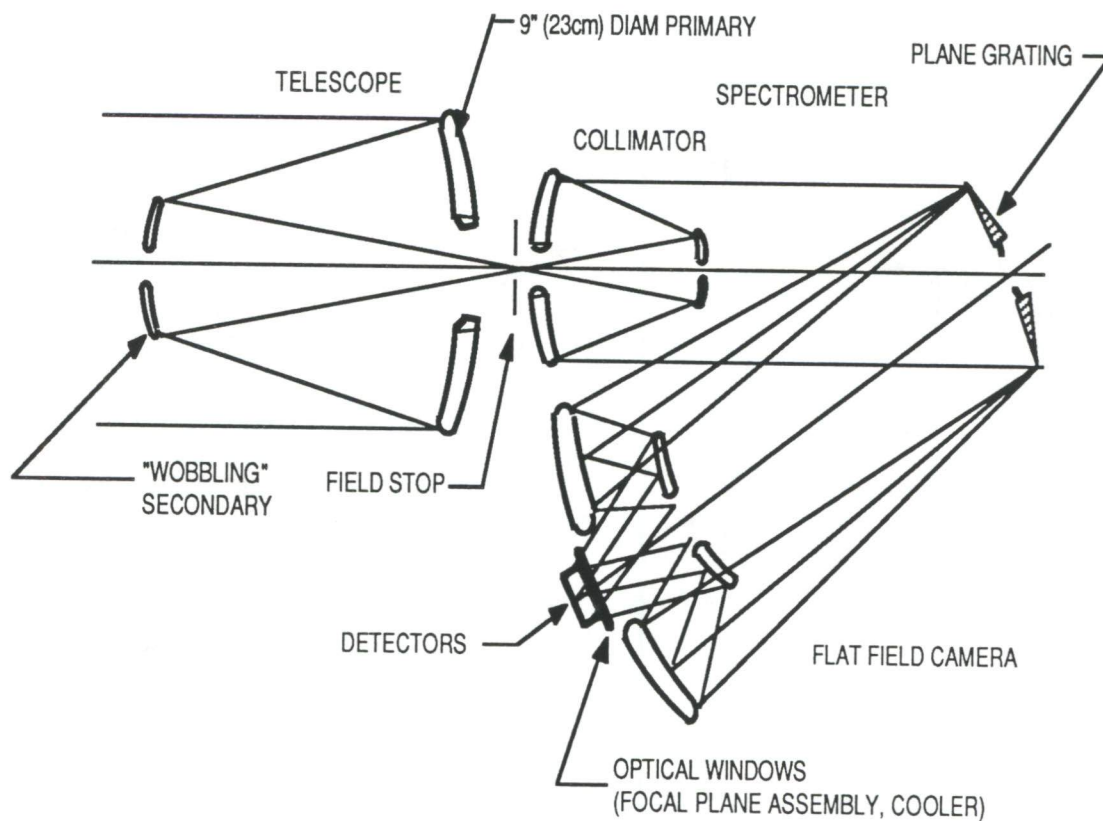


FIGURE 3-4
VIMS OPTICAL LAYOUT

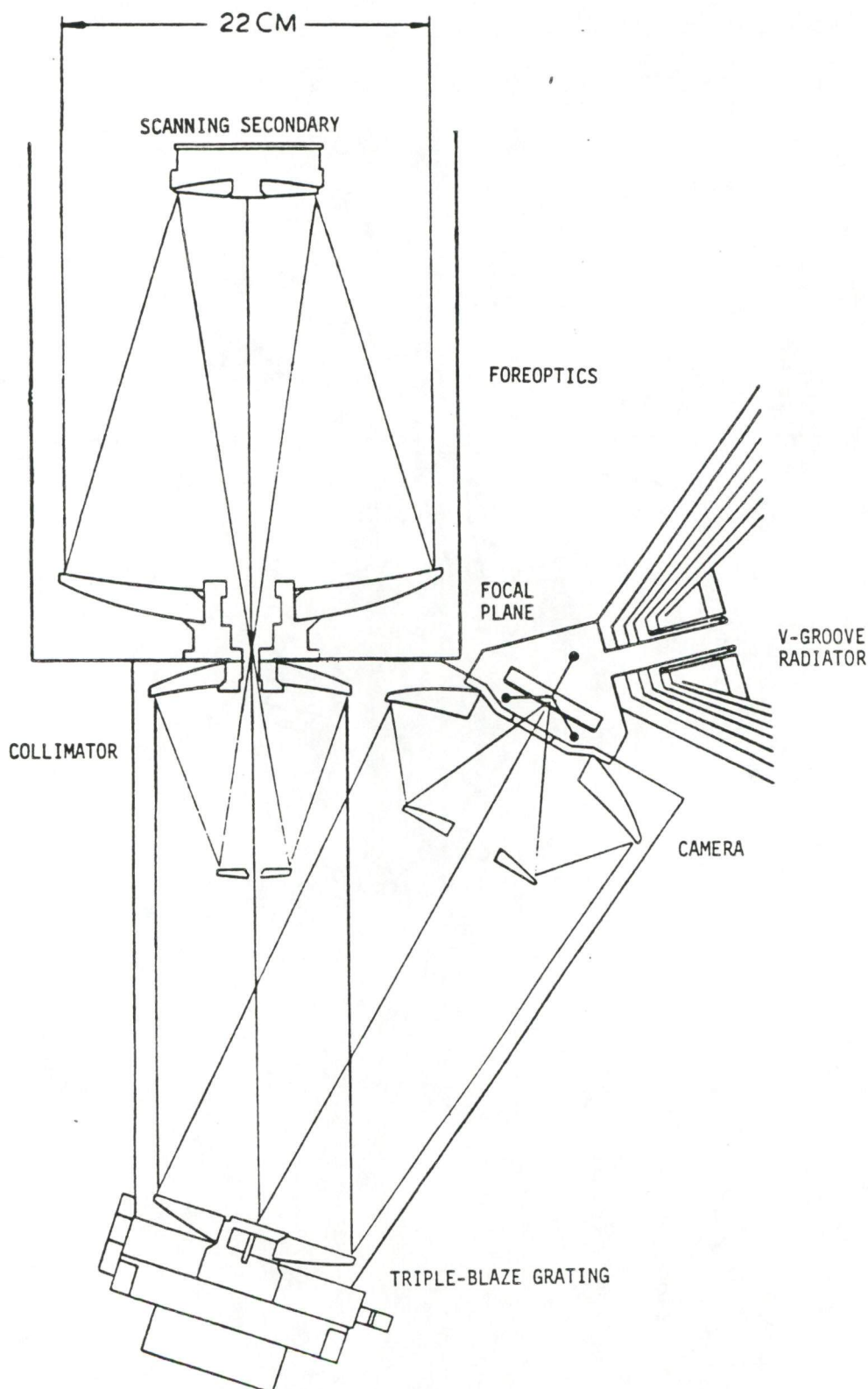


FIGURE 3-5
AVIRIS OPTICAL LAYOUT

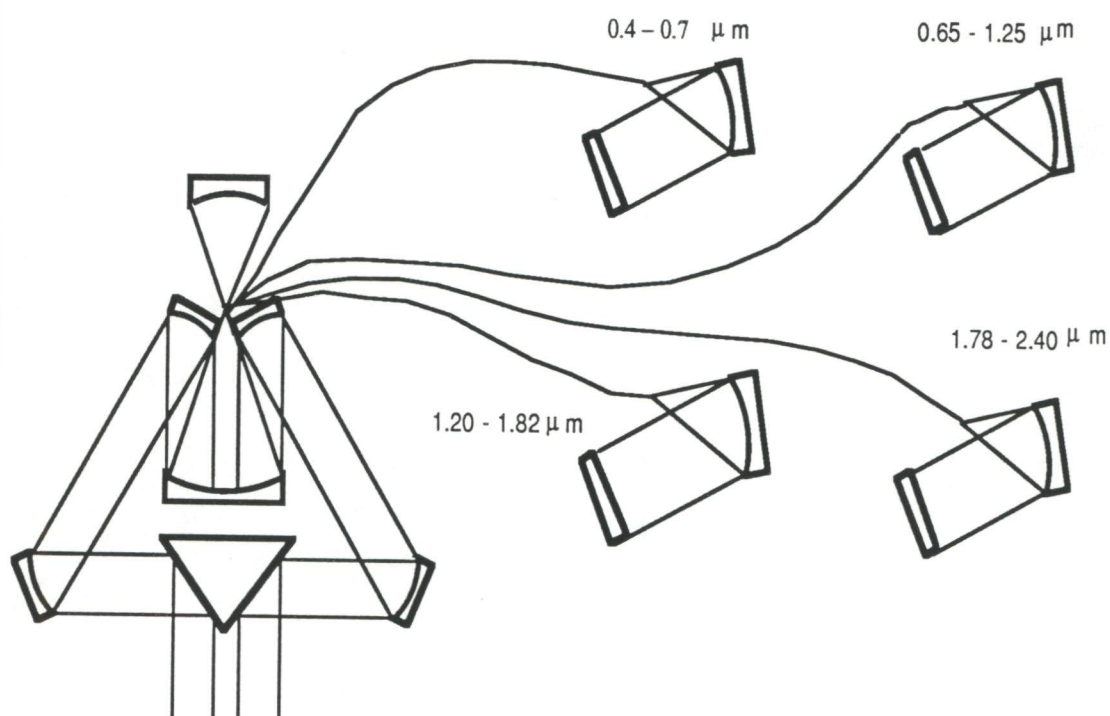


FIGURE 3-6
SISEX OPTICAL LAYOUT

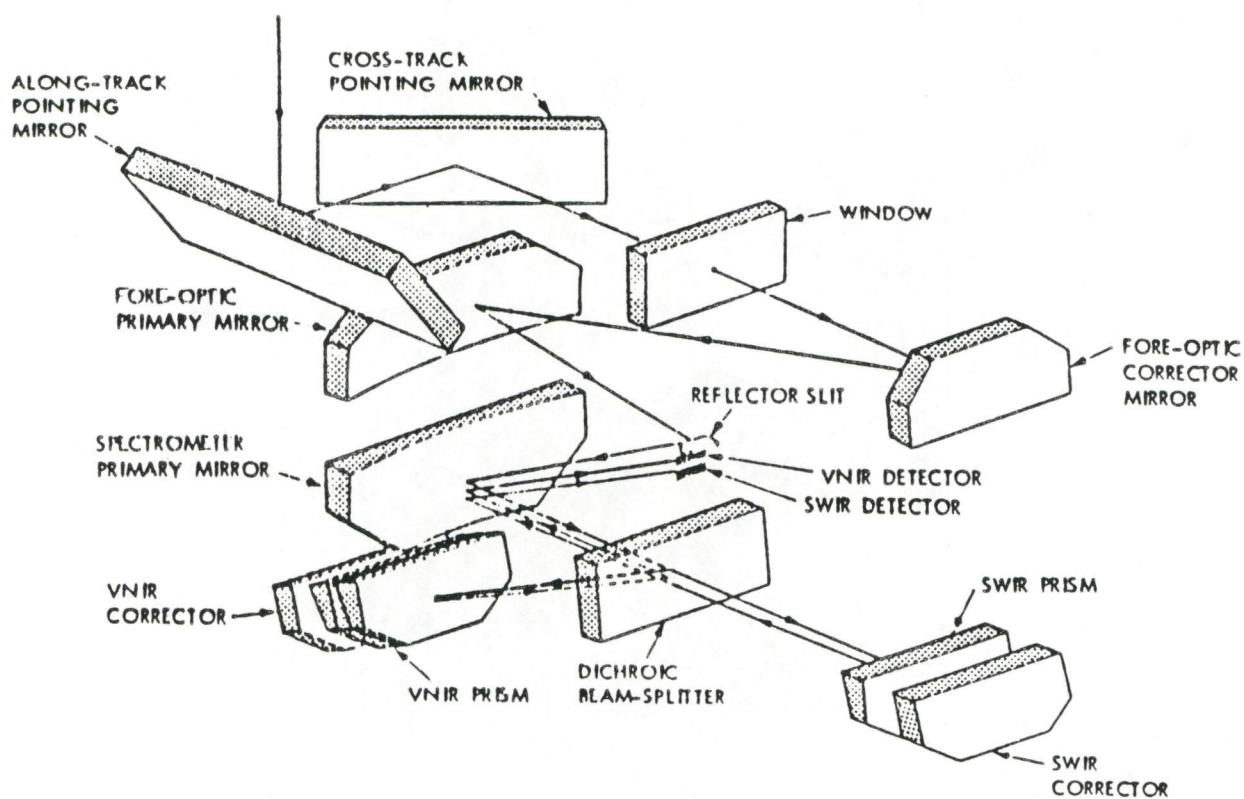


FIGURE 3-7
AIS OPTICAL LAYOUT

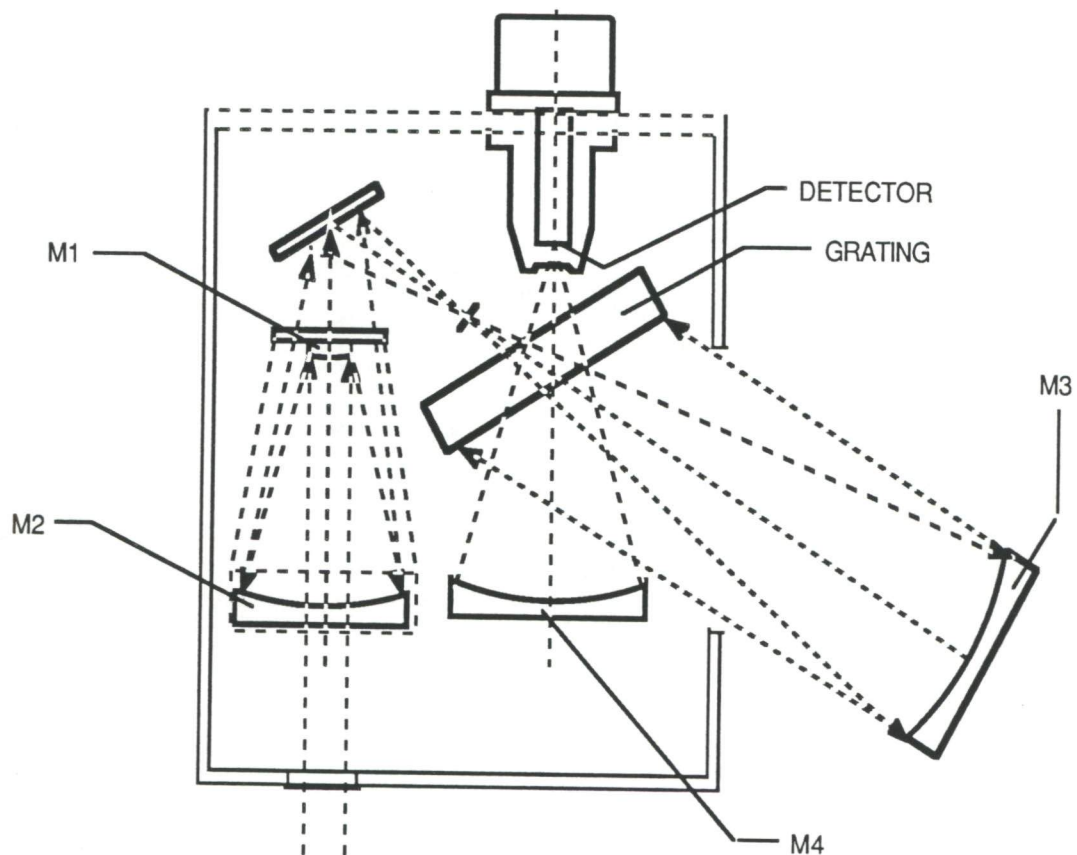
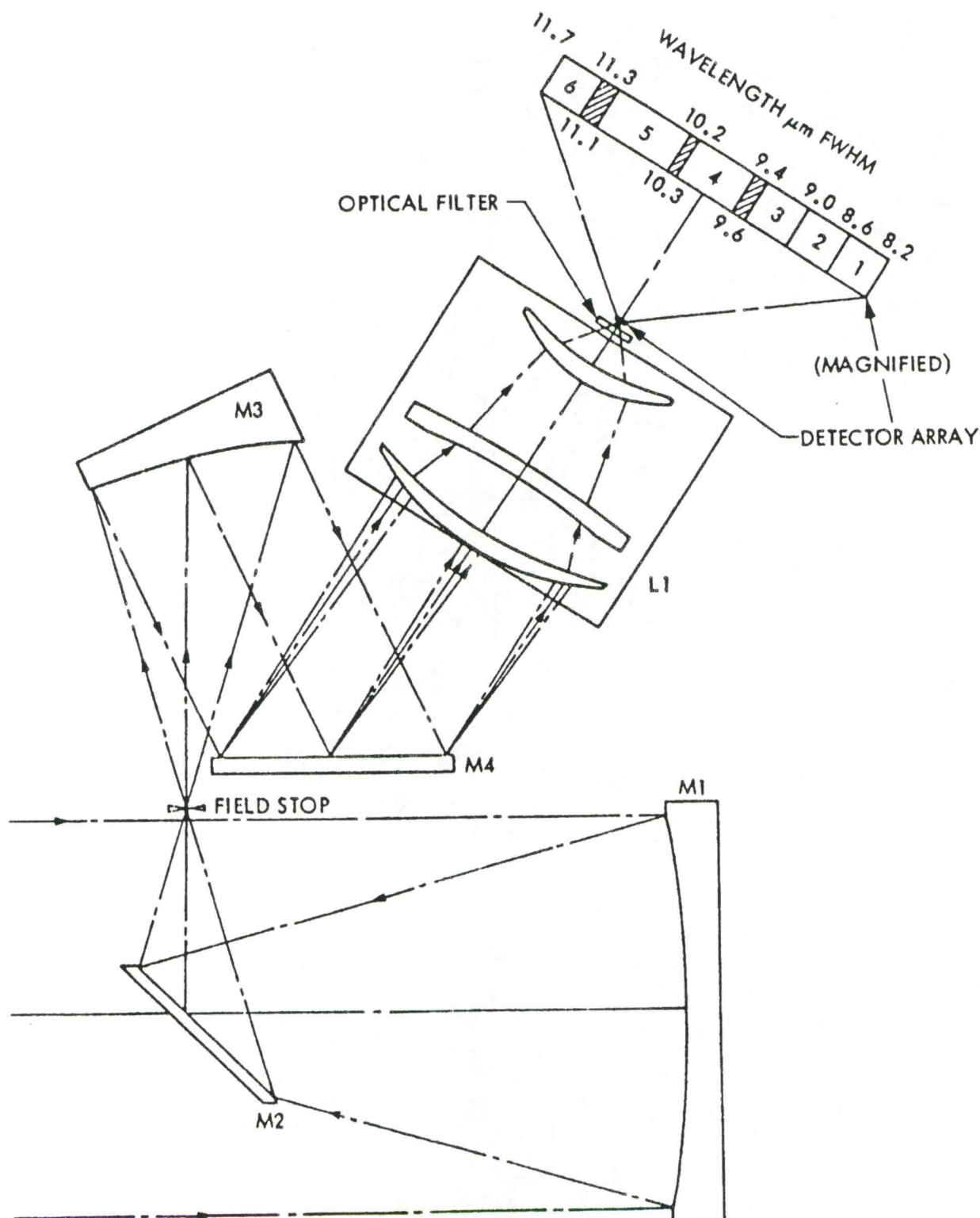


FIGURE 3-8
TIMS OPTICAL LAYOUT



4. Laboratory and Field Spectrometers

4.1 Summary and Conclusions

A wide variety of spectrophotometers has been used for measuring the spectral reflectance properties of materials in the laboratory and in the field. These instruments are either commercially available laboratory or field instruments, or specially designed instruments which have been built to address a specific scientific or technological issue. Our survey of commercially available laboratory and field spectrophotometers has concentrated on those instruments that cover the spectral range of 0.2 to 14 μm at a moderate spectral resolution ($R \approx 100$).

We make the following general conclusions:

1. Most commercially available laboratory spectrophotometers make use of the Fourier transform (FT) technique, which increases the spectral range and resolution beyond what prism techniques can deliver, and removes the problems associated with overlapping orders sometimes experienced when using gratings. FT instruments also offer greater "throughput" and signal-to-noise performance.
2. Most modern, commercially available spectrophotometric instruments are designed for transmission spectroscopy, but they can easily be converted for spectral reflectance measurement, although the "photometric geometry" may not be optimum for some purposes.
3. Special-purpose spectrophotometers designed for specific scientific or technological needs are generally modeled after or reconfigured from commercially available instruments. Some instruments, such as circular variable filter wheel instruments, are barely adequate for the requirements of hyperspectral imaging applications since their spectral resolution is no greater than 1% at best.
4. Hyperspectral field instruments in the 3 to 14 μm spectral region have not been commercially available until very recently. These new instruments make use of a variety of dispersing and data sampling techniques. The versatility of the dual-beam technique makes it superior for many applications. The application of Fourier transform techniques to the field instrumentation makes for small, lightweight instruments.

4.2 Laboratory Instrumentation

Laboratory spectral reflectance instruments have used a variety of optical dispersing techniques: prisms, gratings, circular variable filters, interferometric techniques, and other more exotic, but sometimes extremely useful, methods. Filter techniques give the lowest spectral resolution. Prism and grating techniques give much better spectral resolution but are generally limited in spectral range by certain factors, for example, the wavelength dependence of the dispersing power of the prism, or the overlapping order of the grating. Interferometric techniques, in particular the Fourier transform (FT) technique, offer by far the best combination of spectral range, spectral resolution, and "throughput" (which controls the total amount of time necessary to obtain a given signal-to-noise ratio over the entire spectral range).

Most modern commercial laboratory spectroscopic instruments are designed for spectral transmission work since absorbance measurements are critical for qualitative as well as quantitative analysis of organic and inorganic molecules (work which provides the largest market for this instrumentation). The spectral reflectance properties of various materials can be measured only if specialized accessories are adapted to the spectrometer, or the commercial instrument is suitably modified, or a customized instrument is designed and built. These attachments are either bidirectional (a collimated incidence beam and a collimated emission beam) or diffuse (the incident beam is not collimated and the emission beam is formed from integrating light scattered in all directions from the sample), or some combination of these two methods (e.g., hemispherical reflectance). In any case, the most generalized but not necessarily the most physical measurement is the normal reflectance, R_n , which is defined as the reflectance relative to a Lambertian reflector measured when the angle of the incident light and the angle at which the surface is observed are both normal to the surface (i.e., zero degrees).

The spectral reflectance properties of a given material depend upon the physical state of the material. For this reason, it is somewhat difficult to relate quantitatively the value of spectral absorption coefficients with the value of the spectral reflectance, even though photometric theories (Hapke 1983) would have us believe that such things are possible. The strength and apparent position of some absorption bands seen in reflected light can depend to varying degrees upon the particle size and the photometric geometry (incidence and emission angles). Even the temperature of the sample can influence the presence and position of some spectral features (e.g., the case of sulfur where the 0.5 μm absorption edge is very temperature-sensitive and changes at the rate of two Angstroms/ $^{\circ}\text{K}$ toward longer wavelengths as the temperature of the sulfur increases).

The effects that photometric geometry has on the spectral reflectance properties of materials are well documented (e.g., Grady and Veverka 1983). These effects are caused by the variation of the average photon path through a substance as the incidence and emission angles are changed. Essentially, these changes occur in the absorption probability for a photon as the average path length is increased or decreased. For this reason, it may be difficult to compare at the few percent level (sometimes more) the reflectances obtained for the same material measured by different techniques. For example, absorption bands tend to become deeper as the incidence angle and the emission angle are increased. Because the method of diffuse spectral reflectance measures light integrated over all scattering angles, the depths, widths, and apparent positions of absorption bands will be slightly different from those obtained when the reflectance is measured by the bidirectional technique, which can better approximate the geometry defined for the normal reflectance.

FT-IR spectrometers differ among themselves mostly in the optical configuration and spectral processing facility. Below we describe two units that demonstrate this difference:

Mattson Sirius 100:

Spectral range: 0.2 to 500 μm

Requires various detectors for use of the whole spectral range.

Spectral resolution: 0.125 cm^{-1}

Optics: Corner cube interferometer with KBr/Ge beamsplitter

Computer: All software included with manufacturer-supplied computer.
Most peripherals (plotter, hard disk, etc.) are optional.

Cost: \$46,000 to \$70,000 depending upon system configuration and accessories.

Nicolet 5DXB:

Spectral range: 2.5 to 50 μm

Use of the whole spectral range requires various detectors.

Spectral resolution: 2 to 0.5 cm^{-1}

Optics: Continuous-scan Michelson interferometer with KBr or CsI beamsplitter

Computer: All software included with manufacturer-supplied computer.
Some peripherals are included, most others are optional.

Cost: \$30,000 to \$70,000 depending upon system configuration and accessories.

A variety of special-purpose instruments is available in scientific laboratories around the country, in particular at NASA field centers and several universities. Most of these devices have limited spectral ranges and a wide range of spectral resolution. These devices are not commercially available although they can, in general, be made available for outside research interests. Some examples of institutions with such special-purpose instruments are: Planetary Geosciences Division, University of Hawaii; Cornell University; NASA Johnson Space Flight Center; and Brown University.

Table 4-1 is a list of manufacturers of laboratory FT-IR spectrometers considered in this study.

4.3 Field Instruments

4.3.1 Portable spectrometers 0.4 to 14 μm

Spectrometers can be useful analytical instruments for measurement of materials in the field. The spectral range and resolution of field spectrometers are governed by two factors: (1) the detector, which governs in part the spectral range, and (2) the spectral filtering system, which governs the spectral resolution. The utility of the field instrument is controlled by a number of factors which, depending upon the application, can make some instruments more suitable than others.

The spectral range of most instruments is governed by the spectral sensitivity of the detector. Silicon (Si), which is very easily made into linear arrays, covers the range from 0.3 to 1.05 μm . The infrared spectral region, from 0.7 to 4.5 μm , can be covered by detectors made of lead sulfide (PbS) or indium antimonide (InSb). Wavelength coverage from about 2 to 15 μm requires detectors such as mercury cadmium telluride (HgCdTe) or "mer-cad-telluride".

The spectral resolution is governed primarily by the optical dispersing or filtering system. Circular variable filters (CVF) provide moderate resolution ($R \approx 100$) with relative ease, although care must be taken to "block" the filter outside the desired spectral range. A broadband detector can become contaminated from "leakage" outside the spectral bandpass. Interferometers provide better spectral resolution and better throughput when combined with Fourier transform techniques for reconstructing the spectrum. The advent of small, fast portable computers makes the FT instruments more desirable.

Portable field instruments can be divided into two classes of optical configurations: (1) single beam and (2) double beam. The single-beam instrument looks at one spot at a time as its name suggests. The radiant flux from the sample is measured first and then the "sampling spot" is moved to a reference spot so that a reference spectrum can be obtained. The single-beam instrument requires that the photometric conditions of the sampling session remain constant so that the sample can be compared quantitatively with the reference. The double-beam instrument uses two optical beams to alternately

measure the sample and the reference areas at a frequency near 10 Hertz. This near-simultaneous measurement of the sample and the reference dispenses with the need for constant photometric conditions but requires that the standard and reference spots be within a few degrees of each other in the field of view of the spectrometer.

Summary descriptions of field spectrometers covering the spectral ranges of 0.3 to 3.0 μm and 3.0 to 14 μm that were reviewed in this study are given in Tables 4-2 and 4-3, respectively. More detailed instrument descriptions are given in Tables 4-4 to 4-8.

TABLE 4-1

MANUFACTURERS OF LABORATORY FT-IR SPECTROMETERS

<u>Manufacturer</u>	<u>Instrument</u>	<u>Description</u>
Analect		Fourier transform
Beckman	FT-1000 FT-2000	Fourier transform
Digilab	Qualimatic FTS 50 FTS 10/11 FTS 14/15/20 FTS 60 FTS 80	Fourier transform
IBM	IBM 32 IBM 85 IBM 98	No longer available (1/87) No longer available (1/87) No longer available (1/87)
Joel	JIR 100	Fourier transform
Mattson	Sirius 100 Nova Cygni Cygnus 100 Polaris	Fourier transform Corner cube interferometer
Nicolet	5_X series 10_X series 20_X series 60SX 5DXB 20DXB	Fourier transform Michelson interferometer
Perkin-Elmer	1500 1700 1800	Fourier transform

TABLE 4-2
DESCRIPTION OF FIELD SPECTROMETERS
0.3 to 3.0 μm

Instrument	Spectral Range (μm)	Spectral Resolution	Type	Sampling Speed	FOV
Daedalus AA440*	0.3-2.5	CVF 1-2%	single beam	3 sec.	1.5 deg
GER IRIS #1†	0.4-3.0	Gratings 2-4 nm	dual beam	30 sec.	< 6 deg
GER IRIS #2†	0.4-3.0	Interferometer	dual beam	3 sec.	< 6 deg
NASA/JSC FSS Field spectrometer system	0.4-2.4	CVF 2-3%	single beam	?	?
NASA/JSC FSAS Field signature acquisition system	0.4-2.4	CVF 1-2%	single beam	?	?
Exotech 20C Purdue University	0.4-2.3 0.1%	Gratings	single beam	?	?
NASA/JPL PIDAS~	0.4-2.5	Gratings 0.88 nm-4.8 nm	single beam	3 sec.	1-15 deg 6 deg nominal

* Daedulus Enterprises, Inc., Box 1869, Ann Arbor, MI 48106.

† Geophysical and Environmental Research, Inc., GPO Box 340, NY, NY 10001.

~ Commercial model could potentially be built by Infrared Associates of Boulder, CO (303-444-2009).
 Delivery time is estimated to be 18 months.

TABLE 4-3
DESCRIPTION OF FIELD SPECTROMETERS
3 to 14 μm

Instrument	Spectral Range (μm)	Spectral Resolution	Type	Sampling Speed	FOV
JPL/ PFES Portable field emission spectrometer	2.4-14.5	CVF 1.4%	single beam	60 sec.	1.5 deg
GER IRIS #3	2.5-14.5	2cm^{-1}	dual beam	3 sec.	< 6 deg
NASA/JSC FSS Field spectrometer system	8.0-14.0	Filters $0.5\ \mu\text{m}$	single beam	?	?
Daedalus Under development	3-14.5	CVF	single beam	?	?

TABLE 4-4

**DESCRIPTION OF FIELD SPECTROMETERS:
Daedalus AA440**

FIELD SPECTROMETER: Daedalus AA440

Daedalus Enterprises, Inc.
Box 1869
Ann Arbor, MI 48106

Size:	8.5 x 6.5 x 5 in (photometer head) 12 x 15 x 35 in (backpack)
Weight:	5.5 lbs (photometer head) 45 lbs (backpack)
Spectral Range:	0.4 - 0.8 μm @ 2% Circular Variable Filter 0.8 - 1.3 μm @ 3% Circular Variable Filter 1.3 - 2.5 μm @ 1% Circular Variable Filter
Detector:	Si and PbS
Electronics:	IBM computer-controlled
Dynamic range:	10 bits
Signal/Noise:	?
Acquisition time:	3 seconds
Battery life:	8 hours
Cost:	\$32,500

TABLE 4-5

**DESCRIPTION OF FIELD SPECTROMETERS:
GER #1**

FIELD SPECTROMETER: GER #1

Geophysical and Environmental Research
GPO Box 340
New York, NY 10001

Size:	?
Weight:	10 lbs (photometer head) 15 lbs (electronics) 10 lbs (batteries)
Spectral Range:	0.35 - 3.0 μm @ 2nm (best) Gratings
Detector:	Si and PbS
Electronics:	IBM computer-controlled
Dynamic range:	16 bits
Signal/Noise:	?
Acquisition time:	30 seconds (or more depending upon application)
Battery life:	6 hours
Cost:	\$70,000

Note: GER #2 is a "belt model" under design which will use interferometric techniques

TABLE 4-6

**DESCRIPTION OF FIELD SPECTROMETERS:
PIDAS**

FIELD SPECTROMETER: NASA/JPL PIDAS (Portable Instant Display and Analysis Spectrometer)

Jet Propulsion Laboratory
Pasadena, CA 91009

Size:	small optical head (camera size) large backpack with display "paddle"
Weight:	1 lb (photometer head) 65 lbs (backpack)
Spectral Range:	0.4 - 0.9 μm @ 0.88 nm Grating 0.9 - 2.5 μm @ 4.8 nm Grating
Detector:	Si (512 Reticon array) and PbS (45-element array); cooled
Electronics:	IBM computer-controlled
Dynamic range:	10 bits
Signal/Noise:	variable from 300 to 50
Acquisition time:	2 seconds
Battery life:	2.5 hours
Cost:	\$300,000 - 500,000

TABLE 4-7

DESCRIPTION OF FIELD SPECTROMETER: Portable Field Emission Spectrometer

FIELD SPECTROMETER: NASA/JPL Portable Field Emission Spectrometer

Jet Propulsion Lab
Pasadena, CA 91009

Size:	?
Weight:	80 lbs total
Spectral Range:	2.35-4.5 μm @ 1.4% CVF 4.4 -8.0 μm @ 1.4% CVF 8.0-14.5 μm @ 1.8% CVF
Detector:	InSb and HgCdTe; cooled
Electronics:	Computer-controlled
Dynamic range:	10 bits
Signal/Noise:	?
Acquisition time:	?
Battery life:	6 hours
Cost:	N/A

TABLE 4-8

**DESCRIPTION OF FIELD SPECTROMETERS:
GER #3**

FIELD SPECTROMETER: GER #3

Geophysical and Environmental Research
GPO Box 340
New York, NY 10001

Size:	?
Weight:	60 lbs total
Spectral Range:	2.5 - 14.5 @ 2cm^{-1} Interferometer
Detector:	InSb and HgCdTe; cooled
Electronics:	Computer-controlled
Dynamic range:	16 bits automatic gain control
Signal/Noise:	1000
Acquisition time:	2 - 5 seconds
Battery life:	3 hours
Cost:	\$85,000

5. Spectral Databases 0.2 to 12 μm

5.1 Summary and Conclusions

Libraries on the spectral reflectance properties of various materials are useful for the identification of spectrally active materials in remote sensing data. In general, the spectral reflectance properties in the scene are compared with the spectral properties of the materials in the library (or database) until a unique match is found. (Various comparison approaches are discussed in Chapter 7.)

Our survey of the available spectral reflectance databases has led us to the following conclusions:

1. In general, spectral reflectance databases are not comprehensive since each database has been developed to address a particular scientific or commercial need.
2. There is much diversity in the spectral range and resolution of the available spectral reflectance databases. In fact, much of the available data are in the form of low spectral resolution or broadband observations, and are not applicable to the problem of hyperspectral imaging wherein hundreds of spectral channels are present.
3. Much of the available high spectral resolution, wide spectral range reflectance data exists in the form of publications in the literature or in-house files of commercial concerns. For example, much of the spectral reflectance work on clay minerals remains as separate articles in journal publications and much of the spectral reflectance data on paints and coatings is either proprietary (and sometimes classified) information or available only on a case-by-case basis.
4. The most extensive spectral libraries are for transmission spectra and are available commercially. There is some hope that the application of theories of spectrophotometric scattering can be used to describe, in an adequate manner, the spectral reflectance properties of these materials using the transmission spectra.

It is surprising to find that the spectral reflectance properties of many materials remain relatively uncharacterized and that the existing data remain dispersed in the literature. However, the size of the task of searching for and collecting most spectra ever published is certainly large. The rewards of such an effort are worth considering, but must be weighed against the cost of generating anew, under known and uniform conditions, spectra of the materials most interesting to the specific applications.

5.2 Discussion

Spectral reflectance databases exist for a variety of materials in the 0.2 to 12 μm spectral range. However, these databases are not uniform in nearly all the important parameters such as spectral range, spectral resolution, data format, sample description and experimental conditions. In general, these databases tend to be developed for specific purposes (e.g., mineralogical diagnosis of remote sensing data, or environmental studies of vegetation stress due to disease or nutrient deficiencies) and are not necessarily comprehensive. Also, the spectral range and resolution of each database are determined by the needs of the particular study driving the formation of the database. Many spectral reflectance databases, for instance, are of extremely low resolution (broadband) and of limited spectral range, and have been designed for use with broadband spectral instruments of the Landsat type.

Much of the spectral reflectance data is found scattered throughout the technical and scientific literature. Except in a few cases, these data have been obtained with a specific scientific or technical objective and are not necessarily comprehensive or uniform in spectral range, resolution, sample description, photometric precision, or data format. For example, the data format of the earliest published spectral reflectance databases (e.g., Hunt and Salisbury 1970) is graphical, published in a journal at a scale that is of limited photometric and spectral use when considered in the context of the needs of today. Fortunately, the original data for this particular database have been preserved and incorporated into a more modern database. Unfortunately, this is a rare case and, even in this instance, the sample characterization is weak.

The most extensive databases on the spectral properties of materials contain the spectral absorbance or transmittance of the substance. These databases cover a wide range of samples ranging into the tens of thousands, a wide spectral range (0.25 to 50 microns), and a relatively high spectral resolution (1 to 2 cm^{-1}). Many of the materials contained in the spectral transmittance databases are organic chemicals and solvents of interest to the chemical and biochemical industries, and are useful only for the identification of trace amounts of the substance in a laboratory setting.

In theory, the spectral reflectivity should be calculable given the absorptivity since these two quantities are related in most scattering theories. Unfortunately, it is not clear that current theories of the photometric properties of materials (e.g., Hapke 1981) are adequate to describe the spectral reflectance properties of a material based upon the spectral absorption coefficient alone. If band positions are the only concern, then photometric scattering functions may provide a good estimate of these quantities in the cases where band asymmetries caused by other effects, such as steep continuum slopes, are not too severe. Predictions of band strengths (depths), shapes, and widths may be the most difficult problem for the photometric theory to overcome, since weak and saturated bands probably respond very differently in a multiple scattering environment. In a particulate soil composed of grains of differing composition, albedo, and particle size, there are major scattering asymmetries and nonlinearities which are only now beginning to be sufficiently described by scattering theories, particularly Hapke's theory. Obviously, more effort should be applied toward understanding the relationship between the absorption coefficient on one hand, and absorption band strengths and shapes on the other, if one wants to make use of this large body of spectral data.

Table 5-1 is a summary tabulation of the spectral reflectance databases. The search for such databases focused primarily on those used in remote sensing or with application in remote sensing, covered the spectral range of 0.25 to 25 μm , and involved a large number of spectral channels (> 100) and a spectral resolution much higher than the common broadband system such as Landsat. The tabulation focuses primarily upon databases or libraries that exist as such, and does not include the vast number of small sources in the literature since it is not the intent of this study to produce a comprehensive data library.

Following the summary tabulation is a catalog with eleven entries containing a more complete description of the databases listed in the summary tabulation. Also included for completeness is a summary (Table 5-2) of the databases containing transmittance spectra.

Each catalog entry contains the following information:

1. Database name (either as published or as assigned by this study);
2. General sample category or categories (e.g., rock, mineral, soil, chemical, organic, ceramic, botanical, metal, paint, fabric, planetary);
3. Spectral range and spectral resolution;
4. Instrument(s) used to collect the data;

5. Environmental conditions during measurement (e.g., ambient conditions, vacuum, temperature);
6. Photometric conditions of the measurement (e.g., bidirectional, hemispherical);
7. Number of samples measured in the database;
8. Sample documentation;
9. Database format;
10. Producer of database;
11. Owner (or vendor) and availability of database;
12. Hardware necessary to access the database.

5.3 References

- Hapke, B. (1981), Bidirectional reflectance spectroscopy 1. Theory, *J. Geophys. Res.*, 86, 3039-3054.
- Hunt, G. R. and J. W. Salisbury (1970), Visible and near infrared spectra of minerals and rocks: I, Silicate minerals, *Modern Geology*, 1, 283-300.
- Hunt, G. R. and J. W. Salisbury (1976), Visible and near infrared spectra of minerals and rocks: XI, Sedimentary rocks, *Modern Geology*, 5, 211-217.

TABLE 5-1
SUMMARY OF SPECTRAL
REFLECTANCE DATABASES

Title	Spectral Range (μm)	Sample Category
1. Planetary Gesociences (PGD/HIG/UH)	0.3 - 5.0	Rocks/minerals/ planetary
2. SPAM	0.4 - 2.5	Rocks/minerals
3. USGS (Salisbury)	2.2 - 25	Rocks/minerals/vegetation
4. USGS (Clark)	0.2 - 3.0	Rocks/minerals/planetary
5. NASA/Goddard	0.4 - 2.5	Vegetation
6. USGS (Milton)	0.4 - 2.5	Vegetation
7. LARS (Purdue)	0.4 - 2.5/ 8.0 - 14.0	Vegetation/soils
8. Aston University (UK)	0.3 - ?	Rocks/minerals/vegetation
9. Paint/chemical industry	variable	Paint/coatings
10. JPL	5.0 - 14.0	Rocks/minerals
11. Literature	variable	Wide range of materials

TABLE 5-2

SUMMARY OF SPECTRAL TRANSMITTANCE DATABASE

	Title	Spectral Range (μm)	Sample Category
1.	Sadtler Special Collection Sadtler Research Laboratories 3316 Spring Garden Street Philadelphia, PA 19104	2.5 - 25	Inorganic/ organic chemicals*
2.	Other companies (essentially the same as Sadtler)		

*Sample categories include :

Category	No. of Spectra	Category	No. of Spectra
ATR of polymers	900	Petroleum chemicals	325
Adhesives and sealants	1800	Pharmaceuticals	1670
Agricultural chemicals	700	Plasticizers	270
Coating chemicals	600	Polymer additives	600
Controlled pyrolyzates of polymers	2400	Polyols	270
Dyes, pigments and stains	1800	Rubber chemicals	830
Fats, waxes and derivatives	1500	Solvents	920
Fibers	240	Surface active agents	11900
Flame retardants	600	Textile chemicals	250
Food additives	375	Toxic chemicals	245
Gases and vapors	150	Water treatment chemicals	300
Germicides	300		
Inorganics	1000		
Lubricants	900		
Minerals	440		
Monomers and polymers	12600		
Organometallics	350		

SPECTRAL REFLECTANCE DATABASE CATALOG

ENTRY #1: PGD/HIG/UH

- A. Reference:
Planetary Geosciences Division/HIG Planetary Database
- B. Samples:
Rocks, minerals, meteorites, ices, and compounds of interest to the planetary and terrestrial remote sensing community.
- C. Spectral range and resolution:
($R = \Delta\lambda/\lambda$)
0.35 - 2.5 μm ($R = 100$) primarily
0.25 - 0.5 μm ($R = 100$)
2.5 - 5.0 μm ($R = 30$)
- D. Instrumentation:
0.35 - 1.1 μm Circular variable filter with uncooled Si
0.7 - 5.0 μm Circular variable filter with cooled InSb
0.25 - 0.5 μm Grating monochromator with uncooled Si
- E. Environmental conditions:
Generally room temperature and pressure. Some samples were measured at reduced or elevated temperatures (77 - 700°K) or under vacuum.
- F. Photometric configuration:
Generally bidirectional reflectances. Incidence angle and emission angle may vary among samples and measurements.
- G. Number of samples:
4000+
- H. Documentation:
Well-documented samples from various scientific projects.
- I. Format:
Digital, tabular and graphic
- J. Producer of database:
Planetary Geosciences Division from the work of a variety of scientists and research projects.
- K. Owner:
Planetary Geosciences Division/HIG/UH
2525 Correa Road, Honolulu, HI 96822
- L. Hardware or software needed:
SPECPR software under UNIX operating system or equivalent.

ENTRY #2: SPAM

- A. Reference:
Spectrum Analysis Manager
- B. Samples:
Rocks, minerals, and compounds of interest to the planetary and terrestrial remote sensing community.
- C. Spectral range and resolution:
 $(R = \Delta\lambda/\lambda)$
0.4 - 2.5 μm ($R = 100$)
- D. Instrumentation:
Unknown
- E. Environmental conditions:
Generally room temperature and pressure.
- F. Photometric configuration:
Unknown
- G. Number of samples:
533+
- H. Documentation:
Well-documented samples from various scientific projects.
- I. Format:
Digital, tabular and graphic
- J. Producer of database:
Jet Propulsion Laboratory
- K. Owner:
Jet Propulsion Laboratory
Pasadena, CA
- L. Hardware or software needed:
Unknown; tapes written on machines running VMS.

ENTRY #3: USGS (Salisbury)

- A. Reference:
US Geological Survey Spectral Reflectance Database
- B. Samples:
Rocks, minerals, and compounds of interest to the planetary and terrestrial remote sensing community. Also some botanical samples, primarily leaves of deciduous trees.
- C. Spectral range and resolution:
($R = \text{cm}^{-1}$):
2.2 -25 μm ($R = 2 \text{ cm}^{-1}$)
- D. Instrumentation:
Nicolet FT-IR spectrometer
- E. Environmental conditions:
Generally room temperature and pressure under nitrogen.
- F. Photometric configuration:
Diffuse reflectance
- G. Number of samples:
3000+ (includes variations in particle size, mixtures, etc.)
- H. Documentation:
Well-documented samples from various scientific projects.
- I. Format:
Digital, tabular and graphic
- J. Producer of database:
Dr. John Salisbury
- K. Owner:
Dr. John Salisbury
USGS
Reston, VA
- L. Hardware or software needed:
Unknown.

ENTRY #4: USGS (Denver, CO)

- A. Reference:
US Geological Survey Spectral Reflectance Database
- B. Samples:
Rocks, minerals, meteorites, ices, and compounds of interest to the planetary and terrestrial remote sensing community.
- C. Spectral range and resolution:
($R = \Delta\lambda/\lambda$)
0.25 - 3.0 μm ($R = 200+$)
- D. Instrumentation:
Modified Beckman double monochromator with Insb and Si detectors
- E. Environmental conditions:
Generally room temperature and pressure. Some samples are measured at reduced (77°K) or elevated temperatures, or under vacuum.
- F. Photometric configuration:
Diffuse reflectance using an integrating sphere. Some data in this database are bidirectional (see PGD/HIG).
- G. Number of samples:
5000+ (includes variations in particle size, mixtures, etc.)
- H. Documentation:
Well-documented samples from various scientific projects.
- I. Format:
Digital, tabular and graphic
- J. Producer of database:
Primarily Dr. Roger Clark; in addition, other scientists and researchers working on projects in planetary and terrestrial science (see PGD/HIG).
- K. Owner:
Dr. Roger Clark
USGS
Denver, CO
- L. Hardware or software needed:
SPECPR and UNIX operating system or equivalent.

ENTRY #5: NASA Goddard

- A. Reference:
Unknown
- B. Samples:
Botanical - corn, wheat and soybeans, excised leaves in lab, forested regions with Airborne Imaging Spectrometer (AIS).
- C. Spectral range and resolution:
Varied - broadband for Landsat and Thematic mapper 0.3 - 2.5 μm (0.01 μm resolution with AIS), 0.3 - 2.5 μm with 373 channels
- D. Instrumentation:
AIS
User-built 373-channel instrument
- E. Environmental conditions:
Varied, primarily room temperature and pressure.
- F. Photometric configuration:
AIS is bidirectional using the sun for illumination.
Other instruments are of unknown configuration.
- G. Number of samples:
200+ for lab samples
1000+ for field instruments
- H. Documentation:
Unknown
- I. Format:
Unknown
- J. Producer of database:
Dr. Robin Bell
NASA Goddard Space Flight Center
Greenbelt, MD
- K. Owner:
Dr. Robin Bell
NASA Goddard Space Flight Center
Greenbelt, MD
- L. Hardware or software needed:
Unknown.

ENTRY #6: USGS (Milton)

- A. Reference:
US Geological Survey: Dr. Nancy Milton, Reston, VA
- B. Samples:
Agricultural plants grown in greenhouses, including soybeans, and other crop plants. Some deciduous trees such as red maple and oak. Some of these plants have been "metal"-stressed. Some field measurements are in the database.
- C. Spectral range and resolution:
($R = \Delta\lambda/\lambda$)
0.4 - 0.8 μm ($R = \text{unknown}$)
0.4 - 2.5 μm ($R = \text{unknown}$)
- D. Instrumentation:
Unknown
- E. Environmental conditions:
Room temperature and pressure.
- F. Photometric configuration:
Unknown
- G. Number of samples:
2000+
- H. Documentation:
Unknown
- I. Format:
Digital, tabular and graphical
- J. Producer of database:
Dr. Nancy Milton at the USGS Reston, VA in collaboration with other scientists and researchers.
- K. Owner:
Dr. Nancy Milton
USGS
Reston, VA
- L. Hardware or software needed:
Unknown.

ENTRY #7: LARS (Purdue University)

- A. Reference:
Laboratory for Applications in Remote Sensing, Purdue University
- B. Samples:
Vegetation (crops) and soils.
- C. Spectral range and resolution:
($R = \Delta\lambda/\lambda$)
The spectral resolution is variable depending upon the instrument used. Typical values are:
0.4 - 1.1 μm ($R = 50$)
1.1 - 2.4 μm ($R = 40$)
8.0 - 14.0 μm ($R = 25$).
Some data are with resolutions ranging up to $R = 800$.
- D. Instrumentation:
Various field and laboratory instruments: NASA/JSC field spectrometer system (FSS), NASA/JSC field signature acquisition system (FSAS), and an Exotech 20 C laboratory spectrometer.
- E. Environmental conditions:
Mostly field conditions from helicopters, trucks, and stands.
Some laboratory.
- F. Photometric configuration:
A wide variety of bidirectional measurements in the field using the sun for illumination.
- G. Number of samples:
300,000 field measurements
1,492 lab measurements (duplication of samples unknown)
- H. Documentation:
Well documented
- I. Format:
Digital
- J. Producer of database:
Laboratory for Applications in Remote Sensing
Purdue University
Lafayette, IN
- K. Owner:
Contact: Dr. Chris Johansen
Purdue University
Lafayette, IN
- L. Hardware or software needed:
Unknown.

ENTRY #8: Aston University (UK)

- A. Reference:
Aston University, Remote Sensing Unit Preliminary Report
- B. Samples:
Rocks/minerals/vegetation (limited).
- C. Spectral range and resolution:
($R = \Delta\lambda/\lambda$):
Unknown spectral range but most likely 0.4 to 2.5 μm .
The spectral resolution is unknown. However, it appears that this data library is intended to contain spectral features and signatures such as band positions, band depths, etc., rather than the data itself presented as reflectivity being a function of wavelength.
- D. Instrumentation:
Unknown, probably varied
- E. Environmental conditions:
Unknown
- F. Photometric configuration:
Unknown
- G. Number of samples:
Unknown, probably in the thousands
- H. Documentation:
Unknown. Original request for data to be submitted included:
Aims and objectives of library
Structure of library
Persons involved
Costs and benefits
Details of use
- I. Format:
Unknown
- J. Producer of database:
Probably the National Remote Sensing Center, UK
- K. Owner:
Probably the National Remote Sensing Center, UK
- L. Hardware or software needed:
Unknown.

ENTRY # 9: Paint and chemical industry

- A. Reference:
Various commercial paint and coating companies
- B. Samples:
Pigments, paints, and coatings.
- C. Spectral range and resolution:
($R = \Delta\lambda/\lambda$)
Various: generally 0.3 to 2.5 μm at fairly high spectral resolution
($R > 300$).
- D. Instrumentation:
Commercially available spectrophotometers (see Chapter 4).
- E. Environmental conditions:
Not well constrained but generally room temperature and pressure.
- F. Photometric configuration:
Not well constrained but generally integrating sphere.
- G. Number of samples:
Very large but data are dispersed.
- H. Documentation:
Poor
- I. Format:
Generally graphic
- J. Producer of database:
Varied
- K. Owner:
On a case-by-case basis
- L. Hardware or software needed:
Unknown.

ENTRY # 10: JPL (3-14 μm)

- A. Reference:
Jet Propulsion Laboratory Spectral Emissivity
- B. Samples:
Rocks and minerals.
- C. Spectral range and resolution:
($R = \Delta\lambda/\lambda$)
3 to 14.5 μm ($R = 100$ approx.)
- D. Instrumentation:
JPL Portable Field Emission Spectrometer
- E. Environmental conditions:
Room temperature and pressure.
- F. Photometric configuration:
Bidirectional
- G. Number of samples:
30+
- H. Documentation:
Well documented since these are part of scientific study.
- I. Format:
Digital
- J. Producer of database:
Jet Propulsion Laboratory
Contact: Dr. Anne Kahle
- K. Owner:
Jet Propulsion Laboratory
Pasadena, CA
- L. Hardware or software needed:
Unknown.

ENTRY #11: Literature

Much of the spectral reflectance work available in the 0.2 to 14 μm spectral region remains as published articles scattered throughout the scientific and technical literature. Since the compilation of a database was not part of this project, these sources were not thoroughly researched.

6. Hyperspectral Data Processing Systems

6.1 Summary and Conclusions

An image cube processing system is an integrated package of functions that is able to operate on image data as single-plane two-dimensional data, as single-spectrum (one-dimensional) data, and especially as three-dimensional data, where the third dimension contains spectral information keyed to the pixel locations in the component two-dimensional planes. This three-dimensional entity is referred to as an "image cube" or a "hyperspectral data set." All functions within the processing system work from a common data format so that information generated by one function is immediately available to another function.

Only a limited number of individuals or institutions have developed true image cube processing systems, although many groups have some subset of image cube processing tools available. These latter groups most often have a system or collection of functions that operate on two-dimensional image planes. In addition, many individuals, institutions, and commercial establishments have developed systems of functions that operate only on one-dimensional spectra. In this report, the interest is in those processing systems which combine these two basic sets of operations and are able to operate in both the spectral and image domains. These systems also incorporate functions that integrate the information from these two environments.

Five processing systems that meet these requirements have been identified. These systems are listed in Table 6-1. Descriptions of their capabilities, advantages and disadvantages are given in Section 6.3. None of these systems is sufficiently developed and generalized to be applied as-is to any operational program. The Spectral Analysis Manager (SPAM), Geosciences Array Processor (GARP), and Image Reduction and Analysis Facility (IRAF) systems are the most easily adapted to the applications envisioned here. Of these three systems, GARP is the most generalized and complete.

The nature and composition of a hyperspectral data processing system is often not understood, and so it seems appropriate to describe it in some detail.

6.2 Image Cube Processing System Components

Image cube analysis may be considered to be divided into three main stages: (1) preprocessing, (2) analysis, and (3) display. There is a corresponding set of functions associated with each of these operational stages. These functions are outlined here and complete descriptions of all the components are given in Appendix 6-1.

6.2.1 Preprocessing

The preprocessing operations consist of those sets of functions that are used to:

1. Bring the data into the required or desired format;

2. Calibrate the data;
3. Compute statistics on all or a portion of a data set; and
4. Massage the data to remove noise or enhance certain features.

The preprocessing functions are enumerated below; a complete image cube processing system would have all of these functions available. These and all other functions discussed herein are defined in Appendix 6-1.

1. Versatile data input
2. Smoothing (spatial)
 - a. box filter
 - b. Gaussian deconvolution
3. Filtering (spectral)
4. Geometric rectification
5. Histogram calculation
 - a. 1-dimensional
 - b. 2-dimensional
 - c. n-dimensional
6. Histogram stretches ("rainbows")
 - a. linear stretches
 - b. other stretches
7. Calibration
 - a. on-line calibration standards
 - b. atmospheric correction
 - c. system's response removal
 - d. photometric correction
8. Statistical methods of data enhancement
 - a. principal components
 - b. decorrelation "stretch"
 - c. Fourier transform
 - (1) cross-correlation
9. Convolution to different bandpasses
10. Calculation of statistics
11. Cube transpose

6.2.2 Analysis

Analysis operations consist of those sets of functions which are used to:

1. Identify useful information in a data set;

2. Search for and extract desired information from a data set;
3. Produce products displaying the information.

The following functions are analysis functions; a complete image cube processing system would have all of these functions available.

1. Basic math operations
 - a. image algebra
 - b. image relational operations
 - c. cube algebra
 - d. cube relational operations
2. Classification procedures
 - a. supervised unit mapping
 - (1) histogram-based
 - (a) one-parameter
 - (b) n-parameter
 - b. unsupervised
 - (1) taxonomic ("clustering analysis")
 - (2) discriminant analysis
 - c. interactive
 - d. mixing model-based
 - (1) manual end-member selection
 - (2) automatic end-member selection
3. Spectrum-based operations
 - a. encoding
 - (1) amplitude
 - (2) slope
 - b. identifying/alarming
 - (1) based on reference spectrum
 - (2) based on (n-dimensional) histogram morphology/position
 - c. spectrum extraction
 - (1) based on location in image plane
 - (2) n-dimensional histogram-based
 - d. spectrum normalization
 - e. spectral parameter mapping
 - (1) band center
 - (2) band depth
 - (3) band width
 - f. band fitting
 - (1) Gaussian
 - (2) Cauchy
 - (3) Lorentzian
 - (4) Voigt
 - g. spectrum library
 - (1) on-line spectrum library
 - (2) user-generated library
 - h. spectrum library search procedures
 - (1) search image to match reference spectrum from library
 - (2) search library to match spectrum identified in image

4. Other operations
 - a. image profile/traverse
 - b. contour images (2-dimensional)
 - c. find surface of best fit (2-dimensional)
 - d. edge detection
 - (1) 2-dimensional
 - (2) 3-dimensional
 - (3) n-dimensional
 - e. continuum removal
 - (1) divide cube by single spectrum
 - (2) n-term polynomial for each pixel/spectrum
 - (a) cubic spline
 - (3) Gaussian fit to each pixel/spectrum
 - (4) fit wing of Gaussian, Lorentzian, or Voigt function
 - (5) smoothed spectrum at each pixel
 - (6) blackbody
 - f. derivatives
 - (1) spatial
 - (2) spectral
 - g. thermal correction
5. Spatial feature identification (not applicable here)

6.2.3 Display

Display operations consist of those sets of functions which are used to:

1. Access peripherals such as color monitors and hard-copy printers; and,
2. Display and output images and other products on these peripherals

The following functions are display functions; a complete image cube processing system would have all of these functions available.

1. Software to control
 - a. image display
 - (1) composite images
 - (2) overlay planes
 - (3) cube movies/band scan
 - b. spectrum display
 - c. color manipulation
 - (1) different systems (HSI, RGB)
 - (2) different "rainbows"
2. Software to drive
 - a. color monitor
 - b. hard-copy device
 - (1) black & white
 - (a) spectra
 - (b) images
 - (2) color

6.2.4 Other considerations

Any image cube processing system is bound to have several limitations, including: the number of data channels on which it can operate, the number of dimensions it can access in an image cube, the amount of core memory required, and the variety and kind of peripheral devices that it can control.

There are several other factors to consider in developing an image cube processing system.

1. A system that is powerful in terms of the number of functions that it has available or in terms of the number and sophistication of peripherals that it controls may otherwise be difficult to use.
2. The image cube processing system, to be considered truly general and complete, must be flexible and user-friendly.
3. A manual should be available. A manual is essential if no on-line help capability exists.
4. The system should be interactive, showing results of operations and allowing the operator to change the operation in real time. However, batch operations should also be possible.
5. The code should be organized in such a fashion that it is easy to modify existing functions or add new functions.
6. Software should be documented and easy to understand and modify.
7. The software system should be able to accommodate a variety of data sets; it should not be limited by the number of spectral channels or the size of images on which it is able to operate.
8. Ideally, the system would also be reasonably portable for use with different hardware and operating system environments.

6.3 Survey of Image Cube Processing Systems

Five processing systems meet the requirements for a hyperspectral data processing system, as stated in Section 6.1. These systems are summarized here. Appendix 6-2 contains the addresses and contact persons associated with these systems.

GARP--Geosciences ARray Processor: GARP was developed by the Planetary Geosciences Division of the Hawaii Institute of Geophysics at the University of Hawaii. GARP is an interactive software system for processing n-dimensional arrays of scientific data. A typical array consists of a set of images of the same spatial scene, with members of the set varying in observational parameters such as wavelength, phase angle, and time of observation. (Because of GARP's generalized design, other arrangements of dimensions can also be processed.) GARP provides a comprehensive set of functions for displaying, translating, analyzing, reducing, and geometrically manipulating such arrays. GARP uses a tile-based data format and operates under the UNIX environment on VAX 750 and SUN 3 hardware with IIS-IVAS color display systems; it is in the process of being ported to the VMS operating system (on a VAX 750) also. A version that utilizes

frame-based raster-formatted image cubes and a Transportable Applications Executive (TAE) user interface is currently under development.

AIPS--Astronomical Image Processing System: AIPS was developed by the National Radio Astronomy Observatory. AIPS is an interactive software system designed primarily for processing three-dimensional cubes of data obtained on astronomical objects. AIPS contains many of the generalized software tools needed in an image cube processing system. The data format used by AIPS is sufficiently flexible that it could also be used to operate on other data sets. AIPS operates under the UNIX and VMS environments.

SPAM--SPectral Analysis Manager: SPAM was developed at the Jet Propulsion Laboratory. It is an interactive software system designed for processing data obtained with NASA's Airborne Imaging Spectrometer (AIS). Most of the SPAM functions are designed to deal exclusively with data from this instrument. SPAM is currently under modification to accommodate data from the AVIRIS (Advanced Visible and Infrared Imaging Spectrometer), the successor instrument to the AIS. Additional modifications would be required to use SPAM on other data sets. SPAM operates under the UNIX and VMS environments.

TDRS--TAURUS Data Reduction System: The TDRS system was developed by Dr. Joss Bland as part of his dissertation work at the University of Sussex, England. TDRS is not so much an image cube processing system as it is a collection of image cube processing functions--there is no system executive that controls access to the functions. TDRS was designed primarily for processing observations obtained with the TAURUS interferometer. However, the data format and the available functions are sufficiently generalized that TDRS could also be used to operate on other types of data, following the development of a suitable executive. TDRS operates under the VMS environment.

IRAF--Image Reduction and Analysis Facility: The IRAF originated at the Kitt Peak National Observatory and is now under development by the National Optical Astronomy Observatories in Tucson, Arizona. The IRAF system is a general-purpose image processing system with graphics applications. Although many of the functions which comprise this system are directed toward two-dimensional astronomical image processing, the basic system is designed around the "image cube" concept. Thus, those functions that are not currently set up to access generalized three-dimensional data sets could in most cases be modified to do so. IRAF operates under both the UNIX and VMS environments.

6.4 Image Cube Processing Systems Summary Matrix

Table 6-2 summarizes the capabilities of the five image cube processing systems. The systems are reviewed according to the general matrix of image cube processing system components defined previously.

TABLE 6-1

EXISTING IMAGE CUBE PROCESSING SYSTEMS

- **GARP**

Geosciences **AR**ray Processing System
Planetary Geosciences Division (PGD)
Hawaii Institute of Geophysics (HIG)
University of Hawaii (UH)

- **SPAM**

SPectral Analysis Manager
Jet Propulsion Laboratory (JPL)
Pasadena, California

- **AIPS**

Astronomical Image Processing System
National Radio Astronomy Observatory (NRAO)
Greenbank, West Virginia

- **TDRS**

TAURUS Data Reduction System
Dr. Joss Bland
University of Sussex, England

- **IRAF**

Image Reduction and Analysis Facility
National Optical Astronomy Observatories
Tucson, Arizona

TABLE 6-2

COMPONENTS OF IMAGE CUBE PROCESSING SYSTEMS

A. Preprocessing	GARP	AIPS	SPAM	TDRS	IRAF
1. Versatile data input	•		•	•	
2. Smoothing (spatial)	•	•		•	•
a. box filter	•				•
b. Gaussian deconvolution		•		•	
3. Filtering (spectral)	•		•	•	•
4. Geometric rectification	•	•			•
5. Histogram calculation	•	•	•	•	•
a. 1-dimensional	•	•	•		•
b. 2-dimensional	•	•			•
c. n-dimensional					
6. Histogram stretches	•	•	•	•	•
a. linear stretches	•	•	•	•	•
b. other stretches					
7. Calibration	•	•			•
a. on-line calibration standards		•			
b. atmospheric correction					
c. system's response removal	•	•			•
d. photometric correction					
8. Statistical methods of data enhancement	•	•		•	•
a. principal components	•				
b. decorrelation "stretch"					
c. Fourier transform		•		•	•
(1) cross-correlation				•	
9. Convolution to different bandpasses					
10. Calculation of statistics	•	•	•	•	•
11. Cube transpose	•	•		•	•

TABLE 6-2 CONT'D

COMPONENTS OF IMAGE CUBE PROCESSING SYSTEMS

B. Analysis	GARP	AIPS	SPAM	TDRS	IRAF
1. Basic math operations	.	.	.	.	.
a. image algebra	.	.	.	.	.
b. image relational operations	.	.		.	.
c. cube algebra	.				.
d. cube relational operations	.				.
2. Classification procedures	.	.	.		
a. supervised unit mapping	.	.			
(1) histogram-based	.	.			
(a) one parameter	.	.			
(b) n-parameter	.				
b. unsupervised			.		
(1) "clustering analysis"			.		
(2) discriminant analysis					
c. interactive		.			
d. mixing model-based			.		
(1) manual end-member selection			.		
(2) automatic end-member selection					
3. Spectrum-based operations:	.	.	.		.
a. encoding	.		.		
(1) binary					
(a) amplitude	.		.		
(b) slope	.		.		
b. identifying/alarming	.		.		
(1) based on reference spectrum	.		.		
c. spectrum extraction	.		.		.
(1) based on location in image	.		.		.
(2) n-dimensional histogram-based					
d. spectrum normalization			.	.	.
e. spectral parameter mapping	.			.	.
(1) band center	.			.	.
(2) band depth	.			.	.
(3) band width	.			.	.

TABLE 6-2 CONT'D

COMPONENTS OF IMAGE CUBE PROCESSING SYSTEMS

B. Analysis (cont'd.)	GARP	AIPS	SPAM	TDRS	IRAF
f. band fitting	•	•		•	•
(1) Gaussian	•	•		•	•
(2) Cauchy		•		•	
(3) Lorentzian					
g. spectrum library			•		•
(1) on-line spectrum library			•		
(2) user-generated library			•		•
h. spectrum library search procedures		•			
(1) search image to match reference spectrum from library			•		
(2) search library to match spectrum from image			•		
4. Other operations	•	•	•	•	•
a. image profile/traverse	•	•		•	•
b. contour images (2-dimensional)		•		•	•
c. find surface of best fit (2-dimensional)				•	•
d. edge detection				•	
(1) 2-dimensional				•	
(2) 3-dimensional					
(3) n-dimensional					
e. continuum removal	•	•	•	•	•
(1) divide cube by single spect.	•		•	•	•
(2) n-term polynomial for each pixel	•				•
(3) Gaussian fit to each pixel/spectrum				•	
(4) fit wing of Gaussian, Lorentzian, or Voight function					
(5) smoothed spectrum at each pixel			•		
(6) blackbody					
f. derivatives				•	
(1) spatial				•	
(2) spectral					
g. thermal correction					

TABLE 6-2 CONT'D

COMPONENTS OF IMAGE CUBE PROCESSING SYSTEMS

C. Display	GARP	AIPS	SPAM	TDRS	IRAF
1. Software to control	.	.	.	.	.
a. image display	.	.	.	.	.
(1) composite images	.		.		.
(2) overlay planes	.		.		.
(3) cube movies/band scan	.	.	.		
b. spectra display	.	.	.	.	.
c. color manipulation	.	.	.		.
(1) different systems (HSI, RGB)				.	
(2) different "rainbows"	.	.			.
2. Software to drive	.	.	.	.	.
a. color monitor	.	.	.	.	.
b. hard-copy device	.	.	.	.	.
(1) black & white	.	.	.	.	.
(a) spectra	.	.	.	.	.
(b) images	.	.			.
(2) color			.		
D. Other Considerations	GARP	AIPS	SPAM	TDRS	IRAF
1. Flexibility	.	.	.	.	.
a. to add/change code	.	.	.	.	.
b. user-friendly	.	.	.		.
(1) interactive	.	.	.		.
(2) on-line help	.	.	.		.
(3) useful manual	.	.	.		.
(4) entertaining manual		.			
2. Limitations	x	x	x	x	x
a. number of data channels		x	x		
b. number of dimensions		x	x	x	
c. large memory needs			x		
d. hardware dependent	x		x	x	
e. still under development	x				x

Appendix 6-1. Generalized Image Cube Processing System: Definition of Components

A. Preprocessing

1. Versatile data input: Brings "foreign" data into the native format and can read data from tape or disk. Also has some special capabilities geared to reading data obtained from particular instruments.
2. Smoothing (spatial): Averages or otherwise combines data from two or more pixels, replacing one or more pixels with the new value. The exact replacement scheme depends upon the technique being used. This operation is performed either to remove unwanted noise or distortion from an image or cube, or to enhance large-scale features.
 - a. Box filter: Spatially filters an image cube by calculating a given statistic within a square "window" of pixels. The statistic is generally the mean, median, standard deviation, or variance of the pixels included within the window. The window is progressively moved through the image and the pixel centered in the window is replaced by the derived statistic.
 - b. Gaussian deconvolution: The data points along one or several lines through an image are fit to a Gaussian histogram. The resulting Gaussian curve is then removed (divided out) of the data.
3. Filtering (spectral): Averages or otherwise combines data from two or more channels (wavelength positions). The exact replacement scheme depends upon the technique being used. This operation is performed primarily to remove unwanted noise in spectra.
4. Geometric rectification: Corrects for distortions in the spatial domain or translates to a new spatial coordinate system. Translations include simple image shifts and rotations (perhaps to mutually rectify two or more data sets) and projections to different mapping systems. The distortions arise as a result of variations in aircraft or spacecraft flight characteristics. Even though a sensor may retain the same orientation with respect to the observing platform, motion of the platform relative to the ground or target introduces uncertainty into the apparent spatial location of the observation.
5. Histogram calculation: Computes the number (frequency) of data points (pixels) falling within a given range of values.
 - a. One-dimensional: Plots number or frequency of data points (ordinate axis) versus value (abscissa axis). The spacing between points along the abscissa may be controlled by input from the user.
 - b. Two-dimensional: Produces a two-dimensional image where one side of the image measures the frequency distribution of one plane of data points within a cube, and the second side measures the frequency of a second plane of points. The pixels within this histogram "image" represent the dual occurrence of data values within the two planes. The user may control the range of data values over which the histogram is computed for each plane.
 - c. n-dimensional: An extrapolation of the two-dimensional histogram; produces an n-dimensional cube. Each plane in the cube is a two-dimensional histogram.

6. Histogram stretches ("rainbows"): Resample data from one range of digital values to a new range of values according to some translation scheme. They are used to enhance data values falling within a given range of values (contrast enhancement) or to take advantage of the full dynamic range of a display or recording device (contrast stretching).

- a. Linear stretches: Transformation holds relative separation between data values invariant.
- b. Other stretches: Transformation redistributes spacing of data points from the original data range to the new range. The two most commonly used forms of nonlinear transformation base the new range on a logarithmic distribution of data values or on a Gaussian distribution of data values.

7. Calibration: Brings data numbers obtained by the instrument into a known system of units. It is used to correct for instrument response and atmospheric effects, or to remove the spectral effect of the light source.

- a. On-line calibration standards: The absolute spectral response of calibration standards in common use at a given facility made available as part of the image cube processing system.
- b. Atmospheric correction: The algorithm(s) for a technique or set of techniques used to perform atmospheric backout on image cube data is maintained as a special function within the image cube processing system.
- c. System's response removal: The response of instruments in common use at a given facility is maintained as part of the software of the image cube processing system.
- d. Photometric correction: Derives the photometric or phase function from each spectrum and divides it out.

8. Statistical methods of data enhancement: Techniques based upon the statistics (e.g., mean, median, mode, standard deviation) of the distribution of data values. The assumption is that this distribution represents or condenses useful information.

- a. Principal components: Computes the principal component (or eigenvector transform) images for a given three-dimensional array. This function performs a principal components analysis on the input subarray. The subarray must have three dimensions; the planes of the third dimension are treated as separate variables.

The principal components are the eigenvectors of the covariance matrix of the input data set; they are a linearly independent set of axes vectors, which together describe all of the variance in the entire data set. Because dimensionality must be maintained (if the variables are nondegenerate), there will be as many principal components (eigenvectors) as there were variables in the original data set.

The principal components are based upon the covariance or correlation matrix computed for the data set. The correlation matrix is the covariance matrix computed from a standardized data set (i.e., the data have been recomputed so that each variable has a mean of zero and a standard deviation of one). Standardization reduces the data to a set of comparable "unitless" variables.

The eigenvalues represent the relative lengths of the axes for each eigenvector or principal component and, hence, the relative percentages of the total variance defined by each principal component. For the i^{th} component plane and for n planes, the eigenvectors are of the form:

$$c_1 * x_1 + c_2 * x_2 + c_3 * x_3 + \dots + c_n * x_n$$

where the c 's are the coefficients of the eigenvectors and the x 's are the planes of the original data set. Thus, each new principal component plane is a linear combination of the n original planes.

The coefficients may be used to interpret the interrelationships among the original variables. If, for instance, the coefficient for x_1 is positive and the coefficient for x_2 is negative, the two variables contribute to that principal component plane in an opposite, or reciprocal, sense. Similarly, if the absolute value of the coefficient for x_1 is large (the coefficients range from -1 to +1) and the coefficient for x_2 is much smaller, then the contribution from x_1 to a given plane dominates that from x_2 . The relationships between the variables may be analyzed in this fashion to interpret a given principal component plane.

For the i^{th} component and for n planes, the eigenvectors are of the form:

$$c_1 * x_1 + c_2 * x_2 + c_3 * x_3 + \dots + c_n * x_n$$

where the c 's are the coefficients of the eigenvectors and the x 's are the planes of the original data set. Thus, each new principal component plane is a linear combination of the n original planes.

- b. Decorrelation "stretch": Computes the principal components for a given image cube (or portion of a cube). The process performs a nonlinear histogram stretch on the data values within each principal component plane. It inverts the principal components transformation to reobtain the original set of units, but maintains the values computed in the nonlinear histogram stretch. This process has the effect of enhancing the variation from plane to plane within a data set, or removing statistical correlations from one plane to another.
- c. Fourier transform: A Fourier series (or double Fourier series) is fit across a given direction along a cube. Harmonic or repeating sequences of data values are identified when a match to the Fourier sequence occurs. This technique may also be used to identify and remove patterns of noise within a data set (such as electronic interference within an instrument). It is most often employed to identify underlying patterns within the data values on a scale determined by the separation of the elements of the Fourier series.
 - (1) Cross-correlation: Uses Fourier series analysis to identify correlations or data distributions occurring between two images or image cubes rather than within a single image or cube.

9. Convolution to different bandpasses: Resamples data obtained from one sensor to a new set of wavelength positions corresponding to the channel bandpasses of another sensor.

10. Calculation of statistics: Computes a variety of statistical values for a given data set,

most commonly, the mean, variance, and standard deviation for an input image, image cube, or portion of a cube.

11. Cube transpose: Exchanges the perceived axes of an image cube, so that a new viewing orientation is achieved. This is often done not only for display in different orientations, but because some functions have a faster computation time if the image cube is considered (by the software) to have a particular orientation.

B. Analysis

1. Basic math operations: Combine images or image cubes pixel by pixel, using mathematical operations. This is often done through a "math parser" that accepts an input equation from the user and performs the desired mathematical operation or sequence of operations.

- a. Image algebra: Combines two or more images according to algebraic logic, using the add, subtract, multiply, or divide operations. Also allows combining an image or set of images with a constant value.
- b. Image relational operations: Combines two or more images using the relational operations--equal to, not equal to, less than, or greater than. Other operations may also be included, such as logarithms, exponentiation, and the trigonometric functions.
- c. Cube algebra: Same as image algebra, but allows entire cubes to be combined.
- d. Cube relational operations: Same as image relational operations, but allows entire cubes to be combined.

2. Classification procedures: These are algorithms that section the image cube into a finite number of groups or clusters. The number of groups is generally much less than the number of pixels in a plane of the cube. These techniques are used to identify spectrally similar materials within the data set.

- a. Supervised unit mapping: The data distribution or histogram is examined by the user and boundaries are (subjectively) determined based on the user's understanding of the data set.

(1) Histogram-based: The histogram is displayed and a selected number of boundaries are drawn within the histogram. A specific data value is given to each of these histogram "bins". Pixels falling within each of the bins are replaced with the value selected for that bin.

- (a) one-parameter: The histogram for a single parameter or data plane is examined; a single corresponding image having the same number of units as bins defined in the histogram is produced.
- (b) n-parameter: An n-dimensional histogram is examined. Boundaries are defined within n-space, resulting in a cube of identified "units". Any plane within that cube may be displayed.

- b. Unsupervised: Classifies pixels in an image cube into units based on some

analytical function, rather than on arbitrary boundaries within a histogram.

- (1) Taxonomic ("clustering analysis"): Uses some defined measure of "relatedness" or similarity (most commonly the Euclidean distance computed between data values) to place pixels into units. This also requires a cutoff value for the similarity measure to determine if a pixel falls into a given cluster or not. The objective of the clustering process is to find an optimal number of cluster centers (or "centroids") between two extremum conditions: (a) each point should be at a minimum distance from the center of its cluster (the extremum condition is that, for n points there would be n cluster centers); and (2) the uncertainty of the cluster center with which a given point would be associated is minimized (this is comparable to minimizing the entropy of the system--the extremum condition consists of a single cluster which contains all the data points).
 - (2) Discriminant analysis: Determines a linear combination of the image planes or variables, which defines the maximum difference between two data sets. Discriminant analysis is a comparative measure between two data sets--generally between a known or type area and an unknown area. Units that were identified within the type area may then be directly identified within the unclassified area.
 - c. Interactive unit mapping: Allows the user the option, as intermediate clusters are formed, of moving points or pixels near the edge of a group into another group, as well as the option of changing the cutoff value at each step.
 - d. Mixing model-based: References a set or library of spectral types ("end-members"). Recomputes the spectrum at each pixel as a linear combination of these end-members.
 - (1) Manual end-member selection: The user identifies a set of end-member spectra and extracts these from the library. Each pixel is assumed to include some proportion of each of these end-members.
 - (2) Automatic end-member selection: The principal component planes for the image cube are taken to represent the set of end-members for the data set. A search algorithm is employed to automatically find the end-member set, based on the principal components. The proportion of each end-member is determined based upon the value of that pixel in the appropriate principal component plane.
3. Spectrum based operations: These are functions which operate primarily on the spectra within an image cube; spatial location and interrelationships are secondary.
- a. Encoding: This is a way of condensing the features within a spectrum. It may also be used to reduce the physical size of the data set on disk.
 - (1) Binary: Recomputes the value at each channel or wavelength relative to some defined parameter. In this way, the value at each channel is reduced to a single bit.
 - (a) amplitude: Recomputes the value at each channel relative to the average value of the spectrum. If the value at a channel is

greater than the average value, the data value is replaced by 'one'. If the value is below the average, the data value is replaced by a 'zero'.

- (b) slope: Recomputes the value at each channel relative to the direction of the slope between two channels. If the slope is increasing (i.e., the value at a channel is less than that at the next channel), a 'one' is substituted for the data value. If the slope is decreasing (i.e., the value is greater than that at the next channel), a 'zero' is substituted.
- b. Identifying/alarming spectra: Searches the image cube for specific spectral shapes.
- (1) Based on reference spectrum: Searches the image cube for spectra matching a given input spectrum within certain tolerance limits. The input spectrum may be encoded (in which case the tolerance is given as the number of 1/0 mismatches), or the input spectrum may be in the units of the data set (in which case the tolerance is given as an acceptable range surrounding the input spectrum).
 - (2) Based on (n-dimensional) histogram morphology/position: Given locations within an n-dimensional histogram, pixels having that value or set of values are identified or alarmed.
- c. Spectrum extraction: Selected spectra within an image cube are isolated and treated as individual vectors.
- (1) Based on location in the image plane: Spectra are selected according to pixel locations in an image plane. This may also include the capability of extracting the average spectrum from a designated area within the image cube.
 - (2) n-dimensional histogram-based: Spectra are selected based on their location within a histogram.
- d. Spectrum normalization: There are two basic forms of normalization: (1) a single channel is considered to represent the maximal value for all spectra (and set equal to one in every spectrum) and the values at all other channels are recomputed to maintain proportions; and (2) the area under the spectrum is computed and the values at all channels are recomputed so that this area is equal to one (still maintaining proportions).
- e. Spectral parameter mapping: Spectral bands are automatically identified and parameters describing the location and shape of these bands are computed.
- (1) Band center: The wavelength position of the band minimum, or possibly the band center, is determined.
 - (2) Band depth: Given the wavelength location of a band, the depth of the band is computed relative to some defined continuum value.
 - (3) Band width: Given the wavelength position and depth of a band

(relative to a continuum), the full width at half-height (or "half-depth") of the band is determined.

- f. Band fitting: Spectral bands are assumed to have some predefined, general basic functional shape. This function is computed, with variable input parameters, until the form is obtained that best fits a given band. The following are the functional forms that are most commonly used:
 - (1) Gaussian
 - (2) Cauchy
 - (3) Lorenzia
 - (4) Voight
 - g. Spectrum library: A collection of spectra representing materials of interest that can be accessed by functions within the image cube processing system. This often takes the form of a data base management system.
 - (1) On-line spectrum library: A library of spectra maintained within the image cube processing system, to which all users have access.
 - (2) User-generated library: A library of spectra generated by a given user. Often such a library is composed of spectra extracted from an image cube, which may or may not be identified as representing a particular material.
 - h. Spectrum library search procedures: Routines to look through a library of spectra, extracting spectra from the library based on certain criteria. The criteria often take the form of input spectra to which a match is desired, as a first-order means of identifying the input spectra.
 - (1) Search image to match reference spectrum from library: Extracts a spectrum from the library and searches through an image cube to find spectra within the cube that match the library spectrum.
 - (2) Search library to match spectrum identified in image: Extracts a spectrum from an image cube and searches through the library of spectra to find a match or matches to the cube spectrum.
4. Other operations:
- a. Image profile/traverse: Extracts a vector from an image cube that is not in the "spectral direction"--for instance, extracts a vector corresponding to a given row or column of an image. In its general form, this function may also be used for extracting spectra.
 - b. Contour images (two-dimensional): Connects pixels/points with equal data values, within some defined tolerance.
 - c. Find surface of best fit (two-dimensional): Fits a geometric plane (two-dimensional surface) to a given image plane.

- d. Edge detection: Searches an image or image cube for changes in pixel values, based on some defined threshold value. Replaces the pixels on either side of an edge with proportionately different values, as determined by the severity of the edge. These changes are taken to represent a change in the material in the scene.
- (1) Two-dimensional: Searches for edges in a single plane only.
 - (2) Three-dimensional: Searches for edges in three dimensions.
 - (3) n-dimensional: Searches for edges in n dimensions, such as in an image cube that contains temporal as well as spatial and spectral information.
- e. Continuum removal: Defines and removes a continuum spectrum from each pixel in a cube. The continuum is taken to represent the background spectral response.
- (1) Divide cube by single spectrum: The same single predefined spectrum is divided out of each pixel.
 - (2) n-term polynomial for each pixel/spectrum: A polynomial is fitted to each spectrum in a cube and divided out of that spectrum.
 - (a) cubic spline: A cubic spline is computed for and divided out of each spectrum.
 - (3) Gaussian fit to each pixel/spectrum: A Gaussian function is fitted to each spectrum and divided out.
 - (4) Fit wing of Gaussian, Lorentzian, or Voight function: The wing (i.e., not the central portion) of one of these functions is assumed to represent the shape of the continuum. This curve is fitted to each spectrum and divided out.
 - (5) Smoothed spectrum at each pixel: The spectrum at each pixel is drastically smoothed and divided out.
 - (4) Blackbody: A Planck blackbody curve is fitted to each spectrum and divided out. This form of the continuum is most useful for thermal infrared data.
- f. Derivatives: Computes the derivatives along some direction in a cube.
- (1) Spatial: Computes the derivatives at each pixel in a given spatial direction.
 - (2) Spectral: Computes the derivatives at each channel or wavelength.
- g. Thermal correction: Removes the thermal component from a mid infrared or far infrared data set. This is done by finding the best-fit blackbody function and removing this function. This is generally used to remove the thermal background, thereby leaving the desired reflection or emission spectrum.

C. Display

1. Software to control:

- a. Image display: Displays and enhances two-dimensional images on a color monitor.
 - (1) Composite images: Displays up to three separate images, where the color or gray-level being displayed is a function of the value at a pixel in all three images.
 - (2) Overlay planes: Displays an image (often of "alarmed" areas) on a color plane that is not a function of the colors in other images being displayed. True colors, not mixed colors, are preserved in overlay planes.
 - (3) Cube movies/band scan: Displays the planes or channels of an image cube sequentially in time (i.e., scans through the scene in the spectral domain). This display technique is often used to visually search for or examine changes in spectral response occurring within a scene.
- b. Spectrum display: Displays and manipulates vectors (especially spectra) on a graphics display device. This may be the same device as that used to display images.
- c. Color manipulation: Allows control of the color contrast and choice of color in which a given image or overlay plane is displayed.
 - (1) Different systems (HSI, RGB): Recomputes the color display value based on the two main different systems of color -- HSI (Hue, Saturation, and Intensity) or RGB (Red, Green, and Blue).
 - (2) Different "rainbows": Allows for different histogram or color stretches or contrast stretches to be applied to the display of an image.

2. Software to drive: Peripherals are controlled within the image cube processing system.

- a. Color monitor: Used to display images. Also may be used to display spectra or vectors.
- b. Hard-copy device: Allows for a paper or film copy of an image or spectrum (or spectra) to be created.
 - 1) Black and white: Produces gray-tone copies of images and line graphs of spectra.
 - 2) Color: Produces color copies of images and colored line graphs of spectra. For images, can be either a color printer or a film-writer.

D. Other Considerations

1. Flexibility: The image cube processing system is adaptable to different projects and data sets.

- a. Add/change code: Software is easy to understand, modify, and make additions to.
 - b. User-friendly: Designed to be understood by inexperienced users.
 - (1) Interactive: Provides a menu showing input fields for each function, or otherwise prompts the user for a given input parameter.
 - (2) On-line help: Displays a handy description of each function as part of the basic software.
 - (3) Useful manual: Provides a manual detailing the structure of the image cube processing system and each of the functions and algorithms.
2. Limitations: Inherent limitations within the image cube processing system.
- a. Number of data channels: The system can operate only on a limited number of data channels. This may be due to limitations in available disk space or memory, or the system having been designed to operate only on certain data sets.
 - b. Number of dimensions: The system is limited in the number of dimensions it can access in an image cube. A cube, by definition, has at least three dimensions; a system may be considered an image cube processing system and not be able to access higher-dimensioned data sets.
 - c. Large memory needs: Functions are written so as to require large portions of an image or image cube to be brought into dynamic computer memory.
 - d. Hardware-dependent: The system can access only very specific peripheral devices.

Appendix 6-2. Addresses and Contacts for Systems Surveyed in Section 6

1. GARP:

Geosciences **AR**ray Processing System
Planetary Geosciences Division (PGD)
Hawaii Institute of Geophysics (HIG)
University of Hawaii
Honolulu, HI 96822
Contact: Jonathan Gradie (808-948-6488 /6320)

2. AIPS:

Astronomical Image Processing System
National Radio Astronomy Observatory (NRAO)
Computer Division
Edgemont Road
Charlottesville, VA 22903-2475
Contact: Nancy Weiner (804-296-0328)

3. SPAM:

SPectral Analysis Manager
Distributed by:
COSMIC
Software Information Services
University of Georgia
112 Barrow Hall
Computer Services Annex
Athens, GA 30602
(404-542-3265)

Developed by:
Jet Propulsion Laboratory (JPL)
MS/168-514
4800 Oak Grove Dr.
Pasadena, CA 91109
Contact: Jerry Solomon (818-354-2722 /6257)

4. TDRS:

TAURUS Data Reduction System
Institute for Astronomy (IFA)
University of Hawaii
Honolulu, HI 96822
Contact: Joss Bland (808-948-8319)

5. IRAF

Image Reduction and Analysis Facility
Central Computer Services
National Optical Astronomy Observatories
P.O. Box 26732
Tucson, AZ 85726
Contact: Jeannette Barnes (602-327-5511)

7. Spectrum Identification, Search and Retrieval (IS&R) Techniques

7.1 Introduction

This section serves as an overview to Sections 7.2--*Spectrum identification, search and retrieval capabilities in image cube processing systems* and 7.3--*Spectrum identification, search and retrieval capabilities in spectral processing (only) systems*.

The terms *spectrum identification*, *search*, and *retrieval* are first defined (these are referred to collectively as IS&R). Next, the various contexts in which these operations occur in qualitative and quantitative scientific investigation are described, for example, identifying each unknown in a field data set, locating regions of like materials in a hyperspectral cube, searching for a particular known material in a field data set. Because raw reflectance spectra must be calibrated for observation effects, instrument errors, etc., correction and resampling techniques in association with the above techniques are also discussed in this section.

The processing systems are divided into two major classes: (1) those incorporating automated access to a spectral reference library, and (2) those requiring manually directed comparisons to a set of manually selected reference spectra.

7.1.1 Definition of terms

- Reflectance spectroscopy identification analysis techniques are used to determine the composition of sampled materials by analyzing the signatures of the spectra and comparing them to reference spectra or to known spectral properties. The identification process can be subcategorized as: (1) *classification*, where the unknown is typed into a general category such as basalt; and (2) *characterization*, where the properties of the unknown are determined to a greater level of detail, such as the degree of weathering, presence of contaminants, and grain size. In the context of hyperspectral image cube processing, *identification* refers to the compositional analysis of each spectrum in the cube in terms of a relatively unconstrained set of candidates (in contrast to *searching*, see below).
- Reflectance spectroscopy search techniques are used to locate spectra with a semi-determined/constrained classification (e.g., basalt) or characteristics (e.g., weathered basalt with small grain size). In the context of hyperspectral image cube processing, *searching* refers to the comparison of each spectrum in the cube to a constrained set of candidates, for example, searching for carbonates. In a search procedure, spectra which do not match the candidate set are left unanalyzed.
- Reflectance spectroscopy retrieval techniques are used to locate spectra with well-determined/constrained properties in a set of (typically) identified reference spectra, referred to in this report as a library. Retrieved spectra are often utilized in analysis techniques such as search or identification.

The process for each of these three techniques is shown schematically in Figures 7.1-1, 7.1-2 and 7.1-3.

7.1.2 Reflectance spectra properties used in IS&R

The technique of reflectance spectroscopy is based primarily on spectral signature properties. The specular and diffuse reflectance properties of a pure medium determine spectral features, such as absorption bands. These bands are typically characterized by their center, width, depth and number. Other properties of the spectral signature include slope and amplitude information between bands and band overlaps.

These features may be broadly characterized as invariant or variable over a set of parameters such as grain size, age, lighting, impurity, and instrument calibration. The dimensions of this parametric space include composition of the surface media, the presence of mixtures/impurities in the media, intervening atmosphere, instrument characteristics, instrument calibration and signal-to-noise ratio, and environmental factors such as temperature and pressure.

Assumptions about the stability or invariance of spectral features are critical factors in judging the applicability and effectiveness of the IS&R techniques that are used in the systems described in Sections 7.2 and 7.3. The band centers, for example, are generally invariant over a large number of field conditions, whereas band width can vary with temperature while band depth often varies with material grain size.

The perturbation of spectral features and correction methods are described in the following subsections. The presence of material mixtures can cause additive, multiplicative or nonlinear effects in spectral features. Many factors can perturb the spectral features of a material's measurement, including: the material's temperature, grain size, and coating depth; the presence of contaminants; atmospheric and scattering effects resulting from remote measurement; and instrument response errors.

However, the effects of most of these factors can be removed through various techniques. The remaining spectral features are relatively invariant for pure materials. Some of these techniques are:

- Continuum removal
- Thermal emission
- Atmospheric backout.

7.1.3 Mixture analysis

The general application of IS&R techniques to field data requires methods for analyzing and deconvolving spectra of mixtures of materials. Mixtures of materials that consist of large patches of pure substances (large being on the order of tens of centimeters or more) will produce spectra that are arithmetic averages of the pure components weighted according to the surface area of each component. Mixtures on a more intimate scale, where the patches are on the order of millimeters or smaller, will combine according to a nonlinear scattering law. Mixtures can be vertically stratified, optically thin continuous layers over a substratum, following an approximate multiplicative behavior. Combining end-member spectra in each case, according to the three models, produces quite different mixture spectra.

7.1.4 Overview of reflectance spectroscopy identification techniques

The goals of identification analysis for a reflectance spectrum may be subcategorized as: (1) classification, where the unknown is assigned to a general category, and (2) characterization, where the properties of the unknown are determined to a greater level of detail. The selection of candidates for the identification generally determines which subcategory of identification is being attempted.

The identification analysis techniques used in the systems surveyed in this report may be viewed from several different perspectives. The identification analysis techniques may be considered to be: (1) purely knowledge-based, or (2) a hybrid procedural. Knowledge-based (or data-based) identification analysis techniques require a set of candidate known spectra to analyze the unknown by: (1) comparison of spectral features, and/or (2) channel-by-channel comparison of spectral reflectance values. Hybrid procedural methods used in cube processing systems attempt to find group structure in masses of undifferentiated spectra in the spatial scene; identification of an averaged spectra from each cluster is then attempted using the knowledge-based technique. None of the systems surveyed here is capable of identifying spectra using strictly procedural algorithms that do not require reference or candidate spectra for comparison.

Finally, identification may be considered as a high level technique invoked by an analysis directly, or as a subgoal of the search and retrieval procedures described in the following sections. For systems that analyze only a single spectrum, identification of an unknown is generally attempted against the entire spectral library. In the context of hyperspectral image cube processing, identification refers to comparison of each spectra in the cube in terms of a relatively unconstrained set of candidates (in contrast to searching, which is based on a small set of candidates).

7.1.5 Preprocessing

- Candidate Selection: Manual or automated determination of a set or library of candidate materials/mixtures. Spectral retrieval techniques may be employed to extract spectra from a reference library to form the set of candidates. An example of automated determination in the context of hyperspectral image cube processing is to assume that the identified component materials of an adjacent spatial pixel are candidates for the unknown spectra.
- Envelope Specification: Specification of an allowable error envelope for comparisons, e.g., allowable errors for a channel-by-channel comparison. The envelope selection is often based on the candidates selected. Noisy candidates require a larger comparison envelope but may admit ambiguous comparisons; a very stringent envelope may preclude legitimate identifications.
- Threshold Specification: Specification of the allowable violations of the error envelope.
- Calibration: Application of correction and calibration methods, if necessary, to the known candidates and to the unknown.

7.1.6 Procedural classification

This refers to the application of clustering algorithms in hyperspectral image cube processing to determine groups (often assuming spatial nearest-neighbor relationships) of statistically similar spectra.

7.1.7 Feature comparison

This involves comparison of characteristics of a sample spectrum with parameters for a set of known spectral features, as opposed to comparison of digitized spectra. This process involves several steps:

- Spectral feature characteristic determination, e.g., by Gaussian band fitting to determine band parameters;
- Comparison of the characteristics of the spectral features of the unknown spectrum to those of the reference spectra, using the error envelope and thresholds to quantify the degree of success;

When spectra of mixtures of materials are involved, the analysis requires that permutations and percentages of potential end-members be generated and the resulting spectrum be modeled before the comparison process, and that the comparison of various mixture candidates be evaluated relatively. In general, mixture analysis is only attempted when the number of candidate end-members is small.

7.1.8 Data comparison

This involves comparison of a sample spectrum to a set (perhaps an entire library) of digitized reference or candidate spectra. This technique offers certain computational advantages, since spectral features need not be extracted, but it requires that the sample and reference spectra share the same observation characteristics (e.g., wavelengths, phase angle, temperature, etc.) or that one or both be corrected and synthetically resampled to a reference standard for comparison. This technique involves:

- Standardized calibration of the unknown and comparison candidates;
- Possibly encoding each channel data value of the unknown and comparison spectra to make comparisons more efficient (though some channel information will necessarily be lost); and
- Comparison of each spectrum channel (e.g., distance measures) using the error envelope and thresholds to quantify the degree of success.

Again, analysis of spectra of mixtures of materials requires that permutations and percentages of potential end-members be generated, that the resulting spectrum be modeled before the comparison process, and that the comparison of various mixture candidates be evaluated relatively. In general, mixture analysis is only attempted when the number of candidate end-members is small.

7.1.9 Evaluation of output products

- Estimation of the accuracy of the identification procedure;
- Possible modification of the error envelope or threshold if no identification could be made (for example, the envelope might be relaxed and the identification procedure reiterated);
- Results of the identification may be saved as candidates for subsequent identification of other spectra in the hyperspectral data set, or stored in an output cube map.

7.1.10 Overview of reflectance spectroscopy searching techniques

Search techniques are used to locate spectra with a semi-determined or constrained classification (e.g., basalt) or characteristics (e.g., weathered basalt with small grain size), usually specified in terms of spectral candidates, in a set of (typically) unidentified spectra, here assumed to be a hyperspectral cube. Cube spectra that do not match the candidates are not analyzed further. The output of the search process is a measure of comparison success for each spectra; for a hyperspectral image cube, the product of a search is usually an output map which can be overlaid spatially on the cube containing the unknown spectra. For example, the output map might contain simply a success/failure flag for each spatial pixel, or perhaps a distance measure between the unknown and a reference spectrum.

The search process, then, relies on the same identification techniques described in the previous section. Thus, some of the procedural steps listed below for searching were also presented as identification steps; it should be remembered that *searching* in this report implies a particular problem context (searching for knowns in an undifferentiated hyperspectral cube).

7.1.11 Preprocessing

- Candidate Selection: Manual or automated determination of a set of candidate materials/mixtures. Spectral retrieval techniques may be employed to extract spectra from a reference library to form the set of candidates. An example of automated determination in the context of hyperspectral image cube processing is to assume that the identified component materials of an adjacent spatial pixel are candidates for the unknown spectra.
- Envelope Selection: Specification of a comparison envelope (e.g., allowable error bars for a channel-by-channel comparison). The envelope selection is often based on the candidates selected. Noisy candidates require a larger comparison envelope but this may admit ambiguous comparisons; a very stringent envelope may preclude legitimate identifications.
- Threshold Specification: Specification of the allowable violations of the error envelope.
- Calibration: Application of correction and calibration methods, if necessary, to the known candidates and to the unknown.

7.1.12 Comparison procedure

This involves feature or data comparison as described in the earlier overview of identification techniques. Mixture analysis requires that permutations of potential components and their percentages be generated before the comparison process, and that the comparison of various mixture candidates be evaluated relatively. If the mixture effects are additive, multiple searches against each end-member candidate could be attempted to identify mixture end-members, but their relative percentages would probably not be calculated.

7.1.13 Evaluation of output products

- Estimation of the accuracy of the search procedure;
- Possible modification of the error envelope or threshold. If no identification

could be made, for example, the envelope might be relaxed and the identification procedure reiterated;

- In hyperspectral cube processing, the results of the search may be saved as candidates for subsequent identification of other spectra in the cube or stored in an output cube map.

7.1.14 Overview of reflectance spectroscopy retrieval techniques

Retrieval techniques are used to locate spectra with well-determined/constrained classification (e.g., basalt) or characteristics (e.g., weathered basalt with small grain size), in a set of identified reference spectra, here assumed to be a spectroscopic library or database. (The case where all spectra are requested from the library may be considered a degenerate, though uninteresting, retrieval.) The retrieved spectra (spectral features, attributes, or the digital data sets) are then typically used in analysis techniques such as search or identification.

The retrieval process relies on the identification techniques described earlier. Thus, some of the procedural steps listed below for retrieval were also presented as identification steps; it should be remembered that *retrieval* in this report implies retrieving spectra from a database of identified known spectra.

Retrieval analysis techniques may be grouped into several classifications:

- direct search: an unknown compound is matched either by attributes or by digital comparison with a reference library, giving the closest matches in a report.
- inverse search: an unknown mixture is matched with the library. Compounds (and perhaps their abundances) which might be contained in the mixture are reported.
- Boolean search: the library is polled for compounds which match certain spectral features (e.g., a peak at 3 μm , no peak at 5 μm)

7.1.15 Preprocessing

- Candidate Selection: Manual or automated determination of the set of digital spectra, or spectral attributes/features that will be used as search criteria in the library retrieval. An example of automated determination in the context of hyperspectral image cube processing is the selection of an identified cube (field) spectra as a candidate for an unknown cube spectra; the high-quality library "equivalent" of the identified field spectra is retrieved from the library for comparison with the unknown.
- Envelope Selection: Specification of a comparison envelope (e.g., allowable error bars for a channel-by-channel comparison). The envelope selection is often based on the candidates selected. Noisy candidates require a larger comparison envelope but this may admit ambiguous comparisons; a very stringent envelope may preclude legitimate identifications.
- Threshold Specification: Specification of the allowable violations of the error envelope.

- Calibration to library standards: Application of correction and calibration methods, if necessary, and if a digital spectrum is used as the basis for the retrieval.

7.1.16 Comparison procedure

This involves feature or data comparison for each library member, as described in the earlier overview of identification techniques. Mixture analysis requires that permutations of potential components and their percentages be generated before the retrieval and comparison process, and that the comparison of various mixture candidates be evaluated relatively.

7.1.17 Evaluation of output products

- Estimation of the accuracy of the comparison for each retrieved spectra. If the comparison matches the search criteria to the specified threshold or envelope, the retrieval terminates. If not, the library is queried for the next spectrum.
- Possible modification of the comparison envelope. If no identification could be made, for example, the envelope might be relaxed and the entire retrieval/comparison procedure reiterated.

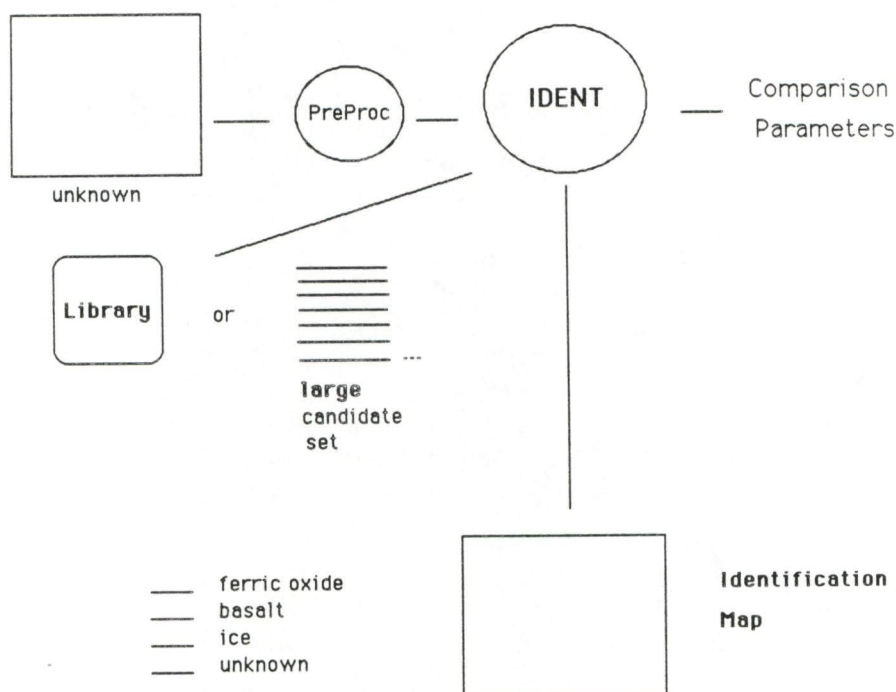
7.1.18 Survey coverage

Sources surveyed for the processing systems described in Sections 7.2 and 7.3 include commercial instrument manufacturers such as Nicolet, commercial spectroscopy database vendors such as Sadtler, government institutions such as the National Radio Astronomy Observatory, quasi-government agencies such as JPL, and universities such as the University of Hawaii. We believe that a nearly complete coverage of these systems has been achieved.

FIGURE 7.1-1

HYPERSPECTRAL IMAGE CUBE PROCESSING SYSTEMS: IS & R CAPABILITIES

Identification Functional Flow



-- Identification of all unknowns attempted

-- Mixture analysis impractical

-- Processing intensive

FIGURE 7.1-2

HYPERSPECTRAL IMAGE CUBE PROCESSING SYSTEMS: IS & R CAPABILITIES

Search Functional Flow

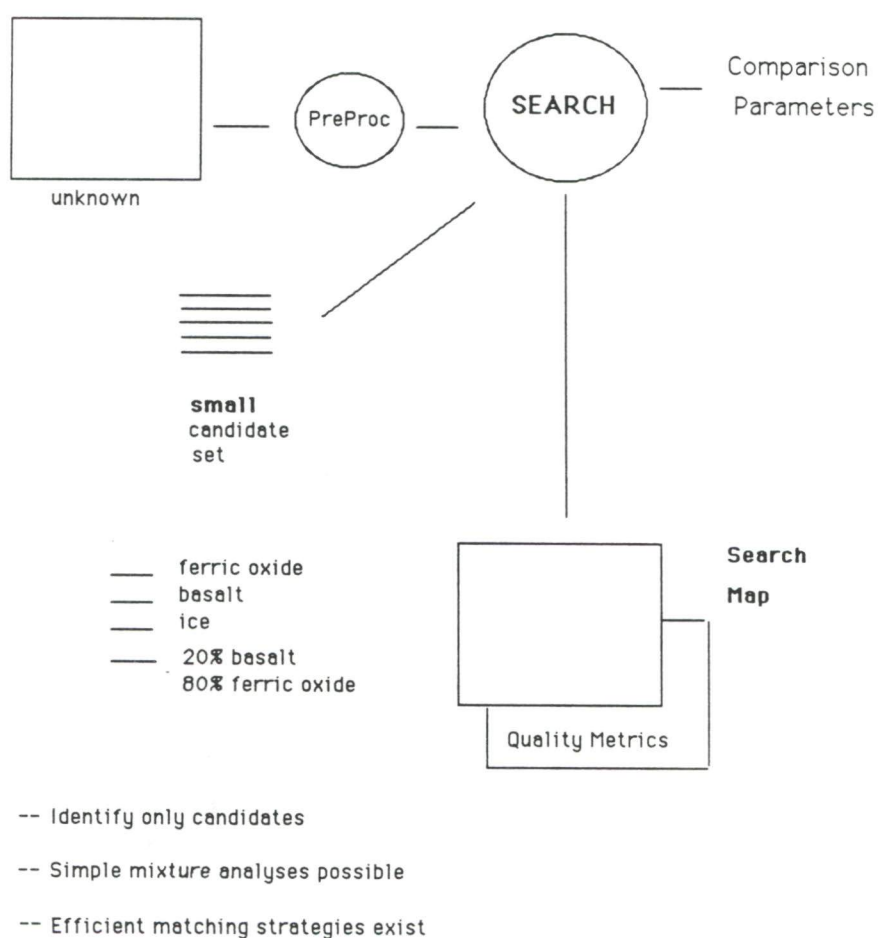
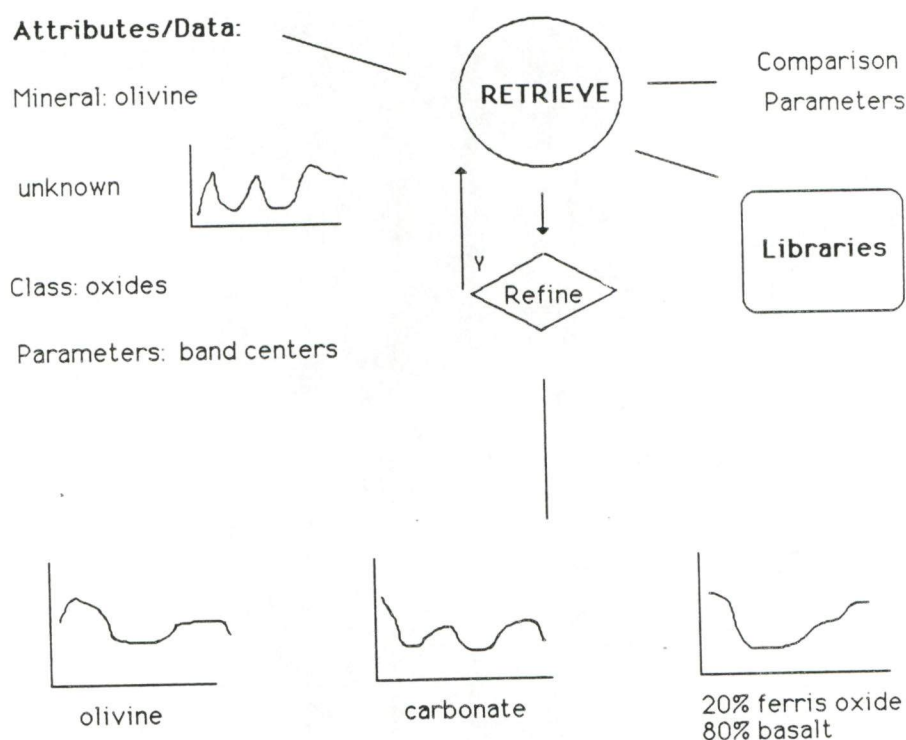


FIGURE 7.1-3

HYPERSPECTRAL IMAGE CUBE PROCESSING SYSTEMS: IS & R CAPABILITIES

Retrieval Functional Flow



- Stringent matches can be supported
- Simple mixture analyses possible

7.2 Spectral Identification, Search and Retrieval Capabilities in Hyperspectral Data Processing Systems

7.2.1 Summary and conclusions

This section describes and compares spectral identification, search and retrieval (IS&R) capabilities in existing hyperspectral image cube processing systems. Terms used in the discussion below are first defined. Second, the processing systems surveyed are described individually, focusing on the IS&R techniques employed. Third, high-level categories of IS&R functionality, application, performance, and other characteristics of hyperspectral image cube processing systems are presented. Using these generalized categories as the basis for comparison, the processing systems surveyed are contrasted using a matrix format. Finally, the systems are discussed as a whole, providing background for Chapter 9 of this report, which presents critical areas for research and development in hyperspectral data processing.

Five systems, listed in section 7.2.3, were surveyed. None of these systems is sufficient to be applied as-is to any operational program processing. To achieve an efficient implementation of the IS&R capabilities described in Section 7.1, construction of a hybrid processing system based on complementary features of the systems surveyed is recommended. Such a hybrid system might incorporate:

- the search methods of TDRS
- the excellent interactive features of SPAM and its spectral library support
- generalized data handling of GARP and IRAF
- host- and device-independent architecture of IRAF
- specialized routines from AIPS and the other systems surveyed.

7.2.2 Definition of terms

- Spectral identification, search and retrieval are defined in detail in Section 7.1.
- Hyperspectral image cubes are data sets obtained from a multispectral (greater than 20 bands) imaging spectrometer which collects a number of spatial images at different wavelengths, usually within the range of 0.3 to 12 μm . The data set is referred to as a cube (more properly, cuboid) since it may be viewed as a stack of registered images taken at various wavelengths. Usually, each planar spatial image is preserved (e.g., the xy-plane) and each spatial pixel is associated with a reflectance spectrum (e.g., parallel to the z-axis).
- Hyperspectral image cube processing systems are used to perform basic hyperspectral cube handling functions, such as display or transposition, cube statistics, cube algebra, dividing a cube by a spectrum, cube transformations, and registration. Hyperspectral data processing systems are described in detail in Chapter 6 of this report. In this section, only processing functions related to IS&R will be discussed.
- A hyperspectral map is a reduced hyperspectral data cube with the spectra of the original cube replaced by a set of characterizing parameters, such as polynomial fit coefficients or the percentage of successful matches in a cube search for a reference spectra. Since only the spectral dimension (previously

wavelength) of the cube is reduced, the output cube can be mapped onto the original for visual analysis.

- Spectrum libraries or databases are collections of reference spectra obtained from laboratory, field, telescope, spacecraft, and other observations. Spectral libraries are described in detail in Chapter 5 of this report. In this section, two types of spectrum libraries will be described: (1) libraries consisting of spectral attributes (e.g., chemical material composition, band centers, etc.), and (2) libraries consisting of reflectance vs. wavelength data sets that are generally resampled and calibrated to a known standard for comparison purposes. Not all of the systems described below incorporate an on-line spectrum library.

7.2.3 Systems surveyed

Five academic and institutional hyperspectral image cube processing systems were determined to support some or all of the IS&R capabilities described in Section 7.1. These systems are surveyed here. Appendix 7.2-1 lists the addresses and contact persons for these systems:

- Geosciences Array Processor (GARP) being developed at the University of Hawaii;
- Spectral Analysis Manager (SPAM) being developed at JPL and distributed through COSMIC;
- Astronomical Image Processing System (AIPS) developed at the National Radio Astronomy Observatory;
- TAURUS Data Reduction System (TDRS) developed by Dr. J. Bland at the University of Sussex; and
- Image Reduction and Analysis Facility (IRAF) developed at the National Optical Astronomy Observatories, Kitt Peak.

Most of these systems are still undergoing revision to accommodate new terrestrial, planetary or astronomical data standards and data from new instruments and upcoming spacecraft missions. Initial surveys indicate that no commercial hyperspectral image cube systems of these types are available.

7.2.4 GARP

The Geosciences Array Processor, GARP, being developed at the University of Hawaii (UH), is a multidimensional hyperspectral cube processing system that provides a comprehensive set of functions for displaying, translating, analyzing and geometrically manipulating data sets of up to ten dimensions.

GARP supports data comparison spectral searches for hyperspectral cubes based on distance measures between a single candidate or reference spectrum and the spectra in the unknown cube. GARP provides several routines for automated feature characterization of the spectra in an unknown cube. The extracted features can then be compared to a single candidate or reference spectrum. GARP does not yet incorporate a spectral library and, hence, does not support spectral identification or retrieval capabilities as defined in Section 7.1.

GARP provides a number of general-purpose analysis routines to assist with analysis functions

necessary for manually assisted spectrum identification and retrieval operations. These include data reduction, statistical characterization of spectral and spatial data (e.g., fitting routines), image cube handling (e.g., transpose of subcube extractions), interactive data displays (movies), etc. These capabilities have been listed in detail in Chapter 6 of this report.

The types of data comparison spectral searches supported by GARP, referred to as alarming, are:

- absolute difference: $\text{abs}(\text{vec}[i,j] - \text{ref}[i]) < \text{diff}[i]$, where *ref* is the reference vector and *diff* is the allowable difference vector;
- relative difference: $\text{abs}((\text{vec}[i,j] - \text{ref}[i])/\text{vec}[i,j]) < \text{diff}[i]$;
- Euclidean distance: $\text{sqrt}(\sum(\text{vec}[i,j] - \text{ref}[i])^2)/n$;
- Hamming distance for binary encodings: number of differing bits between two binary encoded spectra (see the SPAM description below).

The output of the search is a similarity or quality metric map, a success/fail map, and the total number of successful matches. The user inputs the similarity metric used to decide the success/fail value. The similarity value for the difference and Hamming distance alarms is the percentage of successful matches. Frequently the user overlays the success/fail map on the original image to determine whether the comparison thresholds were appropriate.

Several types of spectral feature characterizations are supported by GARP, which can be used to produce similarity maps. The first such method, referred to as band depth mapping I, generates a map in which the data number is the percentage band depth of a specific absorption feature. The user specifies channel numbers for the left- and right-hand edges of the band, which are used to define a straight-line continuum across the top of the potential band and a channel number for the band bottom. Based on this straight line, the continuum reflectance at the same wavelength as the band bottom is computed and the band depth is defined to be:

$$\text{band depth} = 1.0 - (\text{band bottom} / \text{continuum value}).$$

The resulting band depth map is typically compared to the spatial scene as an aid to manual identification.

A second feature extraction method, referred to as band depth mapping II, determines the location of a specified number of bands by identifying the convex hull of the spectrum being processed. Two types of hulls, primary and corrected (incorporating local maxima), may be defined, as shown in Figures 7.2-1 and 7.2-2. After the hull is found, the depths of the bands are found by dividing the hull by the original spectrum, yielding the hull quotient, and computing the maximum depth value in the band channel ranges. Several types of output maps are provided: a data cube of band centers and depths, a success/fail map indicating that a spectrum had a band in a given wavelength and depth range, and a gray-scale map containing the depth of the deepest band found in each spectrum.

A third feature characterization method supported by GARP is referred to as band fitting. Band fitting attempts to fit a specified number of Gaussians to the input spectra (typically transformed to $\log(\text{DN})$ versus $1/\text{wavelength}$) using an unconstrained minimization of the function:

$$F = \sum_{i=1}^n \left[\text{data}(v_i) - \sum_{j=1}^m H e^{\left(-\ln(2) \left[\frac{v_i v_j}{w_j} \right]^2 \right)} \right]^2$$

where n is the number of channels, m is the number of Gaussians being fit, v_j is the data value under

consideration, H_j is the height of Gaussian j , v_j is the center of Gaussian j , and w_j is the full width at half of the maximum of Gaussian j . Band fitting produces band centers, widths and depths, as defined by the Gaussian components, and a root-mean-square percentage deviation. GARP development plans include adding Voigt and Lorentzian functions (Clark 1984, Deming 1973).

7.2.5 SPAM

SPAM, being developed at JPL, is a system for interactive exploratory analysis of AIS imaging spectrometry. SPAM emphasizes the visual display of image data and liberal use of graphics representations for spectral and statistical information. Access to a reference library is tightly integrated into the analysis functions. SPAM is available through COSMIC, the NASA software distribution center, and is documented in the *SPAM User's Guide*.

SPAM relies on a feature extraction operator for spectra in order to compress the spectral information and produce reduced-dimension feature vectors. A pattern identification algorithm is employed for signature matching. Binary encoding of spectral data is used to achieve fast cross-correlation for signature matching (Figure 7.2-3). The following algorithm is used:

Using the notation where (i,j) is the spatial location index, $X_{i,j}$ is the intensity of pixel (i,j) , w denotes wavelength, and L is the total number of spectral measurements per channel, each pixel can be written as an L -component vector

$$\vec{X}_{ij} = [X_{ij}(w_1), X_{ij}(w_2), \dots, X_{ij}(w_L)]$$

If the scale j is defined as the mean of the (i,j) spectral vector,

$$m_{ij} = \frac{1}{L} \sum_{l=1}^L X_{ij}(l)$$

a binary valued L -element vector Y_{ij} is constructed by

$$Y_{ij} = H(\vec{X}_{ij} - m_{ij})$$

where $H(u)$ is the unit-step operator

$$H(u) = \{1, u \geq 0; 0, u < 0\}.$$

In order to characterize the similarity between two binary spectral vectors, the Hamming distance is used:

$$D_H(\vec{Y}_{ij}, \vec{Y}_{mn}) = \sum_{l=1}^L [Y_{ij}(l) \text{ exclusive or } Y_{mn}(l)]$$

To accommodate the variability in spectra of similar materials, the algorithm is run with the use of acceptance thresholds (Goetz 1985).

Encodings of spectra in the general libraries and in the image are calculated whenever an image is read into memory. Spectral plots created synthetically or by SPAM are encoded as necessary when used in

search or identification operations. It appears that amplitude encoding works better for vegetative terrain, and slope encoding is preferred for strictly mineralogical classifications.

SPAM incorporates an on-line spectral library (see Chapter 5) and supports each of the IS&R functions as defined in Section 7.1. The *find* routine attempts to match a specified spectrum against similar spectra in a hyperspectral cube or spectral libraries. An allowable deviation between spectra may be specified in terms of spectral amplitude and slope similarity. The output of this routine is a multicolored overlay of the spatial scene or, in the case of a library search, a list of similar spectra with their amplitude and slope deviations.

The SPAM routine *cluster* segments an image into a number of distinct regions based on similarity of spectra. A noise threshold specifies the maximum number of fluctuations about the mean for amplitude and slope; spectra falling outside these thresholds are regarded as noise. A cluster parameter indicates in how many bands two spectra can differ in amplitude and slope and still be considered identical. The output of this routine is a segmented image corresponding to spectral class plots (Figure 7.2-4). The classes may be merged if desired. Manual and automatic clustering is supported.

SPAM provides routines to break an unknown spectra or a portion of an image cube into its mixture components, given a set of specified reference spectra. There are two modes: (1) the area mode, which analyzes a portion of an image then generates a set of mixture maps, one map per reference mineral (Figure 7.2-5), and (2) the plot mode, which analyzes a plot and then generates a mixture plot and mixture properties for each component mineral. Methods used for mixture analysis include amplitude and slope encoding, Euclidean distance and least-squares fit.

SPAM's feature analysis supports two modes: (1) show all library spectra with features at given wavelengths, or (2) based on the features of a given spectra, search the reference library for matching spectra in the given wavelength region. The width and center of the spectral features are displayed in a bar graph fashion for visual inspection.

7.2.6 TDRS

TDRS, the TAURUS Data Reduction System, was developed by Dr. Joss Bland while at the University of Sussex, England. He is presently at the University of Hawaii's Institute for Astronomy. The TDRS was designed for Fabry-Perot data and has many features relevant to geoscientific data, including: absorption and emission line fitting, continuum removal and fitting, and determination of higher-order properties of spectral lines. TDRS is documented in Bland (1985).

TDRS supports data comparison spectral identification for hyperspectral cubes by finding regions with similar spectral signatures, as characterized by band depth, width, center and baseline. Gaussian fitting techniques are used to determine the band features. TDRS does not incorporate a spectral library and does not support spectral search or retrieval capabilities as defined in Section 7.1.

As with SPAM, TDRS focuses on compressing the spectral information in a large hyperspectral image cube and attempts to accomplish this through parameterization. Figure 7.2-6 shows the TDRS idealized spectral parameters: two emission lines, characterized as Gaussians, and a baseline correction. Figure 7.2-7 illustrates the constraint parameters, which include peak resolution information, continuum division and spectral prefiltering. The TDRS algorithm performs a raster scan over the xy-plane and attempts to recognize how the constraint parameters should be relaxed or constrained for regions with varying spectral properties. The types of regions are characterized as, for instance, noisy spectra, spectra with broad lines, spectra with skewed lines, or spectra with strong continuum variations. Pixels of a given region are connected through the use of bit masks. Associated with each bit mask is a stack containing several sets of constraint parameters. The final stage of the automated TDRS algorithm employs a least-squares fitting algorithm which depends on the number of peaks indicated by the derived constraint

parameters.

In more detail, the steps of the TDRS spectral characterization algorithm are:

Continuum Removal

```

if the smoothing sigma width < 0, then
    heavily smooth spectrum and divide by smoothed spectrum
else
    fit a single Gauss;
    if width > smoothing sigma then
        divide by fitted Gaussian;
    else
        heavily smooth spectrum;
        fit a single Gauss;
        if the new center <> old center then
            divide by new background Gaussian;
  
```

Peak Finding

```

lightly smooth original spectrum;

determine a realistic mean and sigma scatter for spectrum with peaks masked out;

determine positions of peaks in spectrum above the baseline sigma level;

look through peak list for two lines separated by minimum distance between emission
features;
  
```

Least-Squares Line Fitting

```

if no emission lines were found then
    get next spectrum;
else if one line was found then
    fit single Gauss to modified spectrum;
if two lines were found then
    if two lines were well resolved then
        fit double Gauss to modified spectrum;
    else
        fit double Gauss to complete spectrum by converging on
        both components simultaneously by keeping ratio of widths constant;
  
```

Rejection of Bad Fits

```

check parameters of single Gauss and sigma tolerances and store in data block;
  
```

TDRS output products include display of parameter blocks of line fits for further manually directed analysis, and diagnostics such as skewness maps which indicate where symmetric Gaussian fitting may be in error.

7.2.7 AIPS

AIPS, the National Radio Astronomy Observatory Astronomical Image Processing System, is a relatively mature system designed for the processing of astronomical data. It provides support for spectral line cubes, where the third dimension in radio astronomy applications is often frequency or velocity. Facilities are provided for data reduction, calibration, continuum subtraction, fitting, filtering, etc. (AIPS Cookbook).

Use of the AIPS spectral line software requires considerable manual interpretation. Spectral search, as defined in Section 7.1, can be accomplished with the system. Since AIPS is intended for astronomical processing, it does not incorporate a spectral library and, hence, does not support spectral identification or retrieval as defined in Section 7.1.

AIPS provides spectral line software to build and display three-dimensional data cubes, although special programs are needed to build and transpose these cubes and to display them properly. Spectral line imaging is supported through a number of basic data reduction capabilities and advanced profile analysis programs.

The following high-level flow diagram outlines how a typical spectral line data set might be processed in AIPS:

AIPS data reduction strategy

split off a broadband continuum channel or a line channel with a strong signal;
make an image and deconvolve;
self-calibrate the dataset;

if the dynamic range improvement of a line minus continuum image > noise **then**
 correct all channels;
 construct a new cube and page through it;

if a continuum needs to be subtracted **then**
 combine mean continuum images at the outer ends of the band;
 subtract the continuum image from the cube;

if the noise in line-free channels is less than the theoretical noise **then**
 repeat above

as needed, apply advanced profile analysis capabilities:

- display transposed cubes and multiple profiles
- perform baseline removal
- perform spatial smoothing
- reduce the effects of sharp bandpass filtering
 e.g., Hanning smoothing
- blank out regions of bad data
- calculate integral profiles and moments
- perform Gaussian fitting
- perform constrained, nonlinear deconvolution.

Thus, AIPS provides a number of tools that can be used to determine spectral line characteristics. From this spectral signature information, spectral identifications can be made by a trained analyst. However, the individual spectra must be inspected manually through the use of displays, such as that shown in Figure 7.2-8, and statistical characterizations of the dataset as provided by analysis routines,

such as those listed above. Like TDRS, AIPS is designed for optical astronomical data analysis, but it has considerably more generalized functionality (e.g., data set formats, image display support, etc.) than TDRS. AIPS, however, lacks the capability of TDRS to efficiently identify spatial regions having similar spectral signatures.

7.2.8 IRAF

IRAF, the Image Reduction and Analysis Facility developed by the National Optical Astronomy Observatories, provides extensive facilities for general image processing, astronomical data reduction and analysis, scientific programming and general software development. IRAF comprises a virtual operating system, a command language, a general-purpose programming language, a large input/output library, and numerous support utilities and scientific application programs. The system is designed to be transportable to a wide variety of hosts, image displays and graphics devices (Tody).

There are two categories of IRAF optical astronomy packages: one set is intended to be instrument-independent and the other is a set of procedures that have prepackaged parameters for specific NOAO instruments such as the IIDS and IRS. One- and two-dimensional spectral reduction and analysis packages are supported for dispersion correction, flux calibration and general spectral analysis.

IRAF supports user-defined spectral databases for reference (i.e., store and extract) purposes. Since IRAF is intended for astronomical processing, it does not support the spectral identification or retrieval functions defined in Section 7.1 as an integral part of the system. However, an applications programmer could use the library primitives provided with IRAF to construct such functions. As with AIPS and TDRS, a number of packages are supported in IRAF to assist with spectral feature characterization and analysis:

- locating features in a spectrum, time series or image
- finding spectral peaks
- fitting a function to spectra parameter values
- fitting spectra profiles with a five-parameter Gaussian model
- creating, adding to, and listing spectral database contents
- smoothing data by convolution filtering
- continuum analysis
- measuring equivalent width/line strength
- spectrophotometry
- synthetic hyperspectral image cube construction

Thus IRAF, like AIPS, provides adequate tools for manually assisted spectrum identification. It has a very good programming environment and facilities for supporting spectral databases, so it could be augmented for automated IS&R analysis. However, due to the astronomical orientation of the system's users, it is unlikely that such capabilities will be provided by NOAO.

7.2.9 Hyperspectral image cube processing system IS&R comparisons

High-level functionality comparisons for the surveyed systems are given in Tables 7.2-1 through 14. The comparisons are given in matrix format for the IS&R techniques, categorized into:

- Preprocessing
- Candidate Selection
- Envelope and Threshold Selection
- Subcube Selection

- Identification
 - Identification Methods
 - Identification Output Products
- Search
 - Search Methods
 - Search Output Products
- Retrieval
 - Retrieval Methods
 - Retrieval Output
- Processing System Features Computing Environment
 - Hyperspectral Cube Formats
 - Spectrum Library

7.2.10 Discussion of IS&R in surveyed hyperspectral processing systems

Each of the five systems surveyed offers capabilities not available in the others. SPAM is the only system explicitly designed for highly interactive, manually directed and automated spectral identification, search and retrieval operations. However, it lacks the generality of the other systems--GARP and IRAF, in particular--for functional expansion, generalized n-dimensional data set handling and generic image processing functions. AIPS, IRAF and TDRS are targeted for the optical astronomical community, and hence, do not support spectral analysis techniques for terrestrial remote sensing (such as a reference spectral library) and spectral variation analyses (such as mixture analysis). TDRS is unique in its attempt to deal with the large computational requirements of hyperspectral image cube processing by using specialized search and minimization techniques to find spatial regions of similar spectral content. SPAM attempts the same through deterministic clustering routines, but these operate on compressed encodings of the spectra whereas TDRS fits the actual data. To achieve an efficient implementation of the IS&R capabilities described in Section 7.1, it appears necessary to begin by constructing a hybrid processing system based on complementary features of the systems surveyed. Such a hybrid system might incorporate:

- the search methods of TDRS
- the excellent interactive features of SPAM and its spectral library support
- generalized data handling of GARP and IRAF
- host- and device-independent architecture of IRAF
- specialized routines from AIPS and the other systems surveyed.

The hybrid would be very useful for experimenting with data encodings, artificial intelligence (AI) search techniques, advanced hardware utilization, and the incorporation of IS&R techniques into other science analysis techniques.

7.2.11 References

- AIPS Cookbook*, a publication of the National Radio Astronomy Observatory, Edgement Road, Charlottesville, VA.
- Bland, J. (1985), *The Structure and Kinematics of the Ionized Gas within NGC 5128 (Cantaurus A)*, PhD dissertation, University of Sussex (March).
- Clark, R. N. and Rousch, T.L. (1984), Reflectance Spectroscopy: Quantitative Analysis Techniques for Remote Sensing Applications, *Journal of Geophysical Research*, 89, B7 (July), 6329-6340.

Deming, S. N. and Morgan, S. L. (1973), Simplex Optimization of Variables in Analytical Chemistry, *Analytical Chemistry*, 45, 3 (March), 278-283.

Goetz, A. et al. (1985), Imaging Spectrometry for Earth Remote Sensing, *Science*, 1147-1153.

GARP User's Guide, a publication of the Planetary Geosciences Division of the Hawaii Institute of Geophysics at the University of Hawaii, Honolulu, HI.

SPAM User's Guide, COSMIC, Software Information Services, University of Georgia, Computer Services Annex, Athens, GA 30602.

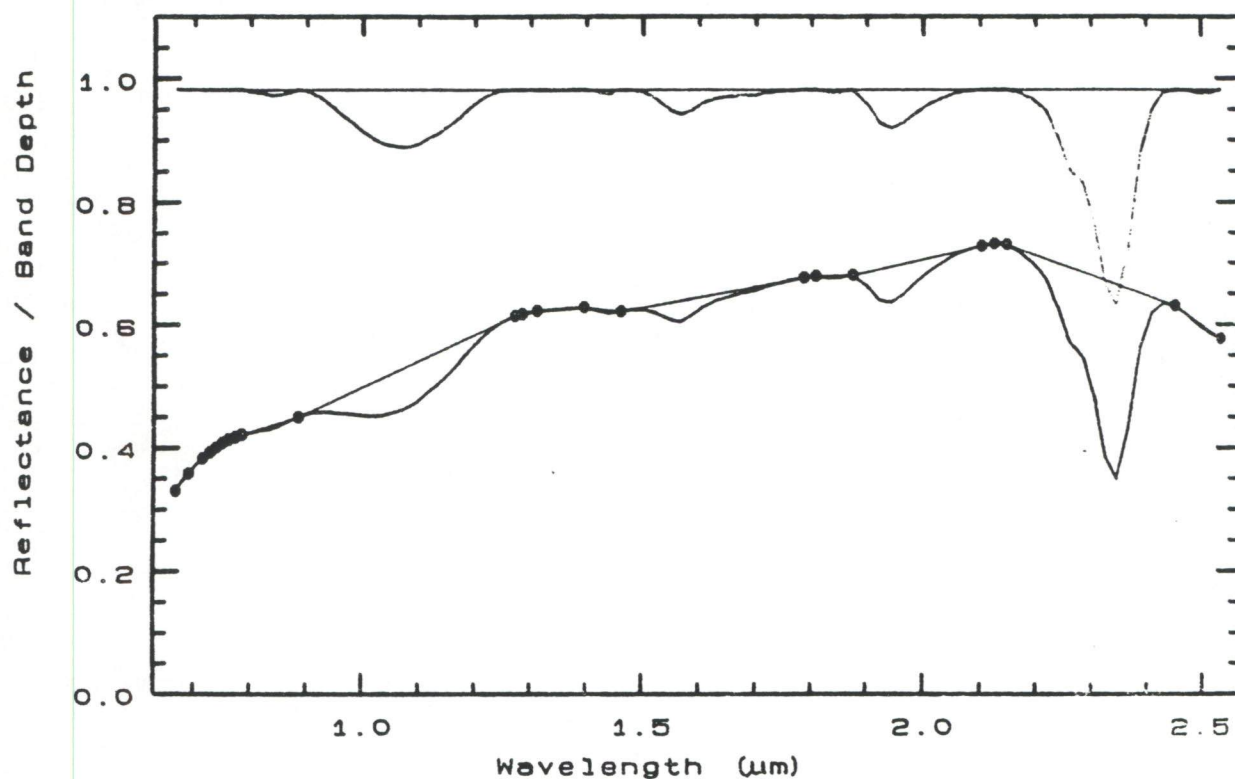
Tody, D., *IRAF Data Reduction and Analysis System*, NOAO internal publication.

Tody, D., *User's Introduction to IRAF Command Language*, NOAO internal publication.

FIGURE 7.2-1

GARP: BAND DEPTH MAPPING

Primary Hull Method



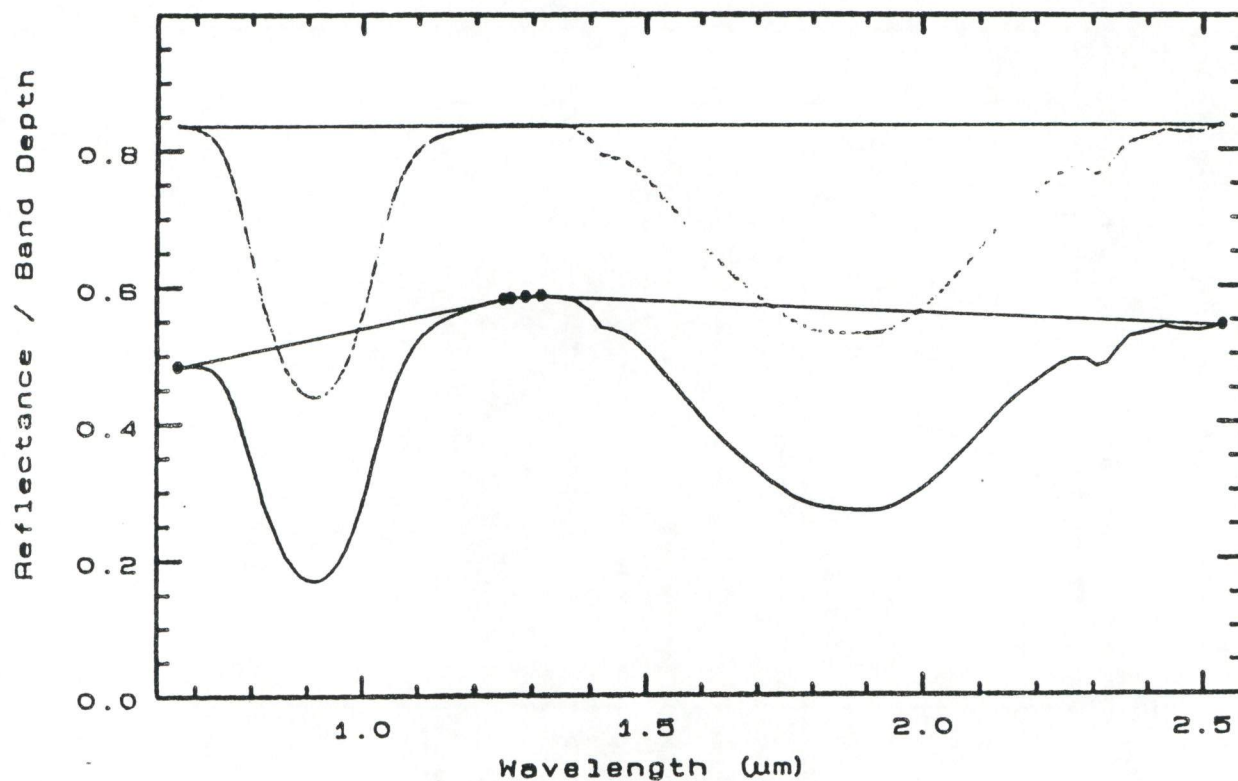
o PYX08 Primary data Values
 PYX08 Hull data values
 PYX08 Band Depths
 PYX08 Quotient Continuum

PYX08da f 1 a1p0016
 PYX08da f 2 a2p1016
 PYX08da f 3 a3p0017
 PYX08da f 4 a4p0016

FIGURE 7.2-2

GARP: BAND DEPTH MAPPING

Corrected Hull Method



o PYX02 Primary data values
 PYX02 Hull data values
 PYX02 Band Depth
 PYX02 Quotient Continuum

PYX02de f 1 81p0018
 PYX02de f 2 82p1018
 PYX02de f 3 83p0017
 PYX02de f 4 84p0018

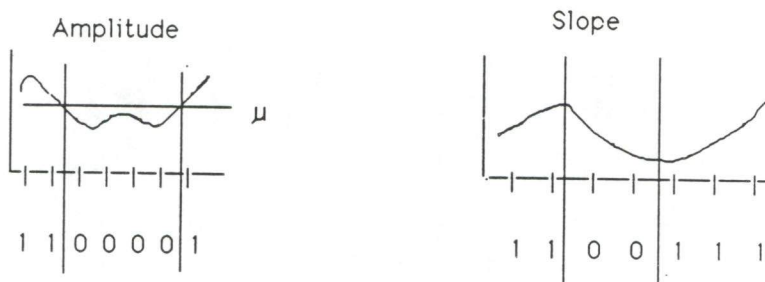
FIGURE 7.2-3

SPAM AND GARP: BINARY ENCODING OF SPECTRA

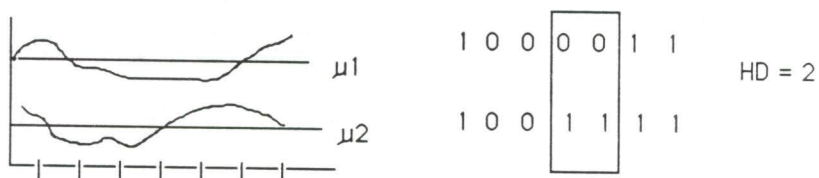
Sample Reduction and Comparison Method

Binary Encoding

One bit per channel
Used in GARP, SPAM



Hamming distance - number of differing bits



Noise discriminator: # bit changes

FIGURE 7.2-4

SPAM: CLUSTERING OUT EXAMPLE

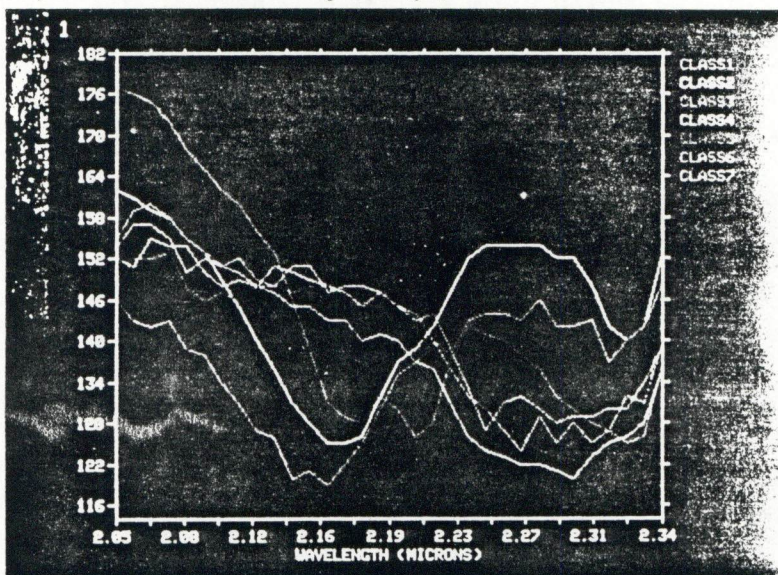
5600 samples were examined
 3393 samples were found to be feature-less

Using clustering thresholds 6 (amp) and 10 (slope).

One moment please . . .

Class 1:	57
Class 2:	448
Class 3:	585
Class 4:	155
Class 5:	42
Class 6:	35
Class 7:	34

Do you wish to save the clustering result?(y/n): Y



READY

MERGE 6 4 5 4 1 4

Do you wish to save the clustering result?(y/n): Y

FIGURE 7.2-5

SPAM: MIXTURE MAP OUTPUT EXAMPLE

mixture area binary alu? ka? no?
Enter area (starting_line number_of_lines): 1 200
Generating mixture maps ...



FIGURE 7.2-6

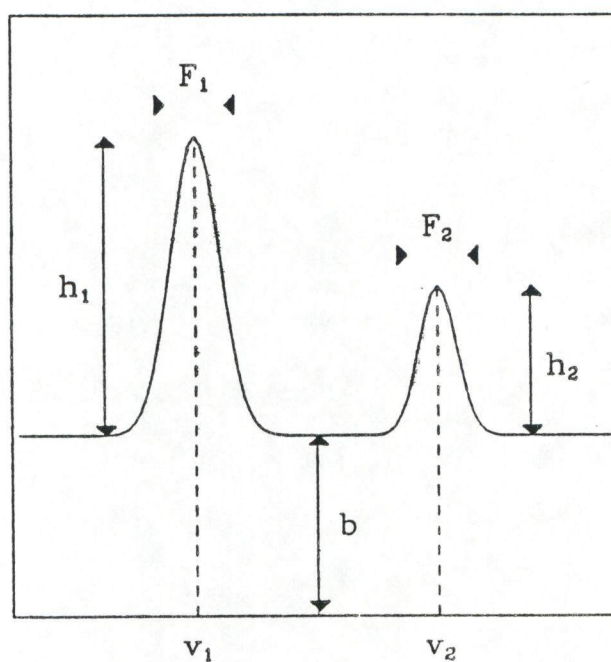
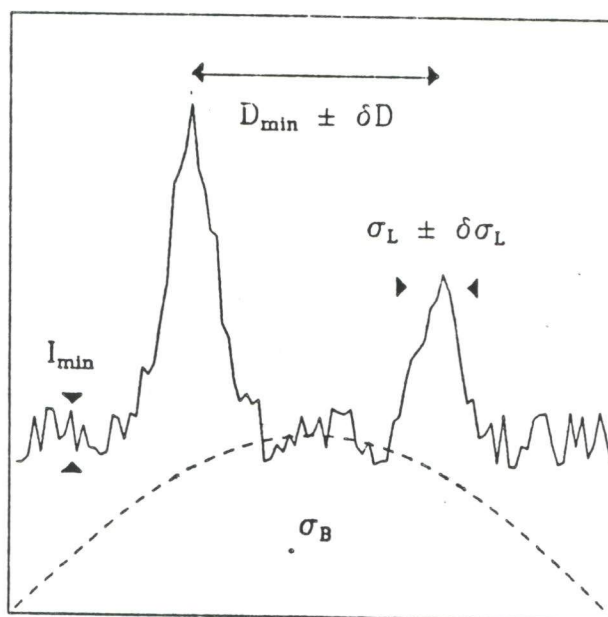
TDRS: IDEALIZED SPECTRAL PARAMETERS

FIGURE 7.2-7

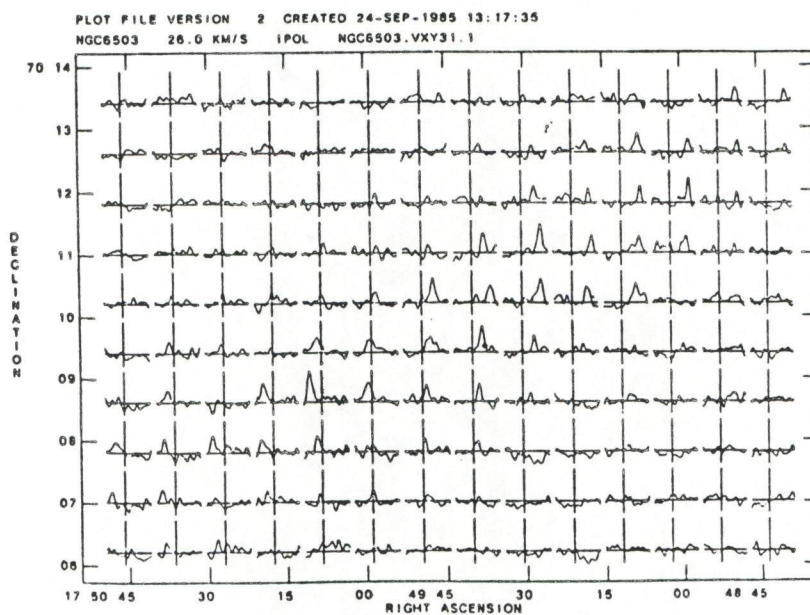
TDRS: CONSTRAINT PARAMETER SET



σ_L - SIGLINE
 $\delta\sigma_L$ - SIGLTOL
 σ_B - SIGBACK
 D_{min} - DMIN
 δD - DMINTOL
 I_{min} - IMIN
 σ_C - SIGCLEAN

FIGURE 7.2-8

AIPS: MULTISPECTRAL DISPLAY EXAMPLE



PLCUB

TABLE 7.2-1

IS & R PREPROCESSING METHODS IN IMAGE CUBE PROCESSING SYSTEMS

		G A R P	S P A M	A I P S	T D R S	I R A F
Filtering						
	box	*				
	deconvolution	*		*	*	*
Derivatives						
	spatial				*	*
Transforms						
	2D FFT			*	*	
Rectification						
	geometric	*		*		*
Curve Fitting						
	polynomial	*		*	*	*
	cubic spline			*		
	Gaussian	*		*	*	
Band fitting						
	Gaussian	*		*	*	*
	Cauchy			*	*	
Corrections						
	calibration stds	*		*		
	instrument error	*		*		
	atmospheric					
	photometric					*
Normalization						
	cube/plane	*				
	cube/spectrum	*	*		*	
Continuum removal						
	straight line	*			*	*
	polynomial	*				*
	Gaussian				*	
	smoothed				*	
Reduction						
	binary amp encodin	*	*			
	binary slope encoding	*	*			
	amp and slope encoding	*	*			
	sparseness compaction	*	*			
	floating pt to integer	*				
	floating pt to byte	*				

TABLE 7.2-2

IS & R CANDIDATE SELECTION IN IMAGE CUBE PROCESSING SYSTEMS

		G A R P	S P A M	A I P S	T D R S	I R A F
Number of candidates	one					*
	many		*		*	*
Source	user library		*			*
	reference library		*			
	spectra from cube	*	*			
	spectra from any cube	*	*			
	synthesized spectra	*	*			
	plot on display		*			
Interactive Selection	single spectrum	*	*			*
	box average		*			*
	regional average				*	
Automated Selection						
	entire library		*			
Channel specification						
	entire spectrum	*	*			
	selectable ranges	*	*			
	deleted points	*	*			

TABLE 7.2-3

IS & R ENVELOPE AND THRESHOLD SPECIFICATIONS IN IMAGE CUBE PROCESSING SYSTEMS

	G A R P	S P A M	A I P S	T D R S	I R A F
Envelope specification					
constant per channel	*				
percentage per channel	*				
abs. diff. per channel	*				
absolute feature					
(1) band centers				*	
(2) centers+widths				*	
adaptive					
Threshold specification					
abs. min matches	*				
percentage min matches	*				
% acceptable matches	*				
max eucl. distance	*				
max hamming distance	*				
(1) amplitude	*	*			
(2) amplitude + slope	*	*			
Noise discrimination					
(1) amplitude		*			
(2) amplitude + slope		*			

TABLE 7.2-4

IS & R SUBCUBE SELECTION IN IMAGE CUBE PROCESSING SYSTEMS

		G A R P	S P A M	A I P S	T D R S	I R A F
Orientation in cube						
	fixed dimension		*			
	any	*			*	*
Channel specification						
	entire spectrum	*				*
	selectable ranges	*	*		*	*
	deleted points	*			*	*
Grouping						
	cluster		*			
	regional				*	
	subcubes	*				

TABLE 7.2-5

IDENTIFICATION METHODS IN IMAGE CUBE PROCESSING SYSTEMS

	G A R P	S P A M	A I P S	T D R S	I R A F
Parameter Mapping					
band center				*	*
band width				*	*
band depth				*	*
Clustering analysis					
supervised		*			
interactive		*			
unsupervised		*			
Comparison Methods					
channel by channel					
(1) rel dif, constant					
(2) rel dif, dif vector					
(3) abs dif, constant					
(4) abs dif, dif vector					
(5) euclidean distance					
(6) hamming distance		*			
features					
Noise detection					
ignore noisy spectra		*			
Mixture analysis					
reference mixtures		*			
modelled					
(1) additive		*			
(2) multiplicative					
(3) nonlinear					
Manual/Visual Aids					
spectral plots	*	*	*	*	*
image overlays	*	*	*	*	*
image movies	*	*	*	*	*
multispectral displays	*	*	*	*	*

TABLE 7.2-6

IDENTIFICATION OUTPUT PRODUCTS IN IMAGE CUBE PROCESSING SYSTEMS

	G A R P	S P A M	A I P S	T D R S	I R A F
Tabulations					
cluster identifications		*			
Visual Display					
image overlays				*	
(1)single id's					
(1)multiple id's		*			
Cube output maps					
identification map					
(1)keyed to tabulation		*			
mixture end-members map		*			
Confidence Levels					
confidence level map					

TABLE 7.2-7

SEARCH METHODS IN IMAGE CUBE PROCESSING SYSTEMS

	G A R P	S P A M	A I P S	T D R S	I R A F
Parameter Mapping					
band center	*			*	*
band width	*			*	*
band depth	*			*	*
Clustering analysis					
supervised		*			
interactive		*			
unsupervised		*			
Comparison Methods					
channel by channel					
(1) rel dif, constant	*				
(2) rel dif, dif vector	*				
(3) abs dif, constant	*				
(4) abs dif, dif vector	*				
(5) euclidean distance	*				
(6) hamming distance	*	*			
Noise detection					
ignore noisy spectra		*			
Mixture analysis					
reference mixtures modelled					
(1)additive		*			
(2)multiplicative					
(3)nonlinear					
Evaluation					
% acceptable matches	*				
distance measures	*			*	
pass/fail, min % matches	*				
pass/fail, max distance	*				
Manual/Visual Aids					
spectral plots	*	*	*	*	*
image overlays	*	*	*	*	*
image movies	*	*	*	*	*
multispectral displays	*	*	*	*	*
statistics on evaluation map	*				

TABLE 7.2-8

SEARCH OUTPUT PRODUCTS IN IMAGE CUBE PROCESSING SYSTEMS

	G A R P	S P A M	A I P S	T D R S	I R A F
Tabulations					
cluster identifications		*			
Visual Display					
image overlays					
(1)single id's	*	*			
(1)multiple id's		*			
Cube output maps					
identification map					
(1)keyed to tabulation		*		*	
mixture end-members map		*			
Confidence Levels					
confidence level map	*				
(1)% acceptable matches	*				
(2)distance measures	*			*	
(3)pass/fail, min % matches	*				
(4)pass/fail, max distance	*				

TABLE 7.2-9

RETRIEVAL PREPROCESSING METHODS IN IMAGE CUBE PROCESSING SYSTEMS

	G A R P	S P A M	A I P S	T D R S	I R A F
Reference standard					
calibration					
resampling					
normalization	*			*	
Reduction					
binary amp encoding	*	*			
binary slope encoding	*	*			
amp and slope encoding	*	*			
sparseness compaction	*	*			
floating pt to integer	*				
floating pt to byte	*				

TABLE 7.2-10

**RETRIEVAL METHODS IN IMAGE CUBE
PROCESSING SYSTEMS**

	G A R P	S P A M	A I P S	T D R S	I R A F
Library search criteria					
spectra name		*			*
attributes		*			*
spectra data values		*			*
features		*			
encodings		*			
Spectral Attributes					
composition		*			
mixture components		*			
Library search methods					
direct					
inverse					
boolean					
Comparison methods					
channel by channel					
(1) rel dif, constant					
(2) rel dif, dif vector					
(3) abs dif, constant					
(4) abs dif, dif vector					
(5) euclidean distance					
(6) hamming distance		*			
Mixture analysis					
reference mixtures only					
modelled					
(1) additive		*			
(2) multiplicative					
(3) nonlinear					
Evaluation					
% acceptable matches		*			
distance measures					
pass/fail, min % matches					
pass/fail, max distance					
input to cube processing					

TABLE 7.2-11

RETRIEVAL OUTPUT PRODUCTS IN IMAGE CUBE PROCESSING SYSTEMS

	G A R P	S P A M	A I P S	T D R S	I R A F
Categories					
classifications		*			*
characterizations					*
Data set output					
cube insertion					
single spectra		*			
Tabulations					
material names		*			*
material attributes		*			*
Visual Display					
image overlays		*			*
(1)single id's		*			
(1)multiple id's		*			
Confidence Levels					
confidence levels					
(1)% acceptable matches					
(2)distance measures		*			*
(3)pass/fail, min % matches					
(4)pass/fail, max distance					

TABLE 7.2-12

COMPUTING ENVIRONMENT OF IMAGE CUBE PROCESSING SYSTEMS

		G A R P	S P A M	A I P S	T D R S	I R A F
Operating System	UNIX	*	*	*		*
	VMS		*	*	*	*
Host	DEC	*	*	*	*	*
	Sun	*	*			*
Language	C	*	*			
	Fortran			*	*	*
Modularity	functions	*	*	*	*	*
	user interface	*	*	*	*	*
Session Control	batch files			*	*	*
	command	*	*	*	*	*
	forms	*				
	session save		*			

TABLE 7.2-13

HYPERSPECTRAL IMAGE CUBE FORMATS IN IMAGE CUBE PROCESSING SYSTEMS

		G A R P	S P A M	A I P S	T D R S	I R A F
cube dimensions	3 N	*	*	*	*	*
axis sizes	AIS only general	*	*	*	*	*
sparse representation	tiles encoded	*	*			
Auxilliary Info	histories abstracts parameter blocks	* *			*	* *
Number of spectral channels	fixed bounded unlimited	*	*	*	*	*
Data types	byte integer floating point double precision	* * * *	*	*	*	* * * *
Subarrays	ranges selectable	* *	*			*

TABLE 7.2-14

**SPECTRUM LIBRARIES IN IMAGE CUBE
PROCESSING SYSTEMS**

		G A R P	S P A M	A I P S	T D R S	I R A F
existence	on line		*			*
	none	*		*	*	
contents	mineralogy		*			
number of members	> 500		*			
organization	attributes		*			*
	data values		*			*
attributes	composition		*			
	location		*			
	instrument		*			
	publication		*			

Appendix 7.2-1. Addresses and Contacts for Systems Surveyed in Section 7.2

1. GARP:

Geosciences Array Processing System
Planetary Geosciences Division/ Hawaii Institute of Geophysics
University of Hawaii
Honolulu, HI 96822
Contact: Jonathan Gradie (808-948-6488 /6320)

2. AIPS:

Astronomical Image Processing System
National Radio Astronomy Observatory (NRAO), Computer Division
Edgemont Road
Charlottesville, VA 22903-2475
Contact: Nancy Weiner (804-296-0328)

3. SPAM:

Spectral Analysis Manager
Distributed by:
COSMIC
Software Information Services
University of Georgia
Computer Services Annex
Athens, GA 30602

Developed by:
Jet Propulsion Laboratory (JPL)
MS/168-514
4800 Oak Grove Dr.
Pasadena, CA 91109
Contact: Jerry Solomon (818-354-2722 /6257)

4. TDRS:

TAURUS Data Reduction System
Institute for Astronomy (IFA)
University of Hawaii
Honolulu, HI 96822
Contact: Joss Bland (808-948-8319)

5. IRAF

National Optical Astronomy Observatories
P.O. Box 26732
Tucson, AZ 85726
(602-327-5511)

7.3 Spectral Identification, Search and Retrieval Capabilities in Spectrum Processing (Only) Systems

7.3.1 Summary and conclusions

This section surveys and compares spectral identification, search and retrieval (IS&R) capabilities in software packages for spectrum processing only, in contrast to the hyperspectral image cube processing systems surveyed in Section 7.2. Most of the software described in this section is proprietary software sold as part of the analysis tools for commercial laboratory spectrometer systems.

First, terms used in this discussion are defined. Second, the processing systems surveyed are described individually, focusing on the IS&R techniques employed. Third, high-level categories of functionality, application, performance and other characteristics for single-spectrum processing systems are presented. Using these generalized categories as the basis for comparison, the processing systems surveyed are contrasted using a matrix format. Finally, the systems are discussed as a group, providing background for Section 7.5, which discusses the application of laboratory systems to remote sensing.

Eight systems and two related algorithms were surveyed. These are listed below in Section 7.3.3. The spectral characterization approaches of the systems fall into three broad comparison categories:

- full spectrum data
- peak/band codings
- derived representations (as in scale space fingerprinting)

Performing spectral searches based on peak information appears to have generally limited utility for reflectance spectra, particularly where mixtures may be present. The peak coding techniques have been motivated largely by disk and processing constraints; parallel processing and special-purpose hardware, such as Digilab's array processor, can help overcome such limitations. Full spectrum analyses are desirable for many reasons, including resolving power, and are very likely required for modeling to be performed dynamically during the identification process (e.g., mixture analysis). The statistical comparison methods and hit quality indices used for full spectrum search in the systems surveyed are all very similar.

Symbolic or encoded spectral representations may be of use for a small spectral population. The development of algorithms for derived representations that are capable of detecting spectral features of fine granularity and that can be consistently applied to many different types of spectra, is an important research area.

7.3.2 Definition of terms

- Spectral identification, search and retrieval are defined in detail in Section 7.1. It should be noted that, as defined in this report, search capabilities are the same as identification capabilities for single-spectrum processing systems.
- Spectrum processing (only) software packages are typically provided by a vendor of a commercial laboratory spectrometer system to perform basic spectrum viewing and manipulation functions, such as display, calibration, and comparison. In this section, only the processing functions related to IS&R will

be discussed.

- Spectrum libraries are collections of reference reflectance spectra obtained from laboratory, field, telescope, spacecraft, and other observations. In this section, two types of spectrum libraries will be described: libraries consisting of spectral attributes (e.g., chemical material composition, band centers, etc.) and libraries consisting of reflectance vs. wavelength data sets that have generally been resampled and calibrated to a known standard for the purpose of comparison. Not all of the systems described below have an on-line spectrum library. Examples of the contents of spectral databases were described in detail in Chapter 5 of this report.
- Baseline removal refers to the measurement and removal of the effects of the darkline response of the spectrometer.
- Continuum removal refers to the estimation and removal of low-frequency spectral features that are not useful in analyzing relatively narrow band features.

7.3.3 Systems surveyed

Several academic and institutional hyperspectral image cube processing systems were determined to support some or all of the IS&R capabilities described in section 7.1. These systems are surveyed here. Appendix 7.3-1 lists the addresses and contact persons for these systems:

- SPECPR, Spectrum Processing Routines, developed at UH and USGS
- Sadtler PC-SEARCH; Philadelphia, PA
- Nicolet SX-SEARCH; Fremont, CA
- Perkin-Elmer SEARCH-3 Expert System; Mountain View, CA
- Mattson SEARCH; Davis, CA
- IBM; Norwalk, CT
- Analect FX Software; Irvine CA
- RELAB, Brown University Department of Geological Sciences; Providence, R.I.

In addition to these systems, the following algorithms for spectral characterization are briefly reviewed:

- Scale Space Fingerprints
- Automated Band Absorption Detection

7.3.4 SPECPR

Spectrum Processing Routines, SPECPR, is a scientist-oriented interactive program for processing one-dimensional arrays. The program is oriented towards processing spectrophotometric astronomical data, but it can be used for general one-dimensional array processing

(Clark 1980). SPECPR was initially developed at the University of Hawaii in the late 1970s by Dr. Roger Clark (now at USGS). Development of SPECPR continues through a user group which includes researchers at UH, USGS, JPL, Brown University, University of Arizona, and others.

SPECPR is a mature system with a large number of display and plotting options, spectrum math operations, and special functions which include continuum removal, band removal, smoothing, interpolation, high-to-low resolution convolution, Gaussian fitting, and many more (SPECPR User's Manual).

The SPECPR file and record format includes provision for a large amount of information on spectral attributes. About half the number of attributes has a fixed format, e.g., time of spectral run, time of processing, coordinates of astronomical body, and angle of illuminating radiation. The remainder is largely free-format or derived information, such as the processing history of the spectra and manual description. Typically, each spectrum has an associated errors record: for the raw spectrum, this may be acquired during the instrument run. The errors represent one sigma standard deviation from the mean and are first computed in the addition routine as a standard deviation of the mean computation. A standard deviation error analysis can be propagated to the final data product through the basic functions (addition, multiplication) and some special math functions. Error analysis is provided in many SPECPR processing routines (e.g., addition, division) to preserve or propagate the errors.

Continuum removal in SPECPR matches two given points of a spectrum and removes the continuum by dividing. The result is scaled to the spectrum file at the two given points by calculating a scaled slope and an intercept (or vertical offset) and converting each data point of the continuum to the scaled continuum. The errors are scaled by a factor given by the ratio of the scaled spectrum to the original spectrum.

To characterize band features, SPECPR provides an interactive routine called *band analysis*. The user displays the spectrum and selects continuum points, and the routine finds the minimum data point (vertical) between the two selected continuum points. A parabola is fitted to the minimum point and the center wavelength is calculated, along with the reflectance on the parabola at that point. A solid vertical line is plotted from this calculated set of coordinates to the continuum and the full width half max (fwhm) is calculated; the fwhm is drawn as a dashed line between the sides of the band. If there are enough channels (e.g., ten) between the two points of the fwhm, the routine will draw a cross at the full width quarter max (fwqm). An asymmetry parameter, band depth, center and fwhm are computed and written to a new spectrum record. Automatic error selection finds the first two points on either side of the channel nearest to the band center and takes one-fourth of the absolute difference as the error value.

The SPECPR routine *spfeatures* takes a wavelength range (only one is currently supported although multiple band searches are planned) and searches a collection of SPECPR records that have been processed by *band analysis* for spectra that fall in the given ranges. The spectrum title, center, error, width, depth, asymmetry and any manual comments are displayed. The user may then retrieve selected records and perform desired analyses.

SPECPR also supports Gaussian fitting. Band information characterized as Gaussians could also be compared and retrieved in a similar fashion, although this has not yet been implemented.

SPECPR runs under most versions of the UNIX operating system and has been ported to the HP, VAX and Sun.

7.3.5 Sadtler PC-SEARCH

Sadtler's PC-SEARCH software was developed by Sadtler to run on an IBM-PC as a stand-alone workstation. The experimental data can be entered manually or through an RS-232 link to

a spectrometer data system that utilizes the JCAMP-DX specification for communications. In addition to peak search, Sadtler software supports searches by chemical name or expression for pre- or postfiltering (Walder).

The search algorithm used to perform spectral searching for both IR spectra and C-13 NIR spectra is based on a peak coding database. In the case of IR spectra, each library entry consists of a peak table generated from the original digital reference spectrum, using a coding algorithm which picks peaks based on the peak being at least 3% T in strength from a local baseline adjacent to the peak. The average number of peaks in the Sadtler database is between 20 and 25 peaks.

The search algorithm is based on set theory, where the unknown spectrum is considered as a set U, containing N peaks as members. Each reference spectrum is considered as a set R, containing M peaks. The intersection of the two sets is denoted as set I, containing K peaks. A perfect match between an unknown spectrum and a reference spectrum would be the case where $N=K=M$, or $I=U$ and $I=R$. This means that every member of U exactly matches a corresponding member of R. In order for two peaks within sets U and R to match and for the match to become a member of the set I, a peak in U must fall within the frequency range of a peak in R, plus or minus a peak tolerance that may be entered by the user as a search parameter or set to a default.

The Sadtler algorithm calculates a Hit Quality Index (HQI) that ranges between 0 and 9990. (The least significant digit is for comparison of peak intensity). Each digit in the HQI is calculated independently of the others and concatenated with the others to obtain the HQI in the form of "ABC". A represents the percentage of peaks in the unknown spectra that have been matched with a peak in the reference spectrum. A is calculated as $A=K/N*9$, where K is the number of peaks that matched and N is the number of peaks in the unknown. B represents the percentage of peaks in the reference spectrum which have been matched with a peak in the unknown. B is calculated as $B=K/M*9$, where M is the number of peaks in the reference. C represents the average difference between peak locations in the unknown and the corresponding peak locations in a reference spectrum. In order for a peak in the unknown to be considered a match, the unknown peak must fall within the peak location of the reference, plus or minus the peak tolerance. The average peak "wobble" is calculated by summing the absolute value of the difference between the peak locations in the intersection set I, and the corresponding peak locations in the reference set R, and then dividing by the number of matching peaks in the intersection set I.

There are two algorithms used in PC-SEARCH:

- forward search
- reverse search

The forward search is a measure of how well the unknown spectrum matches the reference spectrum. The forward search works best when the unknown is a pure or nearly pure compound. Since the A term in the HQI is a measure of how well the intersection matches the unknown, the HQI takes the form ABC, where the A term is weighted the heaviest.

The reverse search is a measure of how well the reference matches the unknown spectrum. The reverse search works best when the unknown contains more than one component. If the unknown is a mixture of chemical compounds, then the search algorithm must account for matching only a subset of the peaks in the unknown. Since the B term in the HQI is a measure of how well the intersection matches the reference, the HQI takes the form BAC where the B term is weighted the heaviest.

To be considered a match and thereby appear in the hit list, the reference must match at least half of its peaks with the unknown, or vice versa. The HQI measure may be misleading in some instances, for example, the case of a simple compound that has only a few peaks, which match very closely with some of the peaks in a more complicated compound.

7.3.6 Nicolet SX-SEARCH

Nicolet's search software, developed to work with its SX and DX FT-IR spectrometer systems, compares the unknown spectrum point by point to each library spectrum and thus attempts to take into account all peak positions, shapes and intensities. Typically this involves some deresolution of the unknown spectrum, depending on the resolution of the database spectra.

For its FT-IR spectral database, Nicolet supports three search routines:

- full
- omni
- peak

The full spectral search directly compares an unknown spectrum to all of the spectra contained in a selected FT-IR database reference library. A match quality metric is calculated (four matching algorithms are available, which are described below) and the best matches are displayed. The omni search is an extension of the full spectral search and enables the investigator to use information available on the unknown, in addition to the IR spectrum itself, for prescreening. Physical properties such as boiling point or density may be used. The peak search compiles a "peak code" for the spectrum and initiates a search of a peak library, which is a condensed and encoded IR library where each spectrum is characterized in terms of its strongest peaks.

The DX and SX full spectral search routines can be performed with any of four matching algorithms:

- absolute difference = $\sum |x_i - y_i|$
- derivative difference = $\sum [|(y_i - y_{i-1}) - (x_i - x_{i-1})|]$
- absolute squared difference = $\sum |x_i - y_i|^2$
- derivative square difference = $\sum [|(y_i - y_{i-1}) - (x_i - x_{i-1})|]^2$

These differences are interpreted as search metrics only in a relative sense. The search algorithms can overcome certain spectral distortions, for example, by compensating for noisy spectra, variations in sampling conditions, or comparisons of reflectance and transmittance spectra. The absolute difference algorithm weighs all points equally and is useful for comparing spectra that have good signal-to-noise ratios, as in Figure 7.3-1, and where the sampling procedures of the unknown and the references are similar. Derivatives enhance peak position information while minimizing intensity information, and tend to favor sharp bands over broad ones. Figure 7.3-2 shows a spectra for which the absolute difference metric would have been inappropriate since the relative peak intensities differ. In this case, the derivative metric is preferable.

The absolute squared difference algorithm weighs large differences more than small ones, which is useful if the signal-to-noise ratio is not optimal. Figure 7.3-3 shows a noisy plot where a search algorithm that is less sensitive to baseline noise and favors strong peaks is appropriate. Since taking derivatives of noisy spectra will increase noise, derivative methods in such a case are not useful. The derivative square difference algorithm is useful for reflectance spectra such as that shown in Figure 7.3-4, since it minimizes the contribution of very large broadbands (which might result from surface reflections) and sharpens the location of the bands. Squaring the terms helps compensate for unreliable relative intensities, which, for example, might occur in areas of strongly absorbing features where little energy is reflected to the

detector.

7.3.7 Perkin-Elmer Search-3

Search-3 is the proprietary software offered by Perkin-Elmer for spectral interpretation and library searches. It is advertised as an expert system due to its interpretive components, which are described below. It is designed for use with the Perkin-Elmer 7000 series computers and either Perkin-Elmer dispersive- or FT-IR instrumentation.

The search software produces an interpretation of the unknown spectrum, in a Possible Structural Unit (PSU) format. A PSU is defined as a molecular fragment, a function group, or a combination of functional groups that can be detected in the IR of a sample by a set of well-defined bands. The development of the PSU is based on the wavenumber position or range for a combination of bands to indicate a well-defined macro-group frequency, and the assignment of a range of intensity values for each PSU band to accommodate relative intensities.

Two main approaches are adopted in the interpretation scheme: compound class-specific, which is for either pure compounds or mixtures that have at least one major component, and general PSU, which is intended to indicate the presence of certain major or minor functional groups. Compounds that contain functional groups that have substantial spectral overlap generally give only a single PSU class that is consistent with the functional group most prominent spectroscopically.

Following the interpretation step, the spectrum is compared to the search library, using PSUs and peak matches to rank the matches. Two libraries are then used: a search-formatted library of compressed peak table information and PSUs, and a spectral view-formatted library based on Sadtler digital spectra. The peak table format allows both peak position and intensity information to be obtained from the relatively high-resolution unknown since the unknown does not have to be deresolved. A minimum %T tolerance is used for the formation of the peak table, as well as "no bands" information.

Figure 7.3-5 illustrates the search functional flow. The input for applying Search-3 to an unknown spectrum is automatically obtained in a digitized format referred to as a peak table (e.g., Figure 7.3-6). A listing of PSUs is derived to give spectral interpretation. The second output involves matching of the unknown spectrum to a spectral library.

Five matching algorithms produce five hit lists. Four of the search algorithms use both the PSU and peak match information to determine the ranking of the library spectra, based on the assumption that the unknown is a single component or a mixture. Various weightings are then applied to the PSU and peak match information. The first algorithm for identifying mixtures imposes no penalty for having extra bands in the unknown. It is biased toward PSU match and so should give better results for unknown mixtures that contain structurally similar components. The second mixture algorithm should give better results for mixtures containing structurally dissimilar components.

7.3.8 Mattson SEARCH

The Mattson Spectral Search Package measures an unknown compound run on a Mattson FT-IR system and searches the unknown against the commercial or user libraries stored in the system.

The search package supports three principal search methods:

- Direct search (4 or 32 cm^{-1} resolution), where an unknown compound is searched against the library, giving the closest matches in the report. A choice

of five metrics is provided: absolute difference, absolute squared difference, derivative difference, derivative squared difference, and Euclidean difference.

- Inverse or reverse search, where an unknown mixture is searched against libraries. Compounds that might be components of the mixture are reported.
- Boolean search, where the libraries are polled for compounds that match certain spectral conditions of the unknown, such as the presence or absence of peaks at specified spectral ranges.

These methods can be combined into one search. For example, one might narrow down the database with a peak search and then use a direct search against the remaining compounds.

There are five Sadtler library components that support the Mattson Search package: (1) a spectra component containing fully digital spectra; (2) deresolved spectra; (3) a name component; (4) reverse search components; and (5) Boolean search components consisting of peak and intensity information.

7.3.9 Digilab

Digilab offers its Search-32 spectral search software for use with Model 3200 Data Systems. Search 32 is a menu-driven software package that supports the installation of commercial spectral libraries, the creation of user libraries, and the identification of unknown spectra by comparison to these libraries.

The libraries can be manually examined by displaying a library entry, plotting the entry, and performing a manual comparison. Automatic searching is provided for one or multiple spectra, against single or multiple commercial and user libraries. The results can then be merged. An unknown can be searched against multiple library files. Libraries of 4, 8, and 32 cm^{-1} resolution are supported for medium- or high-resolution viewing formats and for low-resolution, faster searches.

Full spectral searches are supported by means of spectral subtraction techniques using a library of complete spectra (as opposed to peak encodings). Each spectrum is stored over its spectroscopically significant region. An unknown spectra is converted to the same resolution and is then subtracted in turn from each of the library spectra. The subtraction is performed by scaling the unknown, using the same parameters as the library spectra to form a difference spectrum.

One of four search algorithms, used to calculate the hit quality index, may be selected for the search. Using the notation U_W for the unknown spectrum (where W is the wavenumber), L_{iW} for the i^{th} library spectrum, U for the normalization constant for the unknown, and L_i for the normalization constant for the library spectrum, the hit quality index HQI is defined as:

- absolute value

$$\text{HQI}^2 = \sum_w \left(\frac{|dU_w|}{|U|} - \frac{|dL_{iW}|}{|L_i|} \right)$$

$$|L_i|^2 = \sum_w L_{iW}^2$$

- Euclidean (least-squares)

$$HQI^2 = \sum_w \left(\frac{|U_w|}{|U|} - \frac{|L_{iw}|}{|L_i|} \right)^2$$

- derivative absolute value

$$HQI^2 = \sum_w \left(\frac{|U_w|}{|U|} - \frac{|L_{iw}|}{|L_i|} \right)$$

- derivative least-squares

$$HQI^2 = \sum_w \left(\frac{|dU_w|}{|U|} - \frac{|dL_{iw}|}{|L_i|} \right)^2$$

An HQI near zero indicates a close match. Search-32 produces a list ranked in order of decreasing HQI. According to Digilab literature, the Euclidean algorithm appears to be the best and fastest choice for most spectral search applications. The derivative least-squares and derivative absolute value algorithms attempt, as does baseline correction, to improve search identification by removing interfering effects. Since Search-32 uses baseline correction for both unknown spectra and spectra entered into search libraries, the derivative least-squares and derivative absolute value algorithms may not be helpful.

Regions of the spectra may be masked to remove peaks that the user wished to exclude from the search criteria. When a search is completed, a report is printed listing the spectrum name, the number of the unknown and, from the best fit to the worst, the CAS names, library numbers and hit quality indices (a type of correlation coefficient) of the best matching spectra.

Search-32 can also be used to identify components in mixtures, and allows subtraction of library spectra from a sample spectrum with re-searching of the residual.

Digilab's software capabilities are quite good relative to the other vendors surveyed. Digilab is the only vendor who offers an array processor for its FTS 60, which can display full-resolution spectra in real time and, at the completion of the run, search those spectra against a full-resolution library.

7.3.10 IBM

IBM offers an infrared spectral search package for its IR/44 and IR/85 spectrometers. The search package includes spectrum search, peak search, compound information search, and combined search modes. The spectrum search mode of the search package takes an unknown compound, run on an IBM FT-IR system, and searches the unknown against the libraries stored in the system. The peak search report allows the user to manually input peak locations of unknown compounds and then have this information searched against a database.

The compound information search mode takes advantage of the fact that each library spectrum may be stored with some compound information (as with the Sadtler libraries), such as molecular weight. The compound information can be used as a retrievable database, as well as a method of selectively narrowing a spectrum search. The combined search permits the user to merge the spectrum information and/or peak search modes with the spectrum search mode to make them more selective and specific by incorporating additional information available on the unknown compound.

IBM's spectral search software, though adequate, does not appear to have any innovative

features.

7.3.11 Analect

The standard Analect RFX software package includes autosubtraction, baseline normalization, polynomial smoothing, first through fourth derivatives, peak identification and Kubelka-Munk normalization. It is compatible with the JCAMP-DX specifications for communications.

Analect's database searches use a high-speed vector correlation search program with modules to compress spectra for inclusion in a user-defined database and to search an unknown spectrum against this database or any of several databases available from Analect. The spectrum is treated as a multicomponent vector, measuring the Euclidean distance between an unknown spectrum and the individual spectrum in the library. It thus takes into consideration both absorbance (reflectance) and frequency information.

Analect's search software, by comparison to software of other vendors, appears limited in scope.

7.3.12 Relab

Relab is a spectral analysis package being developed at the Department of Geological Sciences at Brown University under the supervision of Dr. Carle Pieters. At present, its functionality is generally a subset of SPECPR. Relab routines include spectral resampling, noise removal, continuum removal, spectral smoothing and mixture models (Pratt).

7.3.13 Scale Space Fingerprints

(Note: this algorithm is included to broaden the range of spectral representation techniques presented in this report.)

The scale space fingerprints algorithm has been proposed as a method of symbolic spectral representation for material identification systems. The approach involves the creation of a scale space image by Gaussian convolution and then establishing a "fingerprint" by examining the concavities and second-order derivatives for zero crossings (Marr and Hildreth 1980). The resulting description captures band information and relative feature intensities for well-resolved bands of comparable center and width information.

However, the Gaussian smoothing degrades high-frequency information. Hence, scale space fingerprinting may be insensitive to overlapping band information or small spectral features. The sigma used may be difficult to determine and the resulting parameterization error is difficult to estimate. It is questionable whether fingerprints of spectra acquired under similar conditions are comparable if different sigmas are used to derive them. The technique may be sensitive to additive convolution of constituent bands. Nonetheless, because the fingerprint is compact and may be treated either symbolically or quantitatively, this approach is a useful contribution to the problem of reducing the processing and storage requirements of spectral identification.

7.3.14 Automated absorption band detection

(Note: this algorithm is included to broaden the range of spectral representation techniques presented in this report.)

A multiple high-order derivative analysis algorithm has been developed at the

University of Massachusetts which automatically extracts absorption band positions from reflectance spectra (Huguenin and Jones 1986). The algorithm assumes that bands are approximately symmetric about the band center. Continuum contributions, phase angle effects, and broad low-frequency information are said to be suppressed. Overlapping bands with centers as close as 0.3 to 0.5 W (full band width at half maximum intensity) can be resolved, as long as the bands have comparable widths and intensities. The results are said to be relatively insensitive to whether constituent bands convolve additively or multiplicatively. Spectral resolution can be moderately low, requiring only 4 to 8 data points per W.

The algorithm is sensitive to noise, and data smoothing is required. A spectral pattern recognition algorithm statistically characterizes the frequency distribution of intensity variations in a sliding segment across the spectrum. An intelligent control algorithm can then locally adjust the segment lengths for smoothing until high-frequency components of the spectrum are suppressed. A cubic spline is applied then followed by a multiple high-order derivative algorithm for the center point of the sliding segments.

The processing is fully automated and the same standardized procedure is followed for all spectra. No continuum removal or band modeling is needed.

7.3.15 Spectral processing system characteristics

High-level functionality comparisons for the surveyed systems are listed in Tables 7.3-1 through 7.3-10. The comparisons are given in matrix format for the identification and retrieval techniques listed below:

- Envelope and Threshold Specification
- Identification Output Products
- Identification
 - Identification Preprocessing
 - Spectrum Specification
 - Library Specification
 - Identification Methods
- Retrieval
 - Retrieval Preprocessing
 - Candidate Selection
- Processing System Features
 - Computing Environment
 - Data Formats
 - Spectrum Library
 - Performance

7.3.16 Discussion of surveyed processing systems

The spectral characterization approaches of the above systems fall into three broad comparison categories:

- full spectrum data
- peak/band codings

- derived representations (as in scale space fingerprinting)

Performing spectral searches based on peak information appears to have generally limited utility for reflectance spectra, particularly where mixtures may be present. The peak coding techniques have been motivated largely by disk and processing constraints; parallel processing and special-purpose hardware, such as Digilab's array processor, can help overcome such limitations. Full spectrum analyses are desirable for many reasons, including resolving power, and are very likely required for modeling to be performed dynamically during the identification process (e.g., mixture analysis).

The statistical comparison methods and hit quality measures used for full spectrum search in the systems surveyed are all very similar. The development of new distance metrics and adaptive methods for choosing their application would be an important contribution to full data search evaluations.

Finally, symbolic or encoded spectral representations may be of use for a small spectral population. The development of algorithms for derived representations which are capable of detecting spectral features of fine granularity and can be consistently applied to many different types of spectra is an important research area.

7.3.17 References

Clark, R. N. (1980), *A Large-Scale Interactive One-dimensional Array Processing System*, a publication of the Astronomical Society of the Pacific, 92, 221-224, April.

Huguenin, R. L. and Jones, J. (1986), *Intelligent Information Extraction from Reflectance Spectra: Absorption Band Positions*, manuscript from the Remote Sensing Center at the University of Massachusetts, January.

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Pratt, S., Brown University, private communication.

SPECPR User's Guide, a publication of the Planetary Geosciences Division of the Hawaii Institute of Geophysics at the University of Hawaii, Honolulu, Hawaii.

Vendor-supplied literature.

Walder, F., *Optimizing Spectral Search for Various Sampling Techniques and Problems*, memorandum, Sadtler FT-IR Applications Lab.

FIGURE 7.3-1

ABSOLUTE DIFFERENCE ALGORITHM CANDIDATES

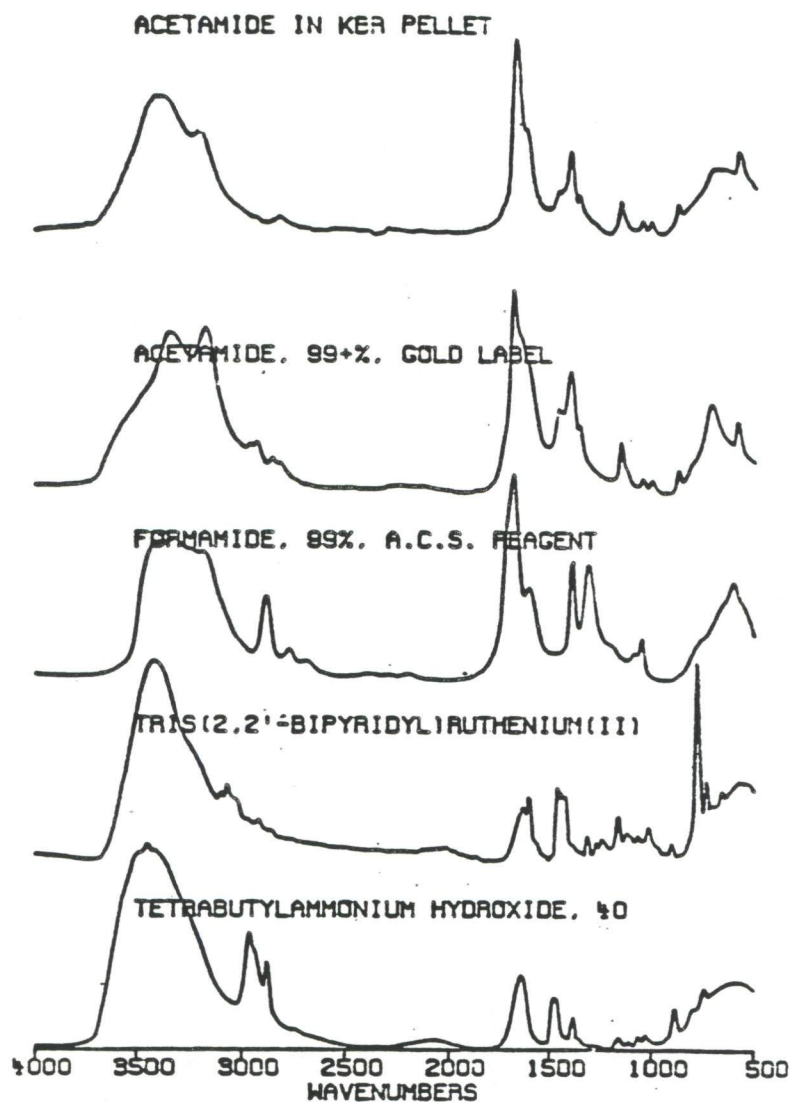


FIGURE 7.3-2

DERIVATIVE ALGORITHM CANDIDATES

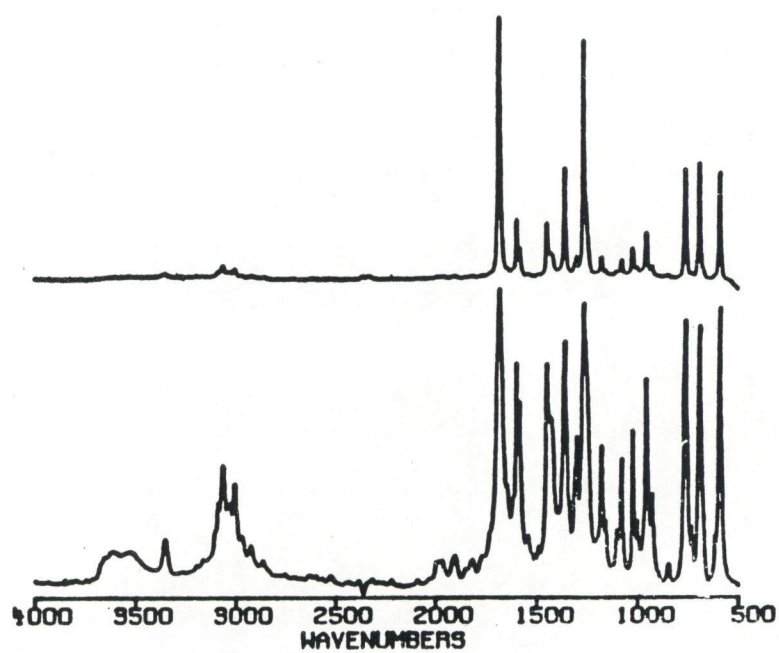


FIGURE 7.3-3

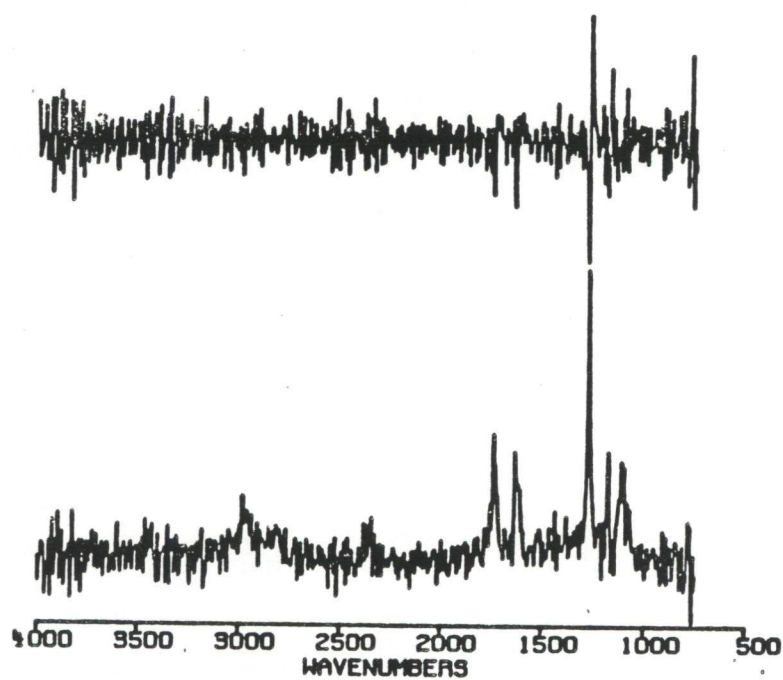
**ABSOLUTE SQUARED DIFFERENCE
CANDIDATES**

FIGURE 7.3-4

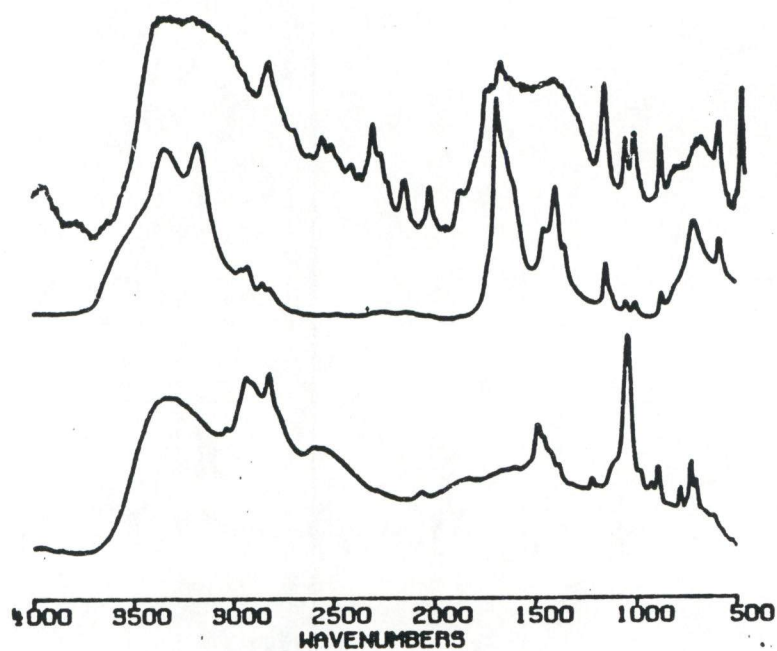
**DERIVATIVE SQUARE ALGORITHM
CANDIDATES**

FIGURE 7.3-5

PERKIN-ELMER SEARCH SOFTWARE OVERVIEW

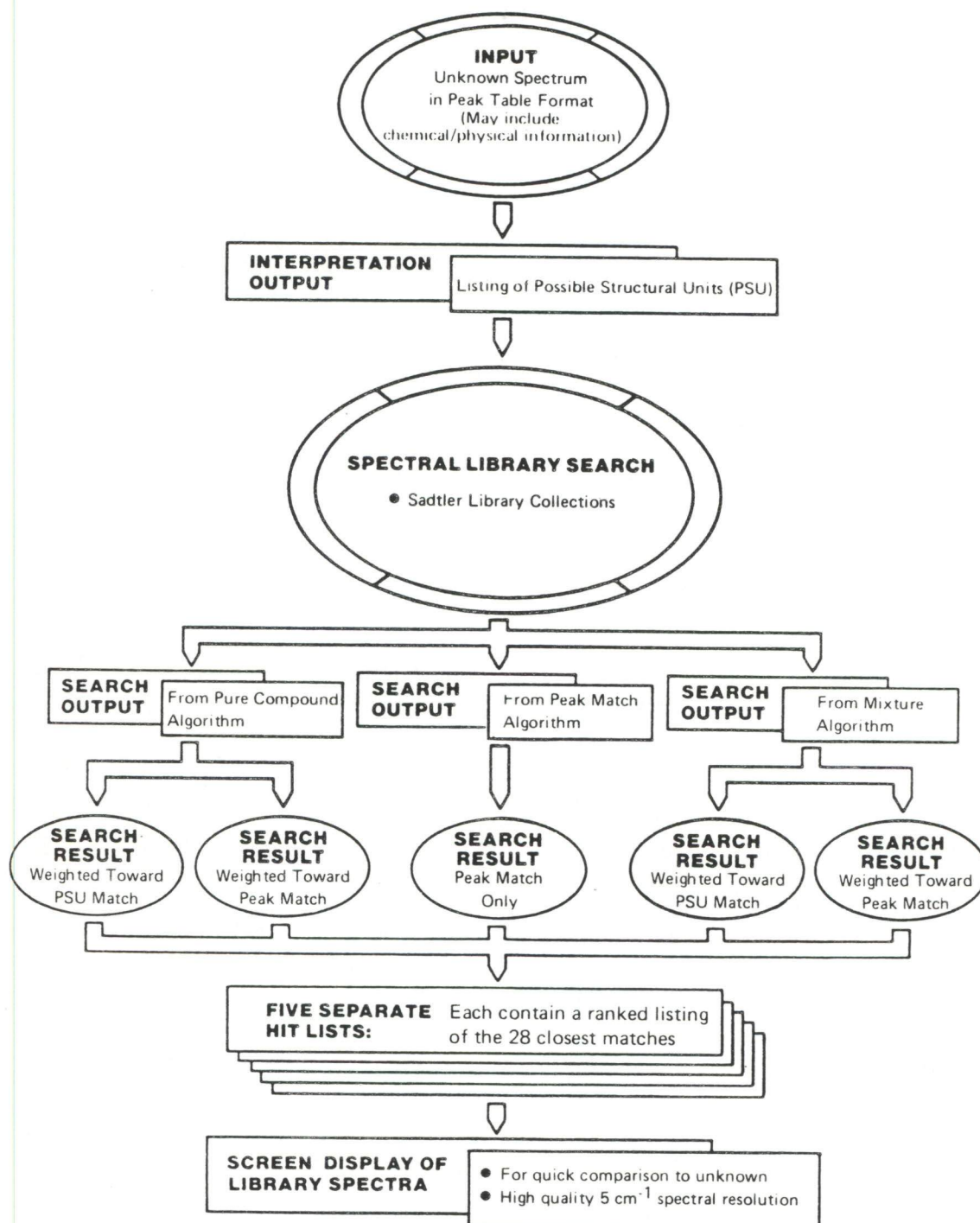
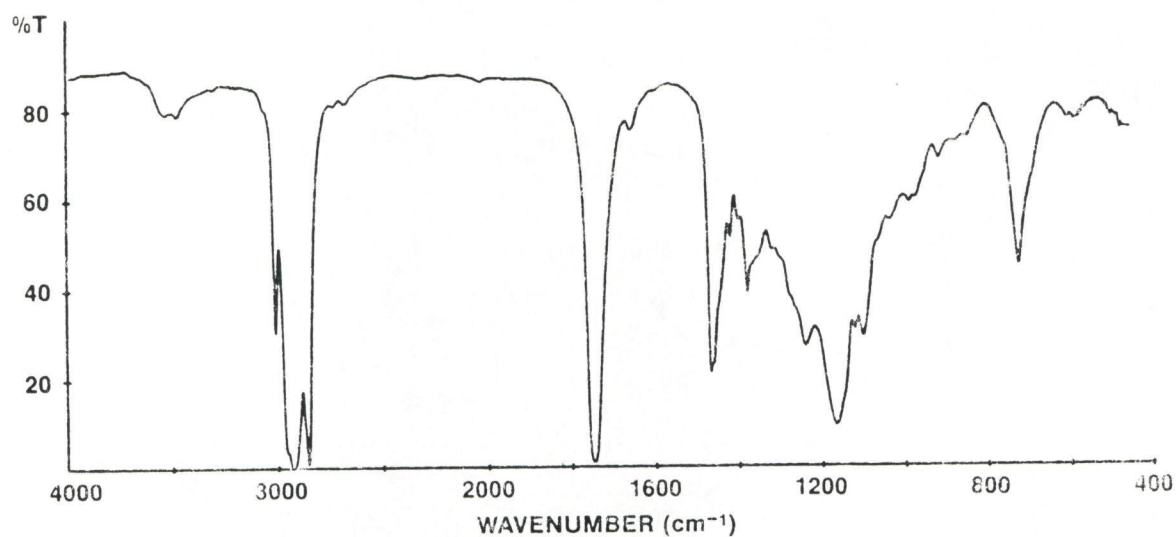


FIGURE 7.3-6

PERKIN-ELMER PEAK TABLE DISPLAY



X:	3551	4000	-	450	1.00	0.20	100.00	T	F	S3	UNOIL
REF:	4000	98.20	2000	98.99	450						
	3531	89.1	3473	88.6	3009	34.3	2924	0.2	2855	0.9	
	2730	91.6	2680	92.3	2335	98.8	2030	98.1	1746	1.1	
	1657	86.0	1465	24.5	1419	59.3	1398	63.4	1379	45.4	
	1239	31.1	1165	10.4	1120	35.6	1100	33.6	1032	63.6	
	987	67.9	971	69.2	915	79.0	723	52.2	585	89.1	
	527	93.1	495	90.3	473	86.7	463	86.6			
END 29 PEAKS FOUND											

TABLE 7.3-1

IDENTIFICATION PREPROCESSING METHODS IN SPECTRUM PROCESSING SYSTEMS

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Filtering									
box					*				
Smoothing									
weighted					*				
Fitting									
polynomial					*				*
cubic spline					*				
Gaussian					*				
Transforms									
FFT		*	*				*	*	
Corrections									
calibration stds		*	*	*	*				*
instrument error									
atmospheric									
thermal									
photometric									
band removal			*		*				*
glitch removal			*		*				
phase									
baseline	*	*	*	*	*	*	*	*	
Normalization									
channel							*		*
Continuum removal									
straight line							*	*	

TABLE 7.3-2

IDENTIFICATION ENVELOPE AND THRESHOLD SPECIFICATIONS IN SPECTRUM PROCESSING SYSTEMS

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Envelope spec.									
peak discrimination	*	*	*	*	*		*	*	
peak tolerance	*								
weight for PSU	*								
weight for peak	*				*				*
weight for PSU -mixtures	*								
weight for peak -mixtures	*								
Threshold spec.									
number matching peaks	*	*	*	*	*	*	*	*	
percentage matching peaks									
absolute difference	*						*		
square difference	*						*		
absolute derivative	*						*		
square derivative	*						*		
number hits to output	*	*	*	*					

TABLE 7.3-3

IDENTIFICATION SPECTRUM SELECTION IN SPECTRUM PROCESSING SYSTEMS

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Channel spec.									
entire spectrum			*		*		*		*
selectable ranges			*		*		*		*
deleted points			*		*		*		*

TABLE 7.3-4
IDENTIFICATION METHODS IN
SPECTRUM PROCESSING SYSTEMS

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Comparison methods									
set theory		*							
vector correlation									
peak apex	*	*			*				
peak apex and intensity	*	*							
presence of bands	*	*	*	*	*	*	*	*	*
absence of bands									
intensity through spectrum			*						
channel by channel				*					
(1) 4 wave				*			*		
(2) 8 wave				*			*		
(3) 32 wave				*			*		
digital to func group	*								
peak-intensity matches	*	*		*	*	*	*	*	
can override algorithm									
forward search		*							
reverse search		*							
boolean search		*							
ignore extra bands									
ignore func. groups	*								
functional group	*								
frequency match									
Research strategies									
1 pass					*				
32 wave, 8 wave									
functional group, member	*								
Presearch strategies									
physical properties	*								
Multiple libraries									
search in succession	*	*	*	*	*	*	*		*
Mixture analysis									
modelled									
(1) additive	*								
Manual/Visual Aids									
derivatives	*				*				
integration	*								
relative peak calc	*								
band int ratios					*				
auto peak calc					*				
rescale					*				*
resize					*				*
spectral plots	*	*	*	*	*	*	*	*	*
multispectral displays	*	*	*	*	*	*	*	*	*

TABLE 7.3-5

IDENTIFICATION OUTPUT PRODUCTS IN SPECTRUM PROCESSING SYSTEMS

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Output type									
classification	*								
characterization	*								
library member	*	*	*	*	*	*	*	*	*
Hit display									
single best hit	*	*	*	*	*	*	*	*	*
multiple hits	*								
multiple hit types									
4 wave		*		*			*		
8 wave		*		*			*		
32 wave		*		*			*		
Tabulations									
search reports	*	*	*	*	*		*		*
hits	*	*	*	*	*	*	*	*	*
Confidence levels									
hit quality index	*	*	*	*	*	*	*	*	*
Justifications									
why assignments made	*								
potential problems	*								

TABLE 7.3-6

RETRIEVAL PREPROCESSING METHODS IN SPECTRUM PROCESSING SYSTEMS

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Reference standard									
calibration					*				*
resampling	*				*				*
normalization					*				*

TABLE 7.3-7

RETRIEVAL CANDIDATE SELECTION IN SPECTRUM PROCESSING SYSTEMS

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Number of candidates									
one	*	*	*	*	*	*	*	*	*
many	*	*	*	*		*	*	*	
Source									
user library	*				*		*		
reference library	*	*	*	*	*	*	*	*	*
spectra from cube									
synthesized spectra							*		
Channel specification									
entire spectrum							*		
selectable ranges							*		
deleted points							*		

TABLE 7.3-8
COMPUTING ENVIRONMENT

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Operating system UNIX VMS				*	*				*
Host DEC Sun PE IBM					*				*
	*			*		*			
Language C Fortran						*			*
					*	*			*
Modularity functions user interface				*	*				*
				*	*				*

TABLE 7.3-9
SPECTRUM DATA FORMATS

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Auxilliary Info									
histories					*				
abstracts					*				
Number of spectral channels									
fixed									
bounded					*				
unlimited									
Data types									
byte									
integer									
floating point					*				*
double precision									

TABLE 7.3-10
SPECTRUM LIBRARY

	P E	S A D T	N I C O	M A T T	S P E C	I B M	D I G I	A N L C	R E L A
Existence									
on line	*	*	*	*	*	*	*	*	*
off line									
none									
Organization									
attributes	*	*	*	*	*	*	*	*	*
data values			*		*				*
peak table	*								
Attributes									
composition	*	*			*				*
location					*				*
instrument					*				*
publication					*				*
User created entries									
from instrument	*				*				
annotations					*				

Appendix 7.3-1. Addresses and Contacts for Systems Surveyed in Section 7.3

1. SPECPR:

Spectrum Processing Routines
U. S. Geological Survey
Mail Stop 964
Branch of Geophysics, Remote Sensing Section
Box 25046 Denver Federal Center
Denver, CO 80225
Contact: Roger Clark (303-236-1332)

2. Sadtler:

Sadtler Research Laboratories
3316 Spring Garden Street
Philadelphia, PA 19104
(215-382-7800)

3. Nicolet:

Nicolet Instrument Corporation
5225-1 Verona Road
Madison, WI 53711
(608-273-5004)

4. Perkin-Elmer:

Perkin-Elmer
Instrument Sales and Service Division
411 Clyde Avenue
Mountain View, CA 94043-2284
(415-961-2050)

5. Mattson:

Mattson Instruments, Inc.
1001 Fourier Court
Madison, WI 53717
(608-833-5515)

6. Digilab:

BioRad Digilab Division
780 Trimble Road, Suite 201
San Jose, CA 95131
(408-435-5530)

7. IBM:

IBM Instruments Inc.
Orchard Park
P.O. Box 332
Danbury, CT 06818
(203-796-9839)

8. Analect:

Analect Instruments
17819 Gillette Avenue
Irvine, CA 92714
(714-660-8801)

9. Relab:

Brown University
Department of Geological Sciences
Box 1846
Providence, RI 02912
(401-863-2417)

7.4 Application of Laboratory Systems and Automated Methods to Remote Sensing

The survey of state-of-the-art spectral data management and analysis techniques presented in Sections 7.1 through 7.3 reveals that some of the functionality of the highly interactive, statistical spectral search software packaged with commercial spectrometers has not been integrated into institutional hyperspectral image cube processing systems. The first part of this section identifies features of the single-spectrum processing systems surveyed in Section 7.3 that would be useful to include in hyperspectral image cube processing systems for remote sensing, such as those surveyed in Section 7.2. The second part of this section discusses in detail the need for and effectiveness of automated methods in spectrum identification.

7.4.1 User Interface

The user interface for most of the commercial software surveyed in section 7.3, such as that provided by Nicolet, is excellent. These software systems feature high-quality graphics, easily learned menus and command language, excellent use of color and hard-copy, and tight integration with the instrument operation. The user interfaces of several of the hyperspectral cube processing systems are not as flexible.

7.4.2 Spectral feature classification

Perkin-Elmer's Possible Structural Unit (PSU) construction, i.e., the grouping together of spectra with similar band characteristics or more general spectral signature properties such as shape, appears to be a useful aid to identification and interpretation. (The PSUs for the Perkin-Elmer reference library are defined by a team of expert spectroscopists.)

7.4.3 Pre- and postfiltering, iterative searches

SPAM uses a one-step retrieval procedure to extract spectra from its database. While this approach is feasible for a small database, filtering the identification or retrieval on known or suspected mineralogical properties, the use of structural units, and other approaches offer obvious gains in efficiency.

7.4.4 Mixture heuristics

Heuristics are needed in hyperspectral cube processing to help estimate, early in the search process, whether an unknown sample is pure, an intimate mixture of a few compounds, or a mixture of many compounds. Perkin-Elmer, in particular, states that their search algorithms help make this determination.

7.4.5 Multiple search strategies

As explained in Section 7.3, the capability to support alternative search strategies (peak-based, data-based, etc.) is useful since the quality of the unknowns in hyperspectral image cubes will typically vary over a much wider range than that of spectra obtained under laboratory conditions.

7.4.6 Multiple comparison algorithms

It is recommended that the five point-by-point numerical algorithms described in Section 7.3 be adopted in hyperspectral identification methods, along with the higher level characterizations, such as PSUs.

7.4.7 Multiple-resolution libraries

The trade-off between efficiency and accuracy of identification is difficult to estimate in a large hyperspectral cube, but heuristics can perhaps be developed to indicate when the faster, low-resolution data point search can be undertaken.

7.4.8 Automated band analysis

SPECPR's band analysis routines and Huguenin's techniques may offer advantages over those incorporated in the hyperspectral systems surveyed in Section 7.2.

7.4.9 Data standards

It may be desirable to add attribute information contained in commercial libraries, such as Sadtler's, to the hypercube standards currently being defined institutionally by JPL and other organizations.

7.4.10 Need for and effectiveness of automated methods

A hyperspectral data set and a companion spectrum library are employed to perform two functions: (1) to determine the location of materials or entities of interest, and (2) to determine the identity of materials or entities at locations of interest. Once a data set of the appropriate area is acquired, both of these functions could be performed using direct spectral matching between a perfectly calibrated hyperspectral field data set and a complete spectrum library. In locating materials with known spectral properties, the spectra of the knowns are used as a template against which the field data are compared. In determining the identity of materials at a given location, the spectra of the unknowns are used as templates against which the spectrum library is compared. If both data sets are "perfect", that is, there is direct and unambiguous correspondence between the spectrum of a material as measured in the laboratory and those obtained in the field, this direct spectral matching will be successful in both determining the identity of unknowns and locating knowns.

Unfortunately, unavoidable imperfections in both the field data and the spectrum library can seriously degrade the efficacy of this strict spectral matching procedure. Imperfections in field data are due to errors that cause deviations from the characterization of the true reflectance of an observed material. There are three major sources of error in field data sets: (1) random error due to finite signal-to-noise ratios; (2) systematic error due to imperfect calibration to reflectance, and (3) the presence of mixtures of materials that produce composite spectra at a given location. The drawback to a practical spectrum library is not error but completeness. Even if the library is used with a perfectly calibrated data set--one with all atmospheric and instrumental effects corrected to levels matching the data quality of the library with a signal-to-noise ratio equal to or exceeding that of the library, and with no spatial elements being mixtures--the library would have to contain, for each material to be identified, a suite of spectra measured under all the physical conditions to be found in the area under scrutiny. These conditions include external variables such as lighting conditions and temperature, and also internal variables such as the physical state of the material (grain size, distribution) or orientation of surfaces. All of these variables, and more, cause significant

changes in the appearance of the spectrum of any material. It is not practical to measure, calculate, or even store the entire suite of possible spectra of a given material. The presence of mixtures infinitely compounds this problem. Even if accurate models were available for calculation of mixtures from end-member spectra, the sheer volume of data prohibits storing all possible combinations of mixtures for even a small suite of end-members. To guarantee a successful spectral match, the library would have to contain, for each material, the entire continuum of spectral variation that corresponds to the variations of physical variables to be encountered in the field. Digitization of this continuum would have to be of resolution finer than the errors in the data set. It is clear that no library could be expected to meet these stringent requirements except for the most restricted cases where some material shows very little variation under the range of measurement conditions to be found in a field observation.

In summary, the utility of strict spectral matching is inhibited by the presence of miscalibration and mixtures in field data, and by the incompleteness of practical spectral libraries.

However, as defined previously, the goal of hyperspectral remote sensing is not to match spectra but to locate known and identify unknown species in a scene. Thus, the information about the precise physical state of materials in the field that strict matching supplies is unimportant to the primary task. Strategies that are insensitive to physical state or to the presence of mixtures can then be developed.

One such strategy is to determine which spectral parameters are relatively invariant with respect to changes in physical parameters. Matching based on derived spectral invariants is far more likely to produce successful identifications than matching of the spectra themselves.

An example of a spectral invariant is diagnostic absorption or emission band centers. For minerals under a wide variety of physical states of grain size, grain size distribution, and ranges of temperature comparable to those found on Earth, the center of diagnostic absorptions is found to be constant, though the band depths and shapes of the spectra change drastically. In this case, a search of a field data set or a library for specific absorptions would be much more fruitful in identification than spectrum matching. The invariant spectral attribute has a physical basis for being stable over an extremely wide range of physical conditions. Other spectral invariants may be the positions of diagnostic absorption features, simple albedos at specific wavelengths, ratios, etc. The utility of this derivation is that these spectral invariants are diagnostic tools that are robust against changes in the physical state of the material to be identified. To identify a desired material, the same analysis applied to the library spectra to derive the values of the spectral invariants is applied to the field data. The values of the invariants derived from the library spectrum are then compared to the values derived from the data to arrive at spectral matches. This procedure does not rely upon strict spectral matching nor on pattern recognition. Rather, it relies upon the values of quantitative spectral parameters derived from the actual variance in the spectral behavior of a material when physical parameters are varied in ways appropriate to the measurement conditions of the field data.

Is this approach robust against errors in the field data? In the case of random error, there is no alternative to enlarging matching envelopes. But due to the fact that invariants will often rely upon more than a single band, the statistical advantage of using more than one independent measurement will help counter the effects of random error.

In the case of systematic error due to miscalibration, invariants derived from wavelengths susceptible to error must be discounted or eliminated. Other sensitive parameters, such as absolute albedo, should also be de-emphasized. A crucial task in the early testing of a system should be the characterization of common sources of error through carefully calibrated test flights.

Lastly, the important, ubiquitous problem of mixtures must be addressed. Most spatial elements in a hyperspectral scene will be composed of mixtures of materials. These mixtures will obey different scattering laws, depending upon their physical condition. For example, mixtures of materials which consist of large patches of pure substances (large being tens of centimeters or more) will produce spectra that are arithmetic averages of the pure components, weighted according to the surface area of each component.

Mixtures on a more intimate scale, where the patches are on the order of millimeters or smaller will combine according to an extremely nonlinear scattering law that favors dark materials over light materials. Mixtures can also occur as vertically stratified, optically thin continuous layers over a substrate. The law in such a case follows an approximate multiplicative behavior. In each of the three models, combining end-member spectra produces quite different mixture spectra. However, diagnostic absorption features will remain visible in the mixture spectra, depending upon the strength and relative abundance of the contaminant.

In conclusion, automation in spectrum identification can be realized in two major areas: (1) the analysis of an individual spectrum for diagnostic spectral features, and (2) the identification of these spectral features in unknown spectra. For some materials with well defined lines, this procedure may be fairly straightforward. For materials with broad absorption features, both of these functions may be considerably more difficult. A major purpose of laboratory measurements will be the evaluation of the detectability of different types of absorption and emission features in varying physical states of the material under scrutiny, and in mixtures with different types of material.

7.4.11 Recommendations

Research into automatic methods should fall into two broad categories:

1. The development of:
 - algorithms for the identification of diagnostic spectral features;
 - accurate models which can generate synthetic spectra of pure materials under a wide variety of physical conditions; and
 - accurate models which can reproduce spectra of mixtures of materials both in absorption and emission.
2. The development of test procedures for evaluating the effectiveness of the automated methods. Test data sets of known targets in the lab and the field are essential to development of a credible identification system.

8. Atmospheric Effects and Their Removal

8.1 Summary and Conclusions

The atmosphere strongly affects the remote sensing measurements of the Earth's surface made from aircraft and spacecraft. Both absorption and scattering effects exist, and these vary with respect to location, altitude, and time. Five methods for attempting to remove the atmospheric effect have been identified. Three of these do not account for variations within a scene. The other two methods, based on: (1) atmospheric models, and (2) mixing models, have been used successfully and are potentially applicable to hyperspectral remote sensing for pixel-by-pixel atmospheric corrections.

In summary, no technique currently exists for performing atmospheric backout on a pixel-by-pixel basis for high-resolution data sets. However, there are techniques under development that have the potential for solving this problem for data in the visible and near infrared wavelength region. Efforts should be directed toward fully developing these techniques.

There are some instances wherein hyperspectral remote sensing is less sensitive to atmospheric effects. If the material to be identified and mapped has a spectrum with a strong absorption feature that is fairly narrow in spectral range and is not near any strong atmospheric absorption, then the atmosphere can be ignored in most of such cases. For broad spectral features and for features near or in atmospheric bands, however, significant corrections must be made.

The burden of atmospheric corrections may be reduced by obtaining a foreknowledge of the approximate conditions existing in the remotely sensed scene. A first-order correction can then be applied as the data are received. The task then becomes one of deriving the additional correction demanded by that specific scene at that particular time. This foreknowledge can be obtained from predictions made from surveys of previous conditions at that scene and by actual weather satellite measurement of broader areas in the same time regime.

8.2 The Problem

Although remote-sensing technologies have seen significant advances over the last decade, particularly in the area of high-resolution spectral sensors, techniques for analyzing the new wealth of data from sophisticated airborne and spaceborne sensors have not kept pace with the development of the hardware. And while many useful methodologies have been developed for the analysis of data from the broadband sensors, such as the Landsat series, detailed analysis of the information available from the new high spectral resolution instruments, such as the Airborne Imaging Spectrometer (AIS), has been hindered by the fact that many important features of the spectra are either masked or distorted by atmospheric effects. Thus, a high priority in current research is the development of analytical methods for atmospheric correction of high-resolution spectral data.

Light passing through the Earth's atmosphere is selectively absorbed and scattered by molecules and particles in the atmosphere. Spectral data obtained through the Earth's atmosphere thus include major contributions from the atmosphere as well as from features of interest on the ground. The atmospheric contribution to the received signal varies in intensity, which is a function of wavelength, temperature, pressure, pathlength, and the nature and concentration of the atmospheric constituents (primarily water, carbon dioxide, and ozone). In some wavelength regions, atmospheric effects can

completely dominate a measured spectrum. Figure 8-1 shows a typical atmospheric transmission spectrum for the wavelength range of 0.5 to 15.0 μm . This spectrum was computed using the LOWTRAN 5b model (Kneizys et al. 1980). This same spectrum is shown in Figure 8-2 with the spectrum of a geological sample (calcite) factored in; the atmospheric contribution clearly dominates the spectrum.

Effects also vary temporally and spatially as atmospheric conditions and angle of the Sun change, and with the altitude of the sensor and the consequent path of the reflected light through the stratified atmosphere. Four atmospheric transmission spectra, computed using the LOWTRAN 5b model, are shown in Figures 8-3 to 8-6 to illustrate these variations. Figures 8-3 and 8-4 illustrate two different pathlengths: Figure 8-3 is for a simulated aircraft flying at 10,000 feet and Figure 8-4 is for a satellite flying above the Earth's atmosphere. In both spectra, an atmospheric model corresponding to typical atmospheric conditions during winter in midlatitude areas was assumed. Figures 8-5 and 8-6 show transmission spectra for the same atmospheric path, but for conditions typical of tropical areas. The most striking aspect in comparing these four spectra is that, although variations do occur, the variations are consistent and basically of the same order of magnitude.

Since the atmospheric component to imaging spectrometer data may drastically differ from pixel to pixel across a given scene, the objective of an atmospheric backout procedure is to deconvolve the desired target signal from the undesired atmospheric contribution. Because of the temporal and spatial variation in atmospheric effects across a scene, a backout done on a pixel-by-pixel basis would be ideal.

8.3 Background

There is only one imaging spectrometer currently in widespread use--the NASA Airborne Imaging Spectrometer (AIS). This instrument obtains data in the wavelength region from approximately 1.2 to 2.4 μm . Because of data availability from this instrument, all of the atmospheric backout procedures for high spectral resolution image data have been developed with reference to this instrument. The three techniques currently in use for performing, at least nominally, an atmospheric backout on AIS data are presented here.

There are additional techniques that exist for use with data sets other than hyperspectral image data. Two of these techniques, with modification, may potentially be applied to perform a full atmospheric correction of hyperspectral image data. These two alternate techniques are also discussed in terms of their potential application to hyperspectral data.

8.4 Techniques Currently in Use

The three techniques developed to perform atmospheric backout of AIS data are: (1) "flat-field" correction; (2) in-scene calibration standard; and (3) statistically based correction. It should be pointed out, however, that none of the approaches currently being employed for AIS data accounts for the across-scene (temporal and spatial) variation of the atmospheric contribution; all assume that a single atmospheric spectrum is sufficient to remove atmospheric effects from an entire scene or a large portion of a scene. This lack of use of sophisticated techniques is largely due to the nature of the data set. The AIS was never intended to be a research instrument; it was developed to evaluate the feasibility of routinely performing Earth-looking high spectral and spatial resolution remote sensing. As a result, the response of this instrument is not well calibrated and this has hindered, if not completely prevented, the development of a rigorous atmospheric backout procedure. These techniques are described below and a summary description is given in Tables 8-1 to 8-3.

8.4.1 "Flat-field" correction

Description: This technique was developed at NASA/JPL by H. Lang, J. Conel and E. Paylor (Lang et al. 1985) to perform atmospheric backout on AIS data. An average spectrum obtained from a "spectrally homogeneous" area is divided out of the entire data set (channel by channel) in an attempt to remove the effects of the solar light curve, the instrument response curve, and the combined atmospheric absorption and scattering spectrum. The solar spectrum may also be removed separately, based on available published solar data (e.g., Arveson et al. 1969). The system's response curve could be similarly removed, but the required data do not exist for the AIS. Field checking may be used to verify the spectral homogeneity of the "flat-field" area.

Assumption: The technique assumes that some area within a scene or image can be identified as being sufficiently spectrally homogeneous as to represent only the effects resulting from the three processes mentioned above. Even if the solar spectrum and instrument response were factored out separately, it is assumed that the atmospheric effects for the entire scene may be represented by a single spectrum. The spectrum extracted from the hyperspectral data is assumed to contain only undesired signal--if this were not the case, then dividing out this spectrum would also remove desired information from the data set.

Applicability: This technique may be adequate for flat, arid or semi-arid regions, as its accuracy relies on the assumption that the atmospheric contribution to the entire data set can be characterized by a single spectrum. However, this is never exactly true even for an arid region. This technique cannot be used for pixel-by-pixel atmospheric backout.

8.4.2 In-scene calibration standard

Description: This approach has been used by several researchers and has also been applied as a modification to the "flat-field" technique. This technique approximates calibration procedures used with laboratory and astronomical data. Under controlled observing conditions--in which the target and sensor remain relatively fixed--calibration is generally done through repeated reference to a material or object of known reflectance that is in close proximity to, and has the same atmospheric pathlength as the target. However, this approach cannot be directly applied to high-resolution spectral data obtained from airborne or spaceborne sensors because of the large ground area surveyed by such instruments. Instead, some material that occurs within the scene is sampled (either during or after the overpass of the sensor) and its spectral characteristics are measured in the laboratory or with a field instrument of sufficiently high resolution.

This sampled material is then treated as a known reflectance standard. The laboratory spectral response of this material is divided out of the pixels corresponding to where the samples were obtained. The spectrum remaining after this division then represents the combined atmospheric absorption and scattering spectrum, as well as the solar and instrument response curves (if these have not been removed separately). Several samples may be obtained for a given scene and each corresponding calibration spectrum is used for calibrating the portion of the scene near where the sample was obtained. (For

an example of the application of this technique, see Mustard and Pieters 1986.)

Assumption: This technique makes two major assumptions. The first assumption is that the atmosphere is homogeneous. However, because several areas may be sampled and measured in the laboratory, some spatial variation in atmospheric effects may be compensated for. Second, the technique assumes that the materials sampled as standards represent the total contribution of the target surface to a given pixel or set of pixels. This assumption may be mitigated by sampling all the materials present in a pixel and integrating their contributions in order to develop a spectrum for the entire pixel. This must be done after data acquisition so that the location on the ground of a pixel in the image may be identified.

Applicability: The accuracy of this technique relies on the assumption that the atmospheric contribution to some portion of the data set can be characterized by a single spectrum. This technique cannot be used for pixel-by-pixel atmospheric backout.

8.4.3 Statistically based corrections

Description: This approach is currently being employed to remove atmospheric effects from imaging spectrometer data. It was developed by A. Green and M. Craig of CSIRO (Commonwealth Scientific and Industrial Research Organization) in Sydney, Australia (Green and Craig 1985). This technique utilizes the fact that the value which the instrument measures may be considered as a linear function of reflectance and irradiance, if the data are converted to logarithms. In this technique, a set of logarithmic averages in both the spatial and spectral domains (specifically, the along-track $[DN_S]$, cross-track $[DN_{CS}]$, and along-wavelength $[DN_\mu]$ averages) is derived from the entire data set or from a specific area of interest. These averages are subtracted from the logarithm of the digital data value ($DN_{S\mu}$) obtained by the sensor, using the formula:

$$\log(R_{S\mu}) = \log(DN_{S\mu}) - \text{avg}(\log(DN_S)) - \text{avg}(\log(DN_{CS})) - \text{avg}(\log(DN_\mu)).$$

Differencing in this domain is the operational equivalent to division in the reflectance domain; this approach may be considered equivalent to dividing a "standard spectrum" from the scene.

Assumptions: This approach has an advantage over the "flat-field" correction method in that it utilizes the entire data set, rather than a single subarea, and so tends to average out atmospheric (and instrument) variation across the scene. However, it also assumes that the averages produced do not include any desirable spectral information, an assumption which is very difficult to examine because the averages used do not refer to any specific physical area. Also, in dividing a single spectrum out of the data, atmospheric homogeneity is assumed across the scene.

Applicability: This technique works well for areas where there is little atmospheric variation across the scene, such as arid or semi-arid regions. The accuracy of the algorithm relies on the assumption that the atmospheric contribution to the entire data set, or a portion of the data set, can be characterized by a single

spectrum. In this case, the smaller the physical area examined, the more likely it is that the average spectrum computed will represent the atmospheric contribution. However, smaller areas will also be more likely to be spatially homogeneous in terms of the number of materials represented; thus, it will be more likely for smaller areas that the computed logarithmic averages will contain desirable as well as undesirable information. This technique cannot be used for pixel-by-pixel atmospheric backout.

8.5 Potentially Applicable Techniques

Two techniques, based on (1) atmospheric models and (2) mixing models, have been successfully used to perform atmospheric backout on remotely-sensed data. Although neither of these methods has yet been applied to a hyperspectral cube data set, both approaches are sufficiently general as to be potentially applicable to such data sets. These two methods are presented here with a discussion of the modifications required to apply them to hyperspectral cube data. A summary description is given in Tables 8-4 and 8-5.

8.5.1 Atmospheric model-based technique

Description: This technique, developed at the University of Hawaii for single remotely obtained spectra (Blake 1983), utilizes the expression of the atmospheric spectral features actually contained in the remotely obtained data, in conjunction with an analytical model of the atmosphere (LOWTRAN, Kneizys, et al. 1980), in order to estimate and remove the atmospheric effects from the remote data. The approach uses an iterative procedure to compare individual, remotely measured, near infrared spectra with LOWTRAN-generated spectra. In this technique the solar spectrum and instrument response curves are first factored out of the data. Then, for a given spectrum (or pixel), the best-fit atmospheric spectrum is found using the LOWTRAN5b model. This spectrum is then factored out of the data.

Assumptions: This technique has been shown to adequately remove atmospheric effects from high-resolution spectral data. The technique assumes that a given atmospheric model, such as LOWTRAN, accurately portrays the atmosphere for a given region. For simplicity's sake, the method as applied references only the primary atmospheric constituent--water. For rigorous applications, other important atmospheric constituents would need to be included in the procedure. Another assumption is that the parameters of the LOWTRAN model can be sufficiently constrained so that the technique can be efficiently applied to a large data set. Another inherent assumption is that the instrument response curves are available for a given instrument. (This is not the case for the AIS--an essentially uncalibrated instrument.)

Applicability: This technique has not yet been applied to hyperspectral image cube data; modification and improvement are required before the algorithm can be tested on such a large data set. The necessary modifications are discussed in Section 8.6.1.

8.5.2 Mixing model-based corrections

Description: This technique was developed at the University of Washington by Adams, et al. (1986) for broadband image data, e.g., Viking Lander data and Thematic Mapper data. Because of the generality of the approach, the technique also has potential application to hyperspectral image data.

This technique defines the atmospheric contribution to a data set as principal components-based end-member spectra, referenced to a spectrum library. The contribution to a given pixel is determined using a linear mixing model of end-member spectra. The principal components (or eigenvector) analysis is used to identify the set of spectral end-members for a scene or portion of a scene. The end-member spectrum corresponding to the atmospheric contribution is identified with reference to a library of candidate spectra. Using a linear mixing model of all the end-members, the specific atmospheric spectrum for each pixel is identified and factored out of the spectrum for that pixel.

Assumptions: Because this technique has not yet been applied to hyperspectral data, the primary assumption is that the method can, in fact, isolate the atmospheric contribution to high-resolution spectral data. Further, it is assumed that the algorithm will produce atmospheric spectra specific to each pixel, rather than some generalized atmospheric spectrum corresponding to the entire scene. Of course, linear mixing models will work only for linear mixing effects; multiplicative atmospheric effects will require nonlinear models.

Applicability: This technique yields good results for broadband data, but has not yet been applied to hyperspectral data; modification would be required before the technique can even be tested for such an application. These modifications are discussed in Section 8.6.2.

8.6 Further Development Required

Of the approaches outlined previously, those that are currently being applied to hyperspectral cube data do not lend themselves to modifications to account for pixel-by-pixel atmospheric variation. However, the other two approaches, which are potentially capable of dealing with single pixel elements, will require some modification to be applicable to imaging spectrometer data.

8.6.1 Modifications to atmospheric model-based technique

The applicability of this technique to image data, rather than to point spectra, must first be determined. The specific changes which would then be required include:

1. Modifications to include all relevant atmospheric constituents: The present iterative procedure must be modified to simultaneously minimize for all constituents the deviations between the measured spectral data and the analytically determined atmospheric spectra (e.g., from LOWTRAN). This might

take the form of a linear programming type approach.

2. Procedural modifications to deal with all pixel elements, instead of single spectra.
3. Efficiency improvements: These would include a study to determine how many pixels must optimally be examined to achieve a satisfactory atmospheric correction.

8.6.2 Modifications to mixing model-based technique

The applicability of this technique to image data, rather than to point spectra, must first be determined. The specific changes which would then be required include:

1. Modifications to address increased number of spectral channels.
2. Modifications to spectral library to include a sufficient variety of potential atmospheric spectra: Alternatively, an approach must be developed to take the place of a strict library search.
3. Efficiency improvements: These would include a study to determine how many pixels must optimally be examined to achieve a satisfactory atmospheric correction.

8.7 References

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- Arveson, J. C., R. N. Griffin, Jr., B. D. Pearson, Jr. (1969), Determination of extraterrestrial solar spectral irradiance from a research aircraft, *Applied Optics*, 8, 11, 2215-2232.
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April 8-10, G. Vane and A.F.H. Goetz (editors), JPL Publication 85-41.

Mustard, J. F. and C. M. Pieters (1986), Abundance and distribution of mineral components associated with Moses Rock (kimberlite) diatreme, *Proceedings of the Second Airborne Imaging Spectrometer Data Analysis Workshop*, May 6-8, G. Vane and A.F.H. Goetz (editors), JPL Publication 86-35.

TABLE 8-1

ATMOSPHERIC BACKOUT TECHNIQUES PRESENTLY IN USE

"Flat-field" Correction

Developed by: NASA/JPL (H. Lang, J. Conel, E. Paylor)

Brief Description:

1. Identify "spectrally homogeneous" area within the scene.
2. Take average spectrum from this area.
3. Divide this average spectrum out of entire scene.

Assumptions:

1. Combined atmospheric absorption and scattering effects across the scene can be represented by a single spectrum.
2. Only undesired components of signal are removed.

Special Software Requirements:

1. Spectrum extraction.
2. Divide image cube by spectrum.

Data Sets Applied to:

AIS, TM, NS-001

General Applicability:

Any data set acquired under highly nonvariable atmospheric conditions.

Limitations:

This technique cannot be used for pixel-by-pixel atmospheric backout.

TABLE 8-2

ATMOSPHERIC BACKOUT TECHNIQUES PRESENTLY IN USE

In-scene Calibration Standard

Developed by: Various persons

Brief Description:

1. Identify "spatially homogeneous" areas within the scene.
2. Obtain samples of these materials from the site.
3. Measure spectra of these materials in the laboratory.
4. Divide these spectra out of appropriate pixels.
(Remainder then represents atmospheric contribution.)
5. Divide atmospheric contribution out of nearby portions of scene.

Assumptions:

1. Combined atmospheric absorption and scattering effects for a large geographic area can be represented by a small number of spectra.
2. Materials sampled and measured in the lab represent total contribution of target surface to a given pixel.

Special Software Requirements:

1. Spectrum extraction.
2. Divide image cube by spectrum.

Data Sets Applied to:

AIS, TM, NS-001, SMIRR, astronomical data

General Applicability:

Data set acquired under highly nonvariable atmospheric conditions.

Limitations:

This technique cannot be used for pixel-by-pixel atmospheric backout.

TABLE 8-3

ATMOSPHERIC BACKOUT TECHNIQUES PRESENTLY IN USE [3]

Logarithmic Residuals

Developed by: CSIRO, Sydney, Australia (A. Green, M. Craig)

Brief Description:

1. Convert data to logarithms.
2. Obtain along-track (DN_s), cross-track (DN_{cs}), and along-wavelength (DN_μ) averages.
3. Remove these averages from the data using the formula:

$$\log(R_{s\mu}) = \log(DN_{s\mu}) - \text{avg}(\log(DN_s)) - \text{avg}(\log(DN_{cs})) - \text{avg}(\log(DN_\mu))$$

4. Reconvert data from logarithms back to original units.

Assumptions:

1. Averages only include undesired spectral information.
2. Atmosphere is homogeneous across the scene.

Special Software Requirements:

1. Logarithm conversion.
2. Capability for calculating pixel averages along various axes.

Data Sets Applied to: AIS

General Applicability:

Any data set acquired under homogeneous atmospheric conditions.

Limitations:

This technique cannot be used for pixel-by-pixel atmospheric backout.

TABLE 8-4

ATMOSPHERIC BACKOUT TECHNIQUES POTENTIALLY APPLICABLE TO HYPERSPPECTRAL IMAGE DATA

Atmospheric Model-Based

Developed by: University of Hawaii (P. Blake, R. Singer)

Brief Description:

1. Remove solar spectrum and system's response curve from data.
2. For a given spectrum/pixel, find best-fit atmospheric spectrum using the chosen atmospheric model (e.g., LOWTRAN).
3. Divide these calculated atmospheric spectra out of the data, pixel by pixel.

Assumptions:

1. The atmospheric model accurately portrays the atmosphere for a given region.
2. The parameters of the model can be sufficiently constrained that the technique can be applied efficiently to a large data set.
3. The system's response curve is available for a given instrument.

Special Software Requirements:

1. Spectrum extraction.
2. Divide image cube by spectrum.

Data Sets Applied to:

Data obtained with UH Planetary Geosciences Division near infrared spectrometer

General Applicability:

Any data set, provided the system's response curve is available.

Limitations:

This technique has not yet been modified for and tested on image cube data. It has only been used for single-point spectra.

TABLE 8-5

ATMOSPHERIC BACKOUT TECHNIQUES POTENTIALLY APPLICABLE TO HYPERSPPECTRAL IMAGE DATA

Mixing Model-Based

Developed by: University of Washington (J. Adams, M. Smith)

Brief Description:

1. Perform principal components analysis.
2. Identify end-member spectra (for each pixel) with reference to spectrum library.
3. Identify end-member spectrum corresponding to atmospheric contribution (for each pixel) using linear mixing model of all end-members.
4. Divide the appropriate atmospheric end-member spectrum out of each pixel.

Assumptions:

1. Method is applicable to high spectral resolution data.
2. Method will successfully identify atmospheric contribution to signal.

Special Software Requirements:

1. Principal components analysis.
2. End-member search routines.
3. Spectrum library.

Data Sets Applied to:

MSS, TM, Viking Lander Data

General Applicability:

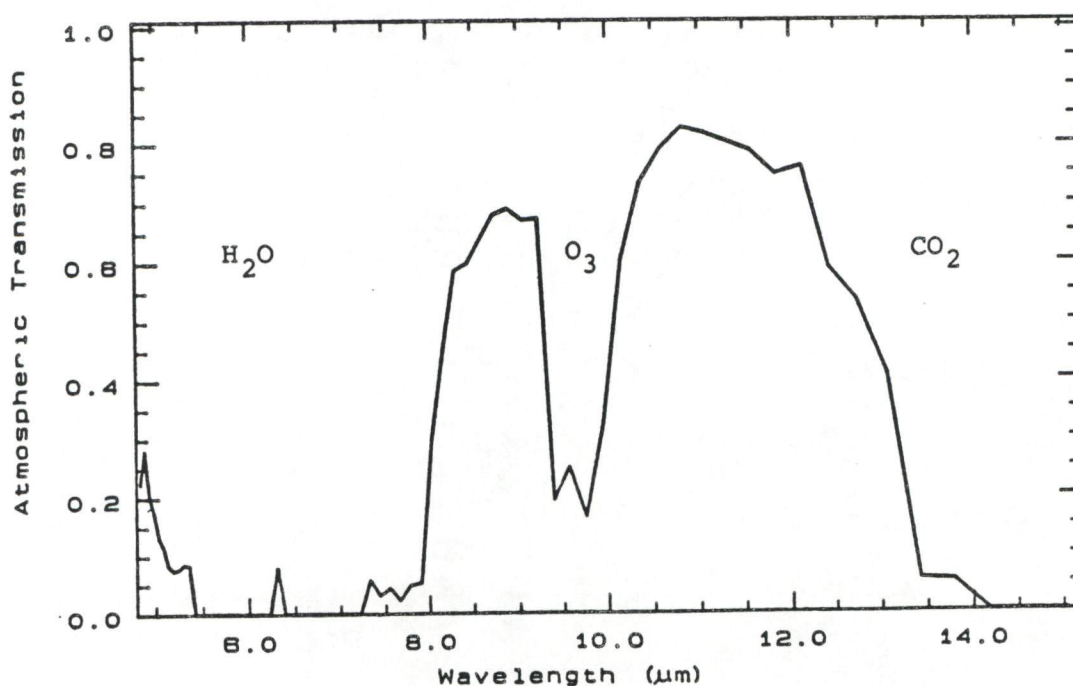
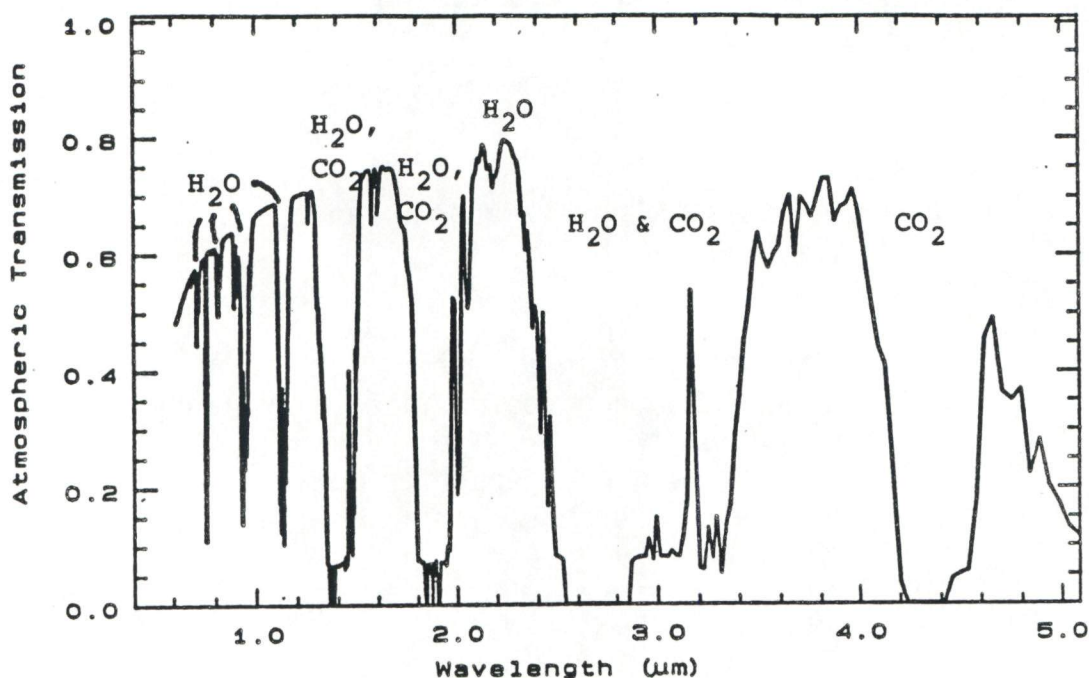
Any data set, assuming applicability to high spectral resolution.

Limitations:

This technique has been applied to broadband image data only and has not been modified for and tested on high spectral resolution data.

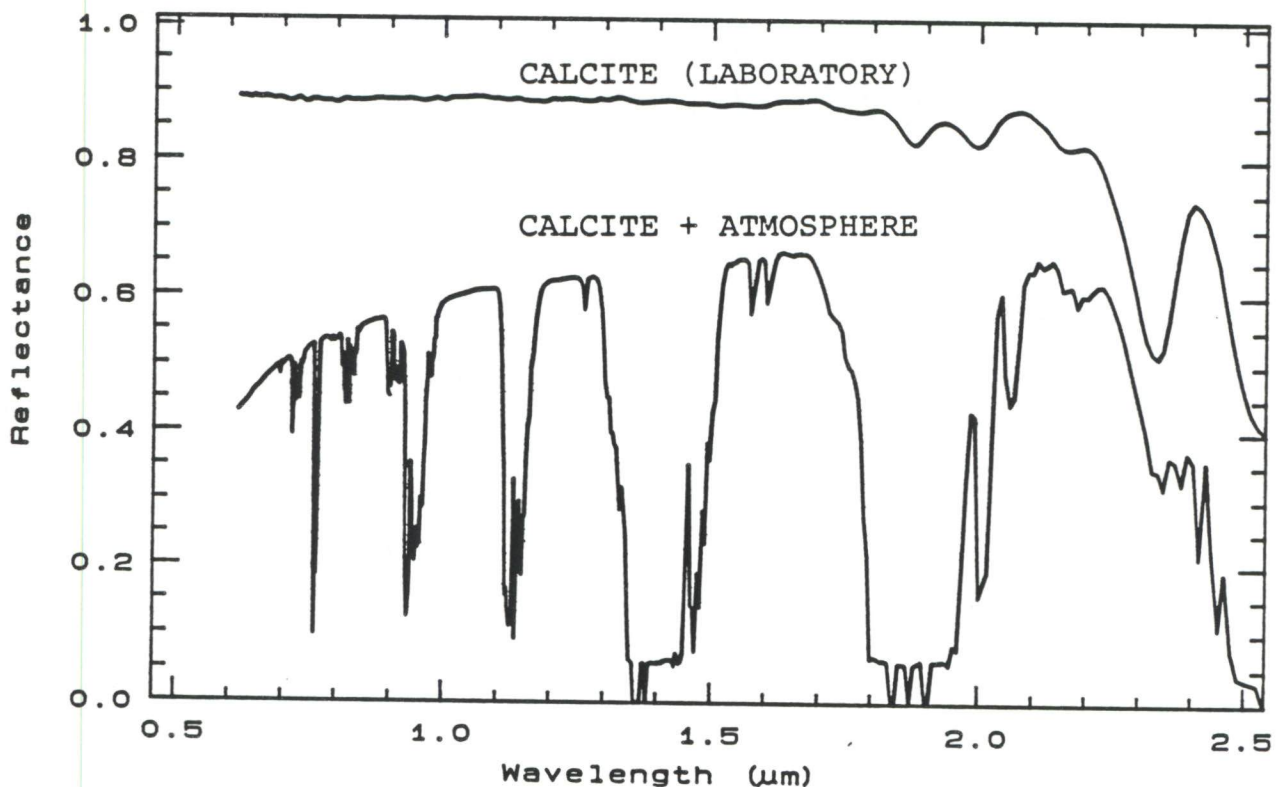
FIGURE 8-1

ATMOSPHERIC TRANSMISSION SPECTRUM (0.5 TO 15.0 μm)



This spectrum was computed using LOWTRAN5b (Kneizys et al. 1980), and assuming the midlatitude winter atmospheric model, with a double vertical path from space to the ground at sea level.

FIGURE 8-2
REFLECTRANCE SPECTRA FOR CALCITE
(0.5 TO 2.5 μm)

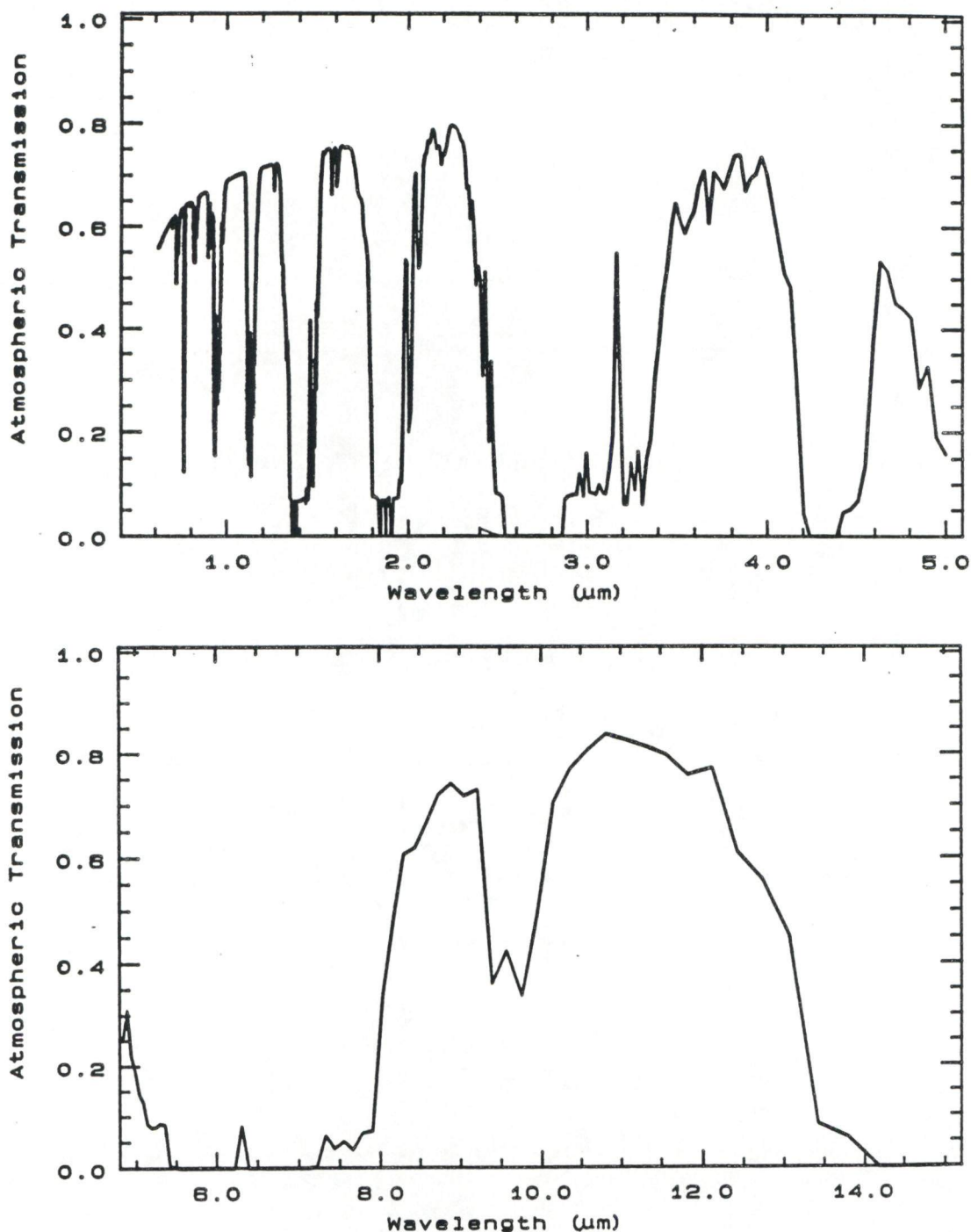


(a) Reflectance Spectrum for Calcite (0.5 - 2.5 μm): The calcite spectrum was obtained on the PGD near infrared spectrometer.

(b) Calcite Spectrum Factored with Atmospheric Transmission Spectrum (0.5-2.5 μm): The atmospheric component was computed using LOWTRAN5b (Kneizys et al. 1980), and assuming the midlatitude winter atmospheric model, with a double vertical path from space to the ground at sea level. This spectrum was multiplied by the calcite sample spectrum to illustrate the effect of viewing a natural surface through the atmosphere.

FIGURE 8-3

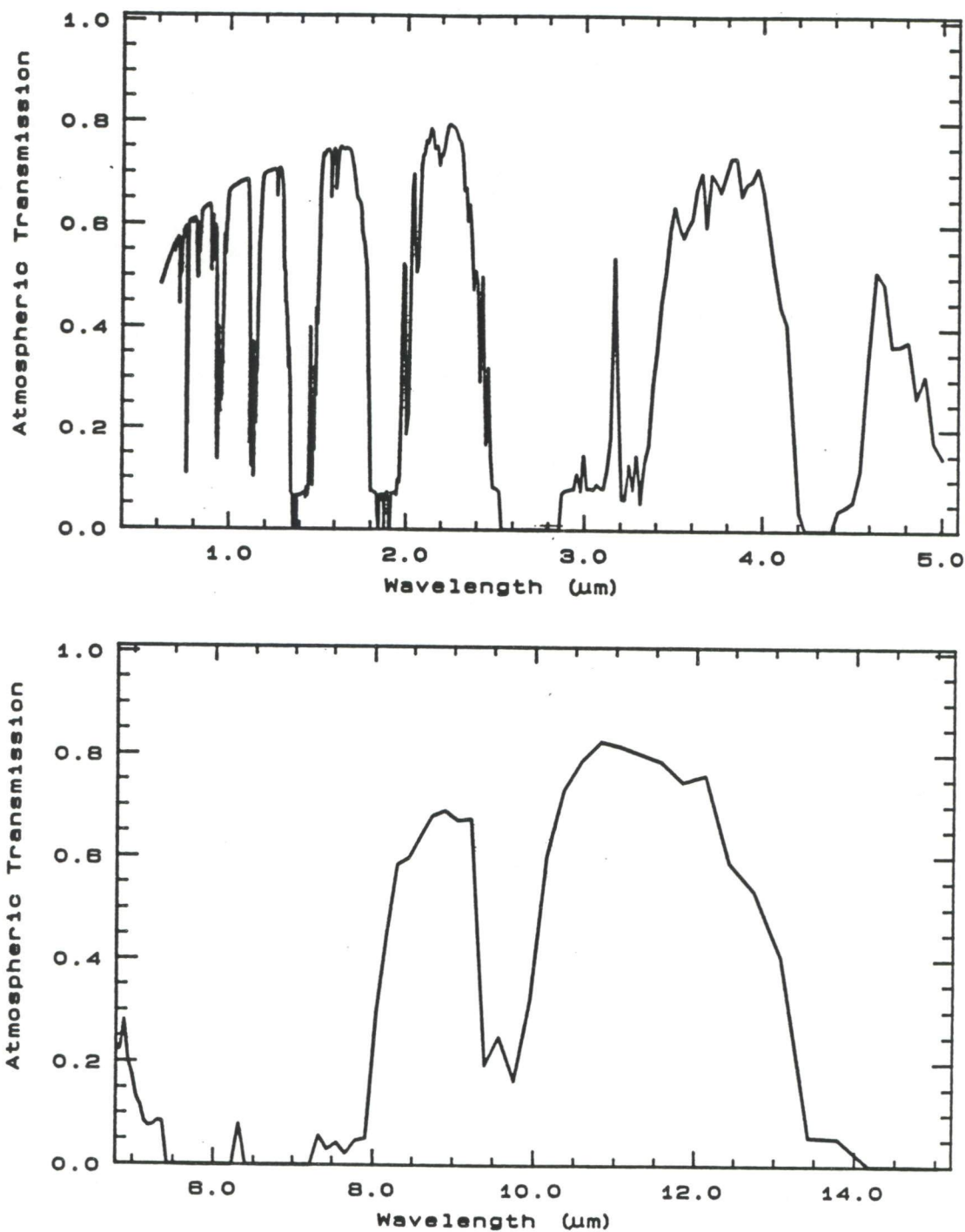
ATMOSPHERIC TRANSMISSION SPECTRUM (0.5 TO 15.0 μm)



This spectrum was computed using LOWTRAN5b (Kneizys et al. 1980). The model used was LOWTRAN's model for a midlatitude winter atmosphere. The spectrum was computed using a double vertical path from space to the ground at sea level and then to an altitude of 3 km (~10,000 ft).

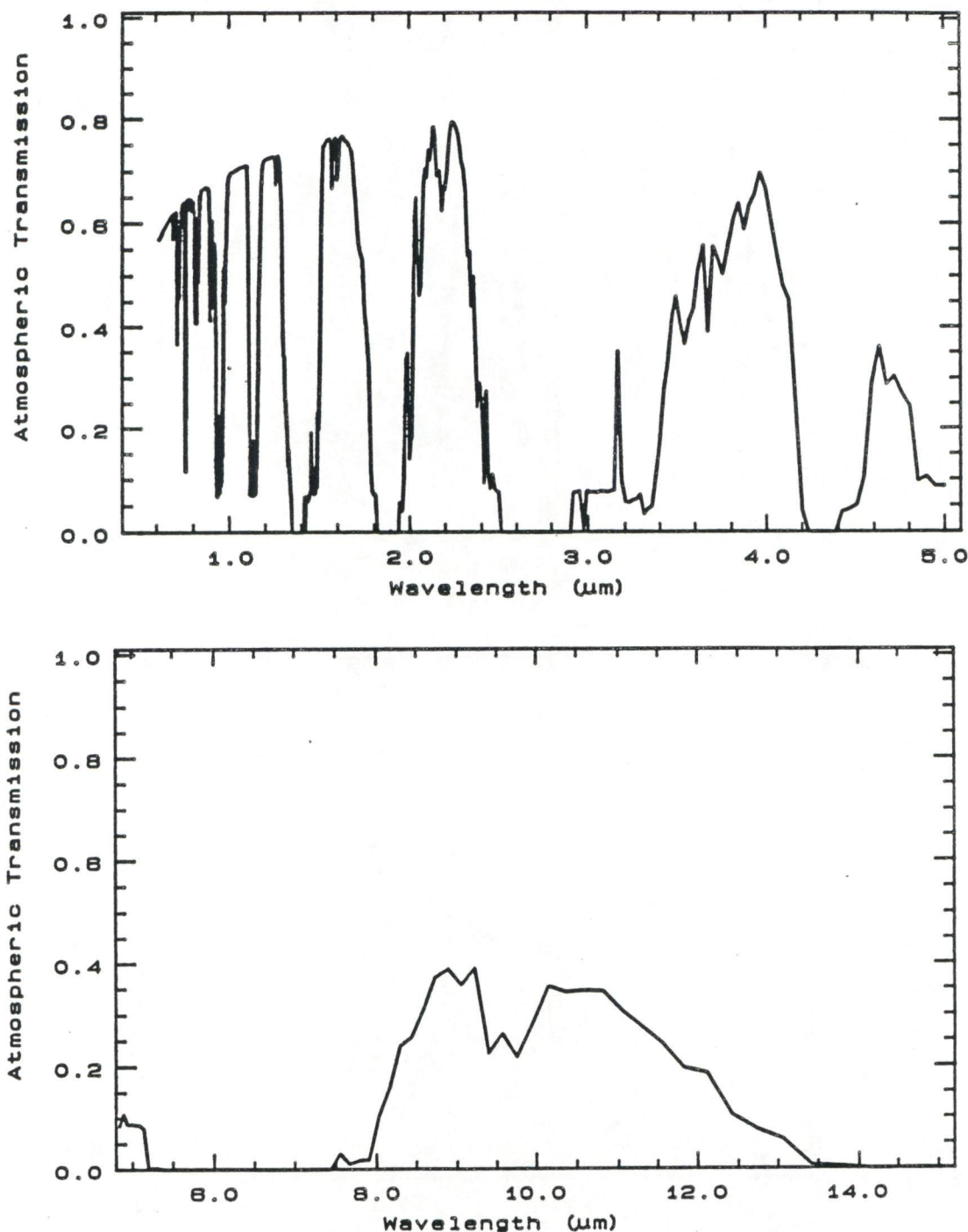
FIGURE 8-4

ATMOSPHERIC TRANSMISSION SPECTRUM
(0.5 TO 15.0 μm)



This spectrum was computed using LOWTRAN5b (Kneizys et al. 1980). The model used was LOWTRAN's model for a midlatitude winter atmosphere. The spectrum was computed using a double vertical path from space to the ground at sea level.

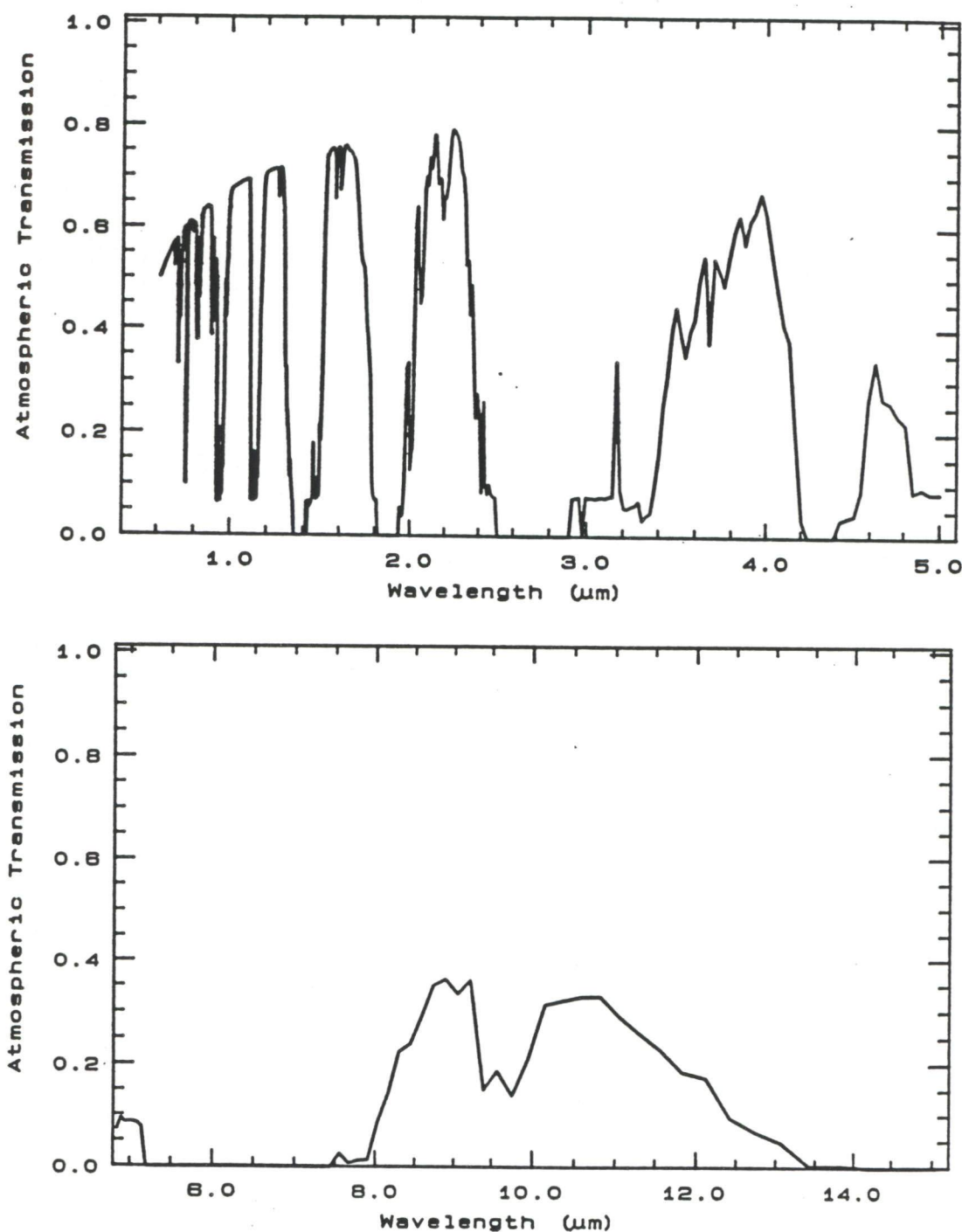
FIGURE 8-5
ATMOSPHERIC TRANSMISSION SPECTRUM
(0.5 TO 15.0 μm)



This spectrum was computed using LOWTRAN5b (Kneizys et al. 1980). The model used was LOWTRAN's model for a tropical atmosphere. The spectrum was computed using a double vertical path from space to the ground at sea level and then to an altitude of 3 km (~10,000 ft).

FIGURE 8-6

ATMOSPHERIC TRANSMISSION SPECTRUM (0.5 TO 15.0 μm)



This spectrum was computed using LOWTRAN5b (Kneizys et al. 1980). The model used was LOWTRAN's model for a tropical atmosphere. The spectrum was computed using a double vertical path from space to the ground at sea level.

9. Critical Areas for Research and Development in Hyperspectral Data Processing

This section outlines technical and scientific areas of hyperspectral image cube processing that are in critical need of basic research and advances in the application of existing technologies, or that require the development of new analytical techniques and technologies. Chapters 3 through 8 of this report provide the background for the following discussion.

9.1 Data Processing and Presentation Application

Advances in remote sensing instrument technology have produced mapping spectrometers for which the volume of data output and complexity present significant challenges. Many of the traditional multispectral analysis techniques implemented on conventional processor architectures become computationally impractical when extended to handle the large number of spectral parameters needed to address advanced spectral identification problems, such as mixture analysis combined with atmospheric backout.

This section presents areas where the development of hyperspectral image cube processing systems would benefit from the application of existing or new hardware and software technologies.

9.1.1 User interfaces

In the near term, it appears that visual inspection of hyperspectral imagery and derived data products will continue to require a significant amount of an analyst's time. Use of alternative command interfaces, windowing, color, sound, and interactive positional devices such as mice, trackballs, and touch screens to augment conventional image and spectral processing environments would greatly enhance the effectiveness of the systems surveyed in Chapter 7.

9.1.2 Distributed processing and data flows

Most commercial image and spectral processing systems are not distributed, and only recently have standards evolved for remote host display of bit-mapped data (e.g., X windows). Architectures incorporating image servers, spectral library database servers, load balancing among networked image processors, highly interactive analyst workstations, and dynamically configurable data flow paths need further study.

9.1.3 Presentation of three-dimensional data

With the exception of hyperspectral cube "movies," which rapidly display each spatial plane of the cube in quick succession, alternative methods of three-dimensional data set presentation, in particular for time-series data, have not yet been exploited in the hyperspectral processing systems surveyed. Techniques used in high-end CAD/CAM systems, such as surface fitting and solids rendering, may be useful.

9.1.4 Presentation of fourth- and higher-dimensional data

As mentioned above, presentation methods for three-dimensional data are not well developed in existing systems. Display techniques, statistical characterizations, and reduction strategies for higher-dimensional data sets, e.g., a hyperspectral cube measured under different viewing geometries, are needed.

9.1.5 Operating system enhancements, massive memories

Extensions to conventional operating systems, such as UNIX and VMS, to support very large memory-resident data segments, very large page sizes, swapping strategies for large data segments, and other memory management schemes are needed. To complement these extensions, processor architectures incorporating massive memories are needed for maintaining a large number of intermediate data products, or for comparison of similar hyperspectral cubes.

9.1.6 High-speed, high-capacity disk subsystems

The creation of large temporary intermediate data products requires advances in disk technologies (e.g., CD-ROMS, WORMS) and compaction techniques for processing; large disk farms are needed to store mission or intelligence data. Data standards for hyperspectral cube attributes are needed to organize such massive collections of data.

9.1.7 Numeric DBMSs, database machines

None of the systems surveyed exploits specialized hardware for the spectral search operations. Conventional DBMSs are generally designed for the storage and retrieval of attribute information. Advances in the hierarchical or connectionist organization of numeric data, and associated search and retrieval schemes would have applicability to many identification, search and retrieval tasks.

9.1.8 Statistical hyperspectral database analysis

Statistical techniques are needed to characterize the contents and relationships between databases of images, single spectra or hyperspectral cubes. Transforms might be developed to enable these statistical metrics and representations to be input to analyses such as mixing models and scene understanding.

9.1.9 Pattern matching and classification techniques

It has been postulated that since imaging spectrometers provide sufficient sampling in the spectral direction in order to obtain unique spectral signatures, a deterministic pattern matching approach is adequate for surface materials identification (Solomon), as opposed to statistical methods. A number of deterministic linear transforms, e.g., Fast Fourier transforms and Walsh-Hadamard transforms, and nonlinear methods, such as binary encoding, have been compared but the nonlinear transforms in particular are not well understood.

9.1.10 Parallel processing

Hyperspectral cube processing naturally lends itself to parallel decomposition,

but none of the surveyed systems has been ported to a parallel processor architecture. One of the commercial spectrometer systems, offered by Digilab, supports an array processor. Development of embedded specialized processors (e.g., for atmospheric backout) functioning in parallel with controlled exploration of the spectral parameter space during identification analysis appears to be a promising engineering area that could utilize existing technologies.

9.1.11 Massively parallel processing

Massively parallel processors, such as the Connection Machine, differ substantially from parallel computers like the Alliant, whose processors are linked in a rigid network configuration. The Connection machine addresses inherent parallelism at the data level, which is a conceptually simpler approach, for problems such as multispectral analysis, and at the same time offers tremendous performance potential. Dynamic linkages between processors help address problems which may be denser in some regions of the parameterization space, and so might be useful for meshing a hyperspectral cube and targeting spectrally unique regions.

9.1.12 Neuro net machines

Neural network processors, which can function as either content-addressable memories or as optimizers, use a form of fuzzy logic to provide fast but approximate solutions to complex problems. Due to the high density of the network, damage to the connections or loss of data in the network does not significantly affect solutions obtained by such architectures; hence, they may be useful for hyperspectral identification where the data exhibit instrument noise or atmospheric interference that obscures spatial or spectral feature information. Rather than operating on digital data, neural networks process analog signals that fluctuate continuously; thus, neural processors may be well suited for external analog input (e.g., from a charge-coupled device). For this reason they inherently can more easily produce weighted decisions from fuzzy, incomplete, or contradictory data than what is achievable with digital logic. Neural computers appear very promising for sorting through spectral libraries to find close matches, or for retrieving database entries that automatically call up related entries as well.

9.1.13 Expert system front-ends

There are a number of areas where expert systems might be of assistance in classifying and identifying spectra, as exemplified in Perkin-Elmer's PSU approach. These were described in Chapter 7.

9.1.14 Learning and autonomy strategies

Adaptive, learning analysis monitors--which can learn the identification strategies of an analyst or learn autonomously by trial and error, and then direct identification analysis autonomously--are needed for extremely large hyperspectral cube data sets. Real time analysis of the data collected by an airborne spectrometer, for example, may benefit from monitors that adapt identification strategies in categorizing recently viewed terrain according to past successes.

9.1.15 Symbolic knowledge representations and processing

Once identified, terrestrial image data extracted using conventional numeric image processing techniques can often be represented symbolically, e.g., buildings or a lake. Image understanding, which can greatly facilitate the identification of components of the image, generally lends

itself to symbolic representation. Advances are needed in the representations and processing capabilities. Ideally, a processing system would combine: (1) the ability to manipulate hyperspectral cubes both numerically and symbolically and to exchange knowledge from these two domains, with (2) monitors, expert systems, and other high-level analysis routines to aid in identification problems.

9.1.16 Coupled image/spectral processing

Often, the spectral identification problem is addressed independently of the scene context in automated hyperspectral processing, although the analyst typically incorporates knowledge of both in the manual identification process. Automated techniques to find spatial neighborhoods with similar spectral signatures, such as those found in the TDRS system, appear promising.

9.1.17 Large data set search and comparison techniques

Experimentation with different search and comparison techniques for very large data sets and databases is needed. Alternative methods of data representation, encoding, and compression can be considered facets of this general research area.

9.1.18 Hyperspectral cube variation

Methods for detecting variations between hyperspectral cubes, e.g., data from the same geographical point taken at different seasons, have not been widely studied.

9.2 Measurement Research Areas

9.2.1 Sampling and measurement techniques

A major need exists for a uniform database of reflectance spectra obtained under similar measurement conditions for use in basic research analyses and model validation. Objectives of this research area encompass further refinement of techniques currently in use to:

- identify the presence of specific minerals and gases and distribution maps for remote sensing applications;
- determination of abundances; and
- estimation of the composition of individual minerals.

9.2.3 Field spectrometer studies

Although considerable laboratory measurement data and unknown remote data sets are available to researchers, there is a lack of intermediate groundtruth data sets. These data sets would emphasize measurements taken:

- of natural surfaces;
- under a variety of environmental conditions; and

- of materials not available in the laboratory.

9.2.4 Instrument calibration studies

None of the terrestrial remote sensing instruments currently in use are well calibrated. Further research is required for:

- performing an accurate calibration;
- initially achieving and then maintaining accurate calibrations; and
- determining scientifically allowable calibration tolerances.

9.2.5 Data reduction and analysis

Methods of handling the very large and multidimensional data sets involved in this area of technology are primitive and inadequate for the rapid and complete analysis required by many applications. Some of the critical areas are:

- image cube formats;
- interactive user interfaces;
- multidimensional displays; and
- expert systems and artificial intelligence approaches.

9.2.6 Mixture analysis

Mathematical models relating fundamental material properties to diffuse reflectance spectra are needed to better utilize laboratory measurements of end-members so that spectra of mixtures and gradations of those materials can be predicted during identification analyses. Research into the effects of differing grain size, shape and optical properties, as well as deconvolving models, is recommended.

9.2.7 Atmospheric backout

No technique currently exists for performing rigorous, pixel-by-pixel atmospheric backout on high spectral resolution remote sensing data. Particular needs are:

- more study of expression of atmospheric features in remote data sets;
- an efficient technique for removing atmospheric transmission effects from remote data sets; and
- an efficient technique for removing atmospheric scattering effects from remote data sets.

9.2.8 Spectral feature characterization

Further research is needed into analytical methods that associate spectral features, including bands, with component materials, and yet are invariant over as many environmental and physical properties as possible. Reduced or compact feature representations that retain this information content are needed for the implementation of efficient spectral identification and search algorithms. Particular needs are:

- suppression of radiative transfer and calibration effects;
- accurate feature resolution;
- interpretation of ambiguities;
- low sensitivity to noise;
- recognition and elimination of false or aliased features/bands;
- robustness treatment of poor spectral resolution and quality; and
- high-volume automation.

9.2.8 Data set synthesis and test procedures

Construction of synthetic test data and evaluation criteria for identification strategies is an important analog to the above basic research areas.

10. Spectral Information Available in Various Spectral Regions

10.1 Assumptions and Context

Of primary interest is the detection and analysis of electromagnetic radiation that: (1) has been intercepted by a material and passively reflected or scattered back to a remote detector, or (2) has been thermally emitted by the surface. For the purpose of this study, the incident radiation can be assumed to be sunlight. The thermal radiation will in most cases be due to the natural temperature of the material, caused by absorption of solar radiation during the day by the material itself and by its surroundings. The thermal radiation could also be due to some internal energy source, including a local "hot" object. It can also be assumed that the detected radiation is scattered or emitted by materials close to or on the Earth's surface, and that the incident radiation and the detected radiation has passed through most of the Earth's atmosphere.

The spectral region of importance is dictated by the above assumptions. The Sun emits radiation most strongly in the visible and near infrared wavelengths between, say, 0.4 and 3.0 μm with a peak at about 0.55 μm (Figure 10-1). The temperature of materials on the Earth's surface is usually in the range of -20°C to 35°C , or about 250°K to 310°K , which means that they emit most strongly in the spectral range of 3 to 20 μm with a peak near 10 μm (Figure 10-2). The Earth's atmosphere absorbs strongly at wavelength shortward of about 0.35 μm , and at wavelengths longward of about 14 μm . Within this range (0.35 to 14 μm), there are serious absorptions due to water and carbon dioxide between 2.5 and 8 μm , with some "windows" of transmission in the 3 to 5 μm region. Also, there are strong water absorptions near 1.4 and 1.9 μm and ozone absorption near 9.5 μm . Figures 10-1 and 10-2 show the general atmospheric transmission spectrum. Thus, we are really concerned with scattered solar radiation in the 0.35 to 2.5 μm spectral region and with emitted thermal radiation between 8 μm and 14 μm . We might also be interested with both scattered sunlight and emitted thermal radiation in the 3 to 5 μm spectral region. A more precise description of atmospheric windows is given in Chapter 8.

10.2 Physics of the Technique

One way to describe scattered and emitted radiation and their information content is through the laws of physics. In principle, this radiation can be described using both Maxwell's equations for the wave nature of radiation, and quantum physics for the particle nature of radiation. Since there are many text books that describe these laws and their application, only a description of the important effects will be given here.

For scattered or reflected radiation, the nature of the interaction between the material and the incident radiation depends on the electrical properties of the material.

10.3 Scattering of Sunlight

This discussion begins by describing the interaction of solar radiation with a particulate surface, i.e., a surface made up of grains of differing size and materials but with the grains much larger than the wavelength of the radiation. Figure 10-3 shows a generalized situation with the various types of interactions possible.

Radiation incident on a particle can be reflected and transmitted at certain angles according to Snell's Law, with certain intensities as described by Fresnel's Equations, and absorbed according to Beer's Law. The key property of the material controlling these is the index of refraction n , which is related to the fundamental electrical properties of the material. The index of refraction is written as a complex number, where the real part n_r controls the amount of radiation reflected and transmitted, and the imaginary part n_i controls the amount absorbed along a certain pathlength. Simple forms of these laws can be written as follows:

Snell's Law

$$n_1 \sin \theta_i = n_2 \sin \theta_t$$

$$\theta_i = \theta_r$$

where 1 and 2 refer to outside and inside (particle) materials, respectively, i refers to incidence, r to reflection, and t to transmission. θ is the angle between the normal vector and the radiation travel vector.

Fresnel's Equation

$$\frac{(n_r - 1)^2 + n_i^2}{(n_r + 1)^2 + n_i^2} = R_N$$

where R is the energy reflected at normal incidence angle.

Beer's Law

$$T = e^{-kl}$$

where T is the energy remaining in the radiation after traveling a pathlength through the material, and k is the absorption coefficient, which depends on n_i .

Scattering Law

$$\Omega = \frac{\lambda}{\pi a}$$

where Ω is the angle of scattering, a is the particle dimension, and λ is the wavelength of the radiation.

The index of refraction is the important parameter, as stated earlier. For a material with a high real and low imaginary index of refraction, there is high reflectance and low absorption; sapphire (aluminum oxide) has this property. For high real and imaginary indices, there is high reflectance and high absorption; conductors (metals) fall into this category. Similar statements can be made for other possible cases.

The size of the particle is important for determining absorption and reflection. The most information about the material is contained in the radiation that enters the particle and is scattered back out of the particle to the observer before it is absorbed by the particles.

Another way to describe the scattering of radiation from a particulate surface is by using a heuristic statistical model. The most important model for this case is the Hapke Scattering Model. It has terms to

describe the direction of scattering and the amount of scattered radiation based on single particle absorbance. In principle, if the indices of refraction of the particle are known, the model can be used to calculate the reflectance spectrum; this, however, has not yet been fully achieved.

10.4 Absorption

The particular interest in this study is the possibility of distinguishing between materials in a remotely sensed scene and, even better, determining the composition of the material. The information to accomplish this is found mostly in the absorption of the radiation, with the angle of scattering (photometric function) being of lesser importance. The important factor is that different materials usually absorb differently as a function of the wavelength of the radiation. This means that a sufficient spectrum of the various materials in the sensed scene must be measured to reveal the differences in absorption. Since what is enough varies widely from material to material, the more of the spectrum measured, the more materials can be distinguished.

To interpret reflectance spectra, one must understand why the absorptions occur. Many books and professional papers have been written describing the various effects, therefore this report gives only a brief introduction to the kinds of effects encountered. It is necessary in this effort to use the particle nature of radiation and deal with quantized packets or radiation particles called photons. A photon energy is related to the wavelength or frequency of radiation by the equation:

$$E = h\gamma,$$

where E is energy, h is the Planck constant, and γ is the frequency of the radiation.

Basically, all absorptions are due to the capture of the photon by some part of the material that has a natural resonance at or near the wavelength (frequency) of the incident photon. The type of resonance varies, depending on what part of the spectrum is involved. In spectral regions where there are no resonances, the spectrum varies slowly with wavelength, depending upon the rate of change of the index of refraction with wavelength (dispersion), and the associated material is difficult to diagnose.

10.4.1 Ultraviolet wavelengths

At wavelengths shorter than about $0.4 \mu\text{m}$, the photon energy is often great enough to free electrons in the material from the host atom and allow them to move freely in that material until they are again captured by an atom and the energy is given up to the crystal lattice or, in some cases, radiated away as light of a different wavelength (luminescence). The electrons may even be ejected from the material (the photoelectric effect). This type of absorption usually sets in rapidly as wavelength is scanned toward shorter wavelengths and remains strong. Essentially, the materials become conducting and behave like metals. The reflectance spectrum will show a sharp decrease in reflectivity toward shorter wavelengths and then remain low far into the ultraviolet. The diagnostic feature is the wavelength of the onset of the absorption.

10.4.2 Visible wavelengths

Beginning in the blue part of the spectrum ($0.4 \mu\text{m}$), photon energies are no longer high enough to eject electrons from most atoms, but it is possible to cause electrons to be exchanged among bonds between adjacent atoms. These charge transfer absorptions usually begin to occur in the blue part of the spectrum and remain strong well into the ultraviolet. The spectrum shows a steep absorption edge and very low reflectance as it is scanned toward shorter wavelengths. Materials that show this effect include those containing Fe^{3+} , Ti^{4+} , and O. Iron oxides are notorious for this effect and

their red color is the result.

There is another important effect due to certain electrons having spin state energy transitions in this region. Particularly important are d-shell electrons in transition element metal ions, such as iron and cobalt. These electronic transition absorptions occur in bands of energy and cause spectra to have well-defined absorption features. Thus, they are very diagnostic. The band wavelength centers are very sensitive to the exact crystal structure in which the ions reside and they are indicative not only of the kind of material but also of the exact composition and crystal structure. Examples of these materials are minerals containing Fe^{2+} ions, such as pyroxene. These absorptions continue to occur into the infrared spectral region to about 2.5 μm .

10.4.3 Near Infrared Wavelengths

Beginning in the 1 μm region and extending to longer wavelengths, the next lower energy absorption effect, molecular oscillations, is encountered. The bonds which hold the atoms of molecules together are constantly stretching and contracting like springs as the atoms jiggle around on these bonds. Such molecular vibrations and rotations have certain characteristic frequencies or resonances. At or near these characteristic frequencies, strong light absorptions occur. The spectra show very well-defined absorption bands that are very diagnostic of the molecule. Important materials showing this effect include water, ice, and carbon dioxide. In fact, molecular absorptions by water, carbon dioxide, and ozone are responsible for strong absorption bands in the Earth's atmosphere.

10.5 Thermal Emission

Materials are made up of atoms and molecules which contain electrons and protons, i.e., charged particles. These atoms and molecules, and thus the charged particles, are constantly moving or vibrating. The amount of vibration is related to the temperature of the material. In fact, it is this motion which is responsible for the effect we call temperature. The higher the temperature, the greater the motion. The important point here is that the charged particles are moving, and a moving charge automatically radiates electromagnetic energy. The higher the temperature, the greater the motion and the stronger the radiation. This radiation is a function of wavelength. The radiation distribution with wavelength moves to shorter wavelengths as the temperature of the radiating material increases. This thermal radiation is described by the Planck Law, which can be written as:

$$B(\lambda, T) = \frac{\epsilon C_1}{\lambda^5 \left[\exp \left(\frac{C_2}{\lambda T} \right) - 1 \right]}$$

where λ is the wavelength of radiation, ϵ is the emissivity of the material (a measure of how efficiently it radiates), and the C_1 and C_2 are constants. B is energy per unit volume per interval of wavelength.

There are many complications involving the temperature differences within the surface layers, and the size of the particles (particles near in size to the radiation wavelength do not radiate very well), but these mostly affect the amount of radiation.

The important effect for this study is the dependence of emissivity on wavelength. As in the case of reflectance and absorption, the amount of radiation and its spectrum depend on the material and its natural resonances, and in particular on the molecules in the material. At wavelengths where molecules

oscillate easily, the thermal emissivity is high and much radiation results compared to other wavelengths. Thus the emission spectrum contains emission peaks that are the analog of the absorption bands in the reflectance spectrum, and these peaks can be very diagnostic of the material radiating.

10.6 Energy Conservation

It is necessary that energy be conserved in the interaction of radiation with a surface. This fact can be very useful. First, all sunlight incident on a surface must either be scattered back into space or be absorbed by the particles. The absorbed radiation must eventually be converted into motion of the atoms and molecules with a resulting increase in temperature, unless it is reradiated according to the process of luminescence. This increase in temperature means more thermal radiation.

Another important law derived from energy conservation is called Kirchhoff's Law. It can be expressed as follows:

$$E_r + E_t + E_a = E_i.$$

That is, the energy reflected plus the energy transmitted plus the energy absorbed must equal the energy incident. For the case of thermodynamic equilibrium and no losses,

$$E_t = 0 \text{ and } E_a = E_e$$

where e signifies emitted. This means that

$$E_r + E_e = E_i$$

E_r is proportional to reflectance and E_e is proportional to emittance. Thus, for unit energy incidence, reflectance plus emittance must equal unity.

$$R + E = 1$$

This suggests that if one knows the reflectance spectrum, one could calculate the emittance spectrum. This, unfortunately, is not usually true because of scattering effects in natural materials. This presents difficulties since laboratory measurements are more easily made in reflectance and field measurements are necessarily made in emittance.

FIGURE 10-1

**SOLAR SPECTRUM WITH
ATMOSPHERIC ABSORPTIONS**

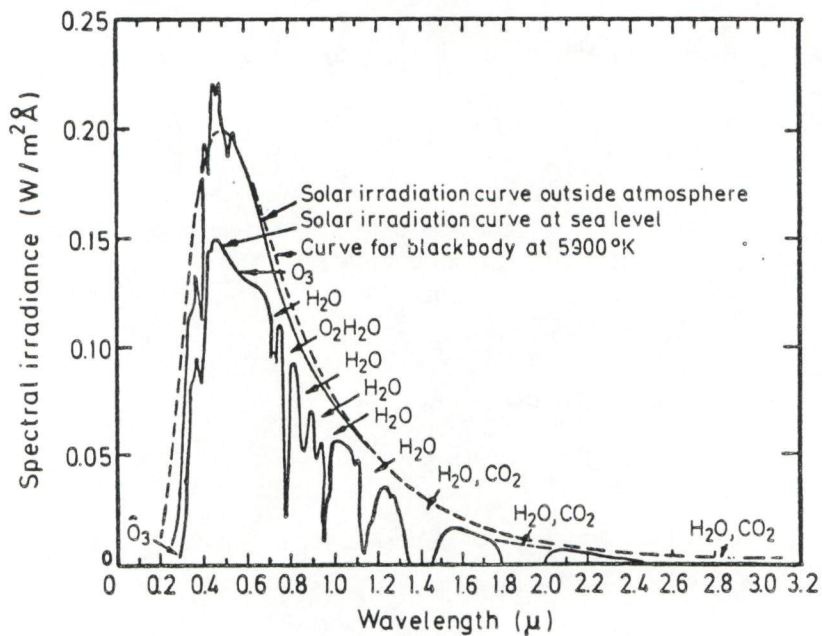


FIGURE 10-2

THERMAL SPECTRUM WITH ATMOSPHERIC ABSORPTIONS

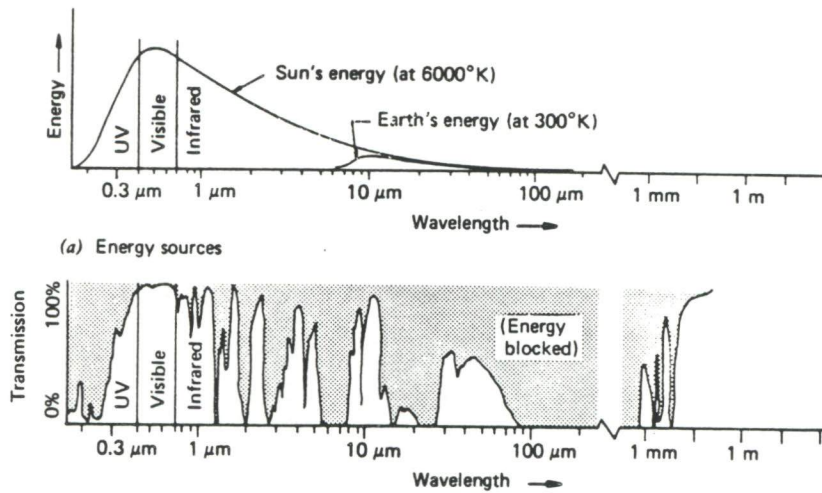
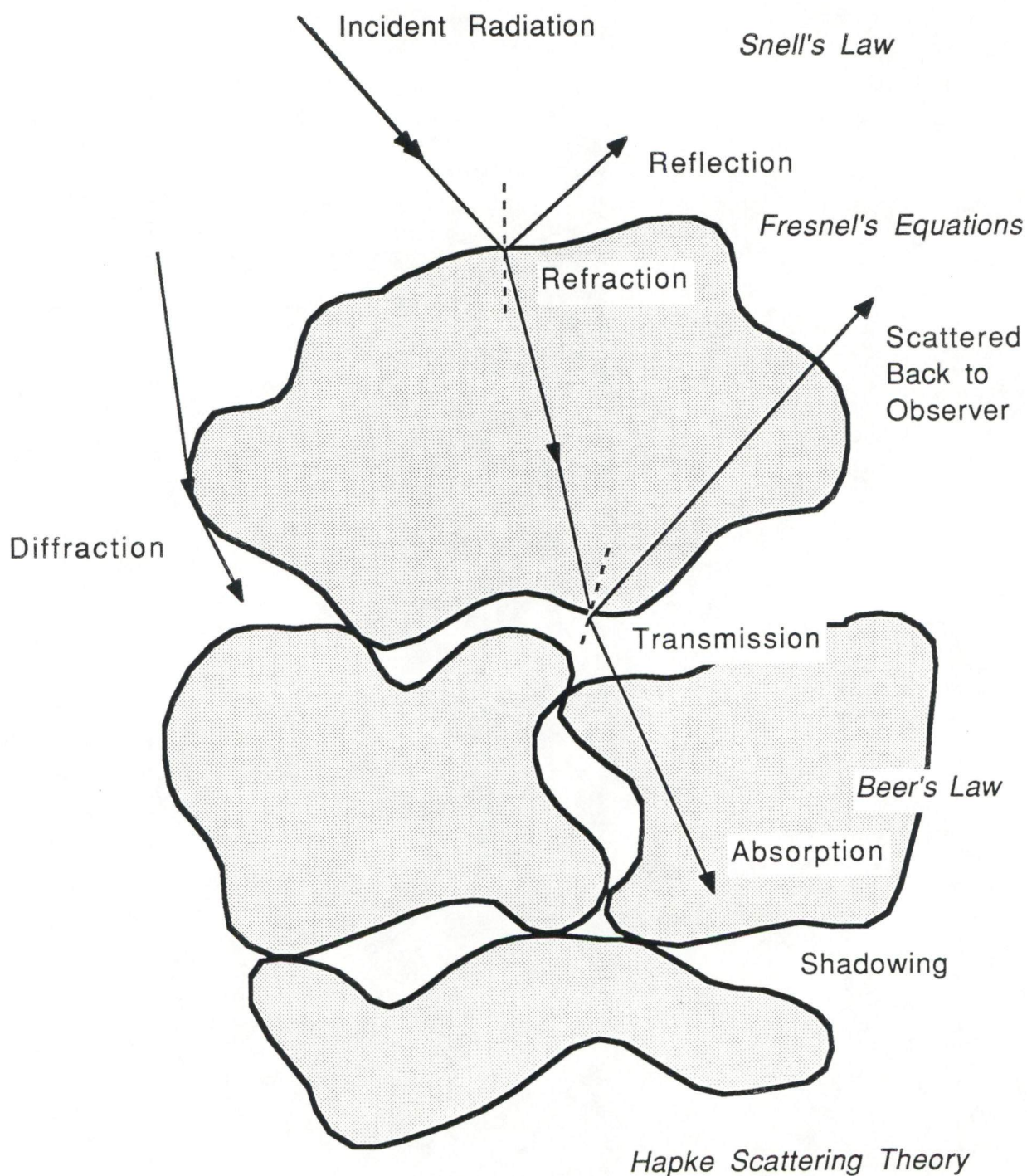


FIGURE 10-3

INTERACTION OF LIGHT WITH
A PARTICULATE SURFACE



11. Polarization Effects

11.1 Summary and Conclusions

The polarized component of light contains information about the surface roughness of the reflecting or emitting object, information about the opaque (degree of reflectivity) content or multiple scattering component of the reflected light, and in some cases, information about the index of refraction (metal content) of the reflecting object. Polarized light can be either linearly, circularly, or elliptically polarized depending upon the surface properties of the object scattering the light.

There is a good theoretical understanding of the nature of polarized light, and of how to detect and measure polarization. The knowledge needed to interpret what the polarized component means in terms of terrestrial materials (either naturally occurring or man-made) is quite limited, however.

Contrast enhancement for imaging (single channel or multispectral) is a particularly useful area. Polarization effects of the atmosphere caused by molecular and aerosol scattering can be used to determine the transmission quality of the atmosphere and to develop time-critical atmospheric backout parameters.

Studies of the polarization effects in absorption bands indicate that measurement of the polarization as a function of wavelength may be a useful technique for absorption band detection and identification in those spectral regions where atmospheric absorptions or transmissions degrade the spectral sensitivity of photometric instruments.

Most studies on terrestrial polarization deal with vegetation and oceanographic applications. Astronomical applications are much more sophisticated and could be applied to the terrestrial hyperspectral imaging techniques.

11.2 Polarized Light in Remote Sensing

The physical properties of a scattering surface can be studied remotely using the photometric (brightness), spectral (wavelength-dependent), and polarimetric measurements. Photometric and spectral effects result from the way in which the intensity of light is affected by the physical properties of a scattering or emitting surface. Polarimetric effects arise from the physical nature of the light itself, as well as from the physical properties of the surface.

Light is composed of electromagnetic waves in which the electric and magnetic fields are perpendicular to each other, and both fields are mutually perpendicular and transverse to the direction of propagation. The orientation of the electric field determines the angle of polarization of the light. In essence, polarized light is light whose vibration orientation exhibits a preference. This preference is described as either linear (in a plane of polarization), circular (left- or right-handed), or elliptical (left- or right-handed) polarization, depending on whether the electric vector has a constant preferred plane of vibration as in the linear case, or tends to rotate as in the circular case, or rotates while the amplitude of the polarized component varies as in the elliptical case.

Unpolarized light is defined as that light which exhibits no long-term preference as to direction of the plane of polarization or to handedness. However, most of the light encountered in nature is polarized to varying degrees since the physical properties of the emitting or reflecting surface define, to varying degrees, a plane or handedness. In theory, one could use the polarization properties of the emitted or reflected light to study certain physical properties of the surface being observed.

Polarized light is generally described in terms of four quantities called the Stokes parameters: I , Q , U , and V . These four quantities are combined together in matrix or vector form to form the Stokes matrix or vector. The first quantity, I , describes the intensity of the light received by the detector. The next two quantities, Q and U , when combined with I describe the linear polarization properties of the light. The final quantity, V , when combined with I describes the circular polarization properties of the light. In general, if A_x and A_y are the amplitudes in mutually perpendicular directions of the electromagnetic waves, then,

$$I = \langle A_x^2 + A_y^2 \rangle$$

$$Q = \langle A_x^2 - A_y^2 \rangle$$

$$U = \langle 2 \cdot A_x \cdot A_y \cdot \cos(g) \rangle$$

$$V = \langle 2 \cdot A_x \cdot A_y \cdot \sin(g) \rangle$$

$$I^2 = Q^2 + U^2 + V^2$$

where the angular brackets enclose time-averaged quantities, g is the phase angle between amplitudes A_x and A_y , and I is the intensity of the light as measured by the detector.

The geometric plane containing the illuminating source (the Sun in most cases), the scattering surface and the detector, is generally referred to as the photometric plane. By defining the photometric plane as the principal reference plane, the Stokes parameter V equals zero because of symmetry. In this case, the linear polarization can be defined as:

$$P(\%) = 100 \cdot Q/I.$$

All four quantities (linear plus circular) are required to describe the elliptical polarization properties of the light. The relative values of these quantities can be directly calculated, in certain circumstances, from the Fresnel equations, which describe the physical aspects of the reflection of light from plane surfaces.

In spite of the fact that there is extra information carried in the polarized nature of the light, most remote sensing studies ignore the polarized component of the light and deal only with the photometric or spectral properties of the light. The reason for this disregard of the polarized component is that for most natural surfaces, the polarization mechanism is complicated and poorly understood. Photometric and spectral information will, in general, suffice for studying the physical properties.

11.3 Sources of Polarization

Polarized light occurs in sky and reflected sunlight scattering from all surfaces (including water, land, roads, buildings and vegetation), and in emitted light (generally at, but not limited to, thermal wavelengths) from any surface. The degree of polarization depends significantly upon the physical properties of the surface and the photometric angles, that is, the angle of illumination and view of the surface. Other nonnatural sources of polarization can be found but these are limited to circumstances not commonly found in the terrestrial environment. These other sources include synchrotron radiation, line emission in strong magnetic fields, and coherent radiation from lasers. Many of these latter sources of polarized light are commonplace in the astrophysical environment.

It is possible to calculate from first principals the polarization of light reflected from a surface, given the index of refraction of the material. Examples for polarization components perpendicular and parallel to the plane of the surface are shown in Figures 11.1 and 11.2 for glass ($n = 1.50$) and for gold and silver

mirrors. Phase changes can occur upon reflection, which can cause the light to become circularly or elliptically polarized depending upon the angle of the phase difference.

Sunlight scattered in a molecular atmosphere is highly polarized in the direction 90 degrees from the source: This scattering, generally described as Rayleigh scattering, is highly wavelength-dependent.

Light scattered by atmospheric aerosols can also be highly polarized. As in the case of molecular scattering, the amount of polarization depends upon the scattering angle. However, the size and shape of the aerosol particles are additional important factors. For simple symmetric shapes, the Mie scattering theory is applicable. As the particles become increasingly irregular, modifications to Mie theory must be employed to calculate and explain the observed polarization effects.

Thermal emission is polarized. For a smooth surface, the emissivity is composed of two components, one parallel and the other perpendicular to the plane of the surface. The parallel component dominates over the perpendicular component since the boundary conditions for the electric vector are more favorable for radiation in that direction.

11.4 Detection of Polarized Light

A wide variety of techniques exists for the detection and measurement of the polarized component of light. In general, these devices use an analyzer or optical device that inhibits the transmission of one preferred direction of polarization, in front of a detector that is sensitive to "nonpolarized light". Rotation of the analyzer causes variations in the amount of light falling on the detector. Comparisons between the angle of rotation of the analyzer and the amplitude of the signal on the detector give both the amount of polarized light and the angle of orientation of any linear polarization.

Analyzers for linearly polarized light include Polaroid sheets, which are thin sheets of polymer molecules aligned in parallel so as to absorb the electric field parallel to the molecules, and half-wave retardation plates which serve to retard one component of the radiation relative to another. Retardation plates are generally made of optically transparent materials that have different indices of refraction for the two orthogonal polarization components. The detection of circularly and elliptically polarized light makes use of quarter-wave retardation plates.

Analyzers can be found that work in nearly all spectral regions from the ultraviolet to the far infrared. In the infrared, the analyzer can be constructed out of thin, appropriately spaced, parallel wires. Retardation plates can be made for monochromatic wavelengths or for broadband applications.

Polarimeters of a wide variety have been made for the study of naturally occurring polarized light. Some are very simple and use a rotating piece of Polaroid film in front of a camera or photometer. Others are quite sophisticated devices for detecting the circular or elliptical polarization at a precision of 0.1% or better. One such device has been developed for astronomical observations by K. Serkowski and T. Gehrels at the University of Arizona. However, the same techniques could easily be applied to terrestrial applications.

11.5 Applications

The polarization state of the reflected light is controlled to a large degree by the macroscopic roughness of the surface. Reflections with a large specular component generally have the highest polarization. Specular reflections tend to arise from shiny, microscopically smooth surfaces such as metal. Reflections with a large diffuse component tend to have a lower polarized component since multiple scattering tends to act to depolarize the scattered light. Diffuse reflections come from vegetation, land, and most other surfaces.

The absolute reflectivity of a surface also controls the contribution of the polarized component to the overall scattering--the darker the surface, the stronger the polarized component relative to the total radiation scattered. Darker surfaces tend to have less multiple scattering since higher orders of scattered light are absorbed. This fact causes the singly scattered, highly polarized component to stand out relative to the total light reflected.

Other factors that control the polarization are the compaction of the surface, the particle size, and the orientation of dominant features in the field of view (for example, pine needles). Polarization is useful in distinguishing the macroscopic and microscopic contributions to the total scattered light.

11.5.1 Contrast enhancements

Polarized light can be used to study the physical properties of the scattering surface in a variety of ways. One method, which is not necessarily related to the scattering properties of the surface, is to use a polarization analyzer to increase the contrast in a scene viewed through a turbid medium such as an aerosol-filled atmosphere.

Scattering in the atmosphere reduces the apparent contrast between the subject under scrutiny and the background, with no increase in the detector sensitivity or the illumination of the scene. However, since the scatterers in the turbid medium are widely separated and scatter light only once, the light scattered in the turbid medium will have only opposite-handed polarization whereas the target will, in general, have both components of polarization. By removing the scattered component polarization, the target/background contrast is enhanced.

11.5.2 Vegetation studies

Wavelength-dependent factors in the polarization can be used to characterize farm crops with significant differentiation. For example, alfalfa leaves have been shown to be significantly different in spectral polarization curves than potato leaves, even though they appear somewhat similar in simple spectrophotometry. This results from the different leaf structure of the two types of plants. Similar results are found for corn relative to potatoes and alfalfa.

The polarization properties of farm soil are very sensitive to the soil moisture content. Higher polarization in wet soil results from a thin film of specularly reflecting water.

Interpretations of the polarization properties of vegetation, including forests, require an empirical approach to understanding. That is, measurements of many diverse areas must be made to gain an understanding of the various ways in which a particular vegetation affects the polarization of the light. In some cases where the polarization effects of a particular vegetation are well understood, e.g., pine trees (aligned needles), it is possible to make statements about the structures below the spatial resolution of the observing instrument.

11.5.3 Spectral reflectance and polarization

The quantity of polarized light reflected from a diffusely reflecting object is a function of the total amount of multiple scattering component. The singly scattered component is highly polarized according to the Fresnel equations whereas the multiply scattered component is depolarized due to the many scatterings. In general, this leads to an inverse relationship between reflectivity and the degree of polarization of the reflected light: light reflected from darker objects is more highly polarized than that reflected from highly reflecting objects.

The relationship described above holds true for spectral reflectance: as the spectral reflectance

varies as a function of wavelength, the polarization of the light at that wavelength changes accordingly. In essence, one could use the polarization as a function of wavelength in order to detect the presence or absence of absorption bands inherent in any material. This method is particularly useful in spectral regions where telluric water vapor or other molecular absorption bands occur.

11.5.4 Ocean studies

The polarization state of light reflected or emitted from the surface of the sea is affected strongly by the surface conditions: oil slicks, vegetation, waves, foam, etc.

Emitted radiation from the sea surface in the range of 2 to 200 microns is polarized according to the Fresnel equations. In general, the polarization of the emitted radiation (usually measured at a wavelength of 10 microns) from a calm sea changes from nadir (looking straight down) to the horizon (looking along a slant path). The polarization will be largest looking toward the horizon along a slant path.

Two important effects must be taken into account when measuring the emitted radiation from a flat area: (1) if the detector system (optics, filters, gratings, detector) is polarization-sensitive, then the measured intensity of emitted radiation may be different from the true intensity; and (2) surface structure (floating materials, waves) may affect the amount of polarization in a nonrandom way.

The first condition must be taken into account when designing any instrument for any wavelength region. The second effect can be used to estimate the degree to which the ocean surface is disturbed.

Skylight reflected from the surface of the ocean can also be used as an indicator of the state of the ocean surface. Sun glint and the angle of polarization can be used to determine both wave height and wave direction.

11.6 Conclusions and Recommendations

The polarized component of light contains information about the surface roughness of the reflecting or emitting object, information about the opaque (degree of reflectivity) content or multiple scattering component of the reflected light, and in some cases, information about the index of refraction (metal content) of the reflecting object. Polarized light can be either linearly, circularly, or elliptically polarized depending upon the surface properties of the object scattering the light.

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Sustaining Excellence in Science and Engineering in the Former Soviet Union

Report of a Conference

SUSTAINING EXCELLENCE IN SCIENCE AND ENGINEERING IN THE FORMER SOVIET UNION

Report of a Conference on February 9, 1993

Co-Conveners of the Conference

**Frank Press, National Academy of Sciences
Richard Getzinger, American Association for the Advancement of Science
John Moore, George Mason University
George Soros, International Science Foundation for the Former Soviet Union**

Working Group Chairs

**Direct Aid - Irving Lerch, American Physical Society
Infrastructural Issues - Gerson Sher, National Science Foundation
Global Scientific Heritage - Robert Hoffmann, The Smithsonian Institution**

**National Academy of Sciences
National Academy of Engineering
Institute of Medicine**

**National Academy Press
Washington, D.C. 1993**

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Support for this project was provided by the International Science Foundation for the Former Soviet Union.

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Preface

Science and engineering in the former Soviet Union represent an asset of great value to the world. Renowned for its prowess in many fields, the scientific enterprise has much to contribute to our knowledge. In addition, science is a force for democracy, and can be expected to reinforce the transition to a democratic, market-oriented society in the former Soviet Union.

The political turmoil and economic tribulations of the last few years pose a grave threat to the survival of the best in natural science, social science, and engineering in the former Soviet Union. Scientists and engineers are being forced to leave their professions in order to survive. Old relationships have been sundered, and new ones are emerging only with great difficulty. The physical infrastructure is crumbling or tragically obsolete. Great research collections and unique data sets, some dating back centuries, are at risk. In short, the enterprise is in a state of intense crisis.¹

The conference that produced the documents included in this report was motivated by the recognition of this crisis and of the fact that sustaining what is best in science and engineering in the former Soviet Union requires the efforts of many organizations. Accordingly, representatives from private foundations, learned societies, government agencies, corporations, universities, and associations were brought together at the U.S. National Academy of Sciences on February 9, 1993, to share their knowledge of the problem and to discuss actions that should be taken. Also participating were colleagues from public and private organizations in Western Europe and Japan and diplomatic representatives from many of the Newly Independent States.

To provide background for the discussions, three individually-authored papers were prepared. Necessarily limited in coverage, the papers nevertheless addressed the three principal aspects of the situation: the need for direct support of individual scientists in this difficult period, the extensive problems in the infrastructure supporting scientists and engineers, and the grim prospect of the possible loss of irreplaceable collections.

Based on these papers, a draft Action Plan was drafted by the conference steering committee.² The purposes of the Action Plan are to identify principles of support, to point to needed actions, and to provide guidance about coordination and management of programs and activities. It deliberately does not attempt to match actions with potential actors. Rather, the

¹See, for example, "Reorientation of the Research Capability of the Former Soviet Union: A Report to the Assistant to the President for Science and Technology," (Results of a Workshop on March 3, 1992), National Academies Press, 1992.

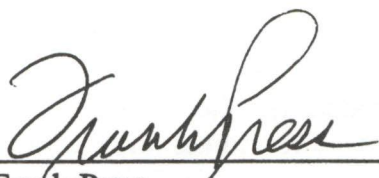
²Committee members included William Blanpied, American Physical Society and National Science Foundation; Sandra Burns, American Association for the Advancement of Science; Gilbert Fayl, European Community; Richard W. Getzinger, American Association for the Advancement of Science; Timothy Goggins, American Mathematical Society; Ernest Henley, American Physical Society; Robert MacPherson, American Mathematical Society; Gerson Sher, National Science Foundation; and Gary Waxmonsky, National Research Council. The committee was chaired by John H. Moore, George Mason University.

intent is to provide a menu of desirable actions, enabling interested organizations, public and private, to choose those that are best suited to their capabilities and interests.

The conference was focused on revising the draft Action Plan. Three Working Groups, one on each of the three major topics, spent most of the day in discussions of those topics. Many of their recommendations for modification and amendment of the Action Plan were then incorporated and the results presented in plenary session. The final document as revised by the conference steering committee is displayed here as the Action Plan.

Programs of assistance to science and engineering in the former Soviet Union are beginning to emerge. Notable among them is the International Science Foundation for the Former Soviet Union (ISFFSU), whose formation was announced by George Soros in December 1992. The ISFFSU will provide support of \$100 million over the next two years. Additional efforts by several learned societies and foundations are also underway, but much more is needed. Readers of this report are strongly urged to work with colleagues to develop programs attacking those problems identified in the Action Plan that are most compatible with their capabilities.

Thanks are due to the staffs of the National Research Council's Office for Central Europe and Eurasia and of the International Institute of George Mason University for their excellent work in support of the conference. The financial support of the ISFFSU is gratefully acknowledged.



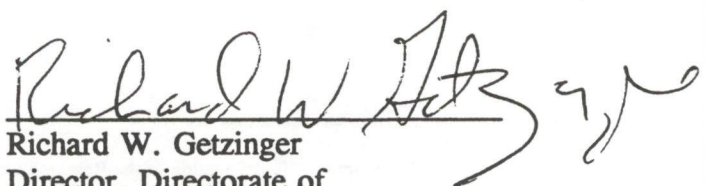
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SUSTAINING EXCELLENCE

IN SCIENCE AND ENGINEERING IN THE FORMER SOVIET UNION

A Conference¹

Washington, D.C.

February 9, 1993

ACTION PLAN

The problems of science in the former Soviet Union are extensive and complex. Their resolution is important for the well-being of international science and to the further development of democratic, market-oriented societies in the former Soviet Union. Many organizations in the West -- governments, foundations, learned and professional societies, universities, and corporations -- are interested in these problems and their possible solutions. A growing number of these organizations are undertaking efforts to aid science in Russia and the former republics. Notable among them is the International Science Foundation for the Former Soviet Union (ISFFSU), which will provide \$100 million over the next two years to support basic research and related infrastructure.

A central issue in the provision of support to excellent science and engineering in the FSU is that of matching support programs to needs. The need is enormous. No single external organization can meet it alone, and there are significant needs that will not be addressed by the ISFFSU, including support for the social sciences, for large-scale research projects, and for training the next generation of scientists and engineers. At the same time, it must be realized that the principal investment in science and engineering in the successor states of the Soviet Union must be made by the peoples of those states. External support can only help to sustain excellence in science and engineering through the transition phase while helping to lay the foundation for the eventual self-sustaining enterprise.

However, high leverage opportunities can be identified. The purpose of this Action Plan is to provide information to organizations to help them plan their programs and to minimize, as far as desirable and useful, unnecessary duplication of effort. It does not presume to direct efforts, but aspires to contribute to a balanced, effective, and comprehensive set of support activities.

This Action Plan reflects the knowledge, expertise, and imagination of the participants in the conference, "Sustaining Excellence in Science and Engineering in the Former Soviet Union." It is hoped that the publication of the Plan will stimulate further dialogue among and concrete action by all those who are concerned about the present and future state of science and engineering in the FSU.

¹The conference was co-sponsored by the National Academy of Sciences, the American Association for the Advancement of Science, the International Science Foundation for the Former Soviet Union, and the International Institute of George Mason University. This Action Plan was developed at the conference.

Steps should be taken at every level to insure that the spirit of international understanding and cooperation which is so necessary to sustain high quality science and engineering in the FSU will continue to be an important element in the development of science and technology in the future. The availability of data and the possibility of developing cooperative projects, where appropriate, should characterize scientific relationships between the FSU and other countries.

The Action Plan's primary focus is on emergency aid to sustain the best in science and engineering during the difficult time of transition. However, it should be taken as a step in the direction of the ultimate goal: to help the FSU to develop a self-sustaining, self-managing system for its science and engineering enterprise.

Participants in the February 9 conference recognized that high level coordination and dialogue among the governments of North America, Europe, Japan, and the states of the FSU has great potential value. The focus of the conference, however, was on the non-governmental sector.

The conference produced a large number of suggestions for action. Among the most important are these:

- Short-term actions to provide emergency aid should be based on scientific merit and should be made directly to individual scientists and small groups. Support should seek to promote open access by FSU scientists to research opportunities and infrastructure, as well as to promote diversification of research among sectors in the FSU -- institutes, universities, industry, and emerging institutions.
- Support for the scientific infrastructure, including telecommunications, books and journals, research management capabilities, and the human infrastructure, should be undertaken as a matter of high priority.
- The irreplaceable collections of physical data and specimens in the FSU, as well as its unique pedagogical techniques in certain fields, represent a heritage of enormous value to the world and should be rescued from impending loss. Steps should be taken to publicize newly available collections throughout the world scientific community.
- New programs of support for science and engineering should be widely publicized within the FSU.
- An international network of information and operations centers should be established to insure better coherence of programs, to avoid duplication, and to catalyze follow-up activities. The network should include nodes within the FSU.
- Periodic consultations should be undertaken among relevant organizations in all concerned countries to exchange information and monitor progress of scientific efforts.

SUSTAINING EXCELLENCE

IN SCIENCE AND ENGINEERING IN THE FORMER SOVIET UNION

ACTION PLAN

1. General Principles

- 1.1 In all support programs, bear in mind the twin objectives of strengthening international science and engineering and developing democratic, market-oriented institutions in the FSU.
- 1.2 Design emergency support programs and enlist FSU cooperation keeping in mind the ultimate objective of creating a self-sustaining, self-managing system for the scientific and engineering enterprise of the FSU.
- 1.3 Make all awards on the basis of competitive merit review, as determined by independent evaluators.
- 1.4 Make awards directly to individuals rather than institutions, and support groups in cases of awards larger than the minimum. Consider including support for institutions in which the individual or group works.
- 1.5 Seek to insure open access by FSU scientists and engineers to research opportunities and infrastructure.
- 1.6 Make special opportunities available for newly established investigators and graduate students, both individually and through their mentors.
- 1.7 Seek broad distribution of awards, geographically and by discipline.
- 1.8 Encourage diversification of research and collaboration among sectors in the FSU -- Academy institutes, universities, industry, and emerging institutions.
- 1.9 Motivate partners in the FSU to share concrete responsibility in all external assistance programs.

2. Direct Grants to Individual Researchers and Small Groups

- 2.1 Place highest priority on emergency aid in the form of small grants and stipends to selected scientists and engineers as a first step towards developing a self-sustaining, self-managing system.
- 2.2 Make grants sufficiently flexible to allow for support of modest research needs, such as supplies and minimal equipment, in addition to salaries.

2.3 Develop and strengthen the basis for long term collaborative research involving FSU scientists and engineers with scientists and engineers from other countries.

2.4 Provide support for special activities.

- Support special educational programs that have contributed to excellence (special seminars for secondary school teachers, student Olympiads, etc.).
- Provide support for exceptional secondary school mathematics and science programs.
- Support workshops in the FSU, especially those involving foreign scientists and engineers.
- Support special summer and winter schools in the FSU.
- Give special consideration to activities designed for younger investigators.

2.5 Provide support for international travel on a limited basis.

- Develop mechanisms to coordinate requests for travel from FSU scientists and engineers invited to present papers at professional meetings.
- Encourage professional societies to help support travel by FSU scientists and engineers to society meetings.
- Conduct professional meetings in the FSU.
- Include funds for travel to international professional meetings in direct aid grants to FSU scientists and engineers.
- Provide support for short-term research visits by FSU scientists and engineers to Western research institutions.

3. Infrastructure Support

3.1 Telecommunications

- Provide low-cost packages of basic computer equipment needed for e-mail; develop and share lists of e-mail addresses.
- Facilitate network access and expedite equipment exports.
- Seek to influence FSU policy-makers to make telecommunications widely accessible to their scientific communities at reasonable cost.

- Help persuade them to give high priority to establishing efficient, low-cost telecommunications systems, for example by financing high-visibility demonstrations of practical systems.
- Provide them with information about the value of networking.
- Facilitate remote access to scientific databases at reduced cost.

3.2 Books, journals, and libraries

- Make grants to professional societies to support journal subscriptions, electronic transmission, and CD-ROM databases.
- Support procurement and installation of CD-ROM equipment in selected FSU S&T facilities.
- Seek to replace missing back issues of selected journals in several central institutional libraries.
- Coordinate and support shipment and distribution of journals and equipment to the FSU.
- Negotiate with publishers to secure appropriate fees for provision of journals, including electronic access.

3.3 Human and Institutional Infrastructure

- Give special priority to programs that create new linkages among FSU researchers and with user communities. Support should be emphasized, for example, for high quality university researchers; young investigators, graduate students, and undergraduates; activities that involve cooperation between academy, university, and/or industrial laboratories; and high quality applied research with potential industrial applications.
- Utilize expertise of national and international organizations with experience in supporting and conducting industrially oriented research to help with developing linkages between research and industry
- Assist the implementation of training opportunities in research management, science and technology policy, competitive merit review, accreditation, university administration and commercial application, technology transfer, S&T marketing, and intellectual property rights (IPR) and legal protection.
- Solicit donation and/or sale of surplus computers and equipment from Western manufacturers and government laboratories.

- Include non-FSU researchers as active research partners, especially in the applied research area, to help show how to bridge the gap between research and application.
- Develop general directories of research institutions and discipline-specific directories of individuals in the FSU. Make directories of Western research institutions available in the FSU.
- Support the formation of broadly based, representative science and engineering societies and support viable existing societies.

4. Scientific Heritage (Collections and Data Sets)

4.1 General observations

- Ensure mutual accessibility to collections and archives for both local and international experts, and promote the open availability of scientific data.
- Develop complementary roles for private sector and governmental organizations with respect to identification and preservation of collections and data sets.

4.2 Collections of objects

- Utilize existing inventories of collections and archives (including rare books), and develop action plans based upon them.
- Develop annotated directories of presently uninventoried collections and archives in each field.
- Develop strategies for long-term protection, preservation, and growth of collections and archives.
- Organize joint teams with access to discretionary resources to assess requirements for insuring the preservation of high priority collections and archives, to make on-the-spot disbursements where necessary.

4.3 Data sets

- Develop or endorse established protocols and promote data sharing.
- Develop annotated directories of presently uninventoried data sets in each field.
- Develop strategies for long-term protection and preservation of data sets.

- Provide support for joint efforts in digitizing, computerization, management, maintenance, and growth of existing data sets.

5. Procedural considerations

5.1 Management and coordination

- Encourage on-going donor consultation; share facilities for the transfer of financial and material resources to the FSU among donors.
- Provide support for an open, accessible information system for managing and tracking financial support, including all significant sources.
- Support the creation of information and operations centers for the logistics of providing financial and equipment support to the scientific and engineering communities of the FSU. Such centers ideally should have broadly based support from government, private foundations, and industry.
- Through professional and learned societies and foundations, organize advisory and coordinating committees to develop plans, procedures, and principles for development of assistance programs.
- Use Western scientific and engineering institutions as organizing bodies for coordinating direct aid efforts and forming advisory committees.
- Handle IPR issues arising from cooperative programs on a case-by-case basis, but encourage the FSU governments to adopt IPR laws that are consistent with Western practice.
- Use existing centers in the FSU wherever possible to coordinate the distribution of journals and equipment.

5.2 Publicity

- Publicize opportunities for support throughout the FSU scientific communities, using widely distributed national media and through joint newsletters involving both FSU and Western organizations.
- Use non-FSU organizations -- foundations, societies, corporations, government agencies -- active in the FSU to help with the publicity effort.
- Publicize the availability of newly accessible databases, collections, and research facilities among scientists outside the FSU.

**DIRECT AID TO SCIENTISTS IN THE SUCCESSOR
STATES OF THE FORMER SOVIET UNION: A CASE STUDY
OF THE PHYSICS COMMUNITIES**

Background Paper

by

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**SUSTAINING EXCELLENCE IN SCIENCE AND ENGINEERING
IN THE FORMER SOVIET UNION**

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Preamble

It is difficult to generalize from the experiences of one scientific community in the former Soviet Union (FSU) to characterize the problems, find potential solutions, develop operations, and formulate the rules applicable to conditions in other disciplines. This paper is, therefore, a case study based on experiences of the U.S. physics community in dealing with its counterparts in several nations of the FSU since 1992. Although the paper makes no claim to applicability beyond physics, the authors are grateful to colleagues in the American Astronomical Society (AAS) and American Mathematical Society (AMS) who have also established significant programs with their FSU counterparts and have generously shared their experiences with us. Our colleagues in the European Physical Society are also undertaking extensive efforts to support colleagues in both the FSU and East-Central Europe and have surveyed the status and needs of both research and academic institutions there. Several of the recommendations in Section 3 are based on their experiences and expectations.

The reasons for the difficulties faced in attempting to generalize beyond one community are inherent in the nature and history of Soviet science. Whereas the biological, behavioral, and social sciences were subject to direct political intervention, the mathematical and physical sciences were largely insulated from such control because atomic and nuclear physics especially were seen as instruments of state policy and a source of state power. Thus the elite physicists occupied a position of privilege in the Soviet State. Despite the emergence of seeds of dissidence in the market of freely circulated ideas which flourished in many of the most important physics institutes, the Academy and institutional structure maintained the strictest controls over the scientific establishment which was distinguished by a large measure of passivity and acquiescence to central authority.

Diminished productivity was often compensated by bloated and inefficient organizational structures. Upon the collapse of the Soviet State, these centers of excellence were deprived of essential resources and services and, unfortunately, self-management did not immediately emerge owing to the legacy of central control. In addition, the separation of the research institutes from the universities has left the latter in a depleted state, incapable of supporting major research initiatives.

The problem now is to assist FSU science to preserve its best endowed communities and traditions so that it will be granted the time and resources needed for restructuring. This paper focuses on provision of direct aid to investigators in the quantitative sciences as a case-study of one approach for solving the broader problem of sustaining the best of science -- and engineering -- in the former Soviet Union. The types of direct aid that will be accomplish that objective will necessarily be somewhat discipline specific. In much of experimental physics, chemistry, and the biological sciences, FSU scientists require modest supplies and instruments, in addition to salaries and stipends, in order to pursue their research. Since these items can often be obtained only in the West, funds for short-term visits which include a moderate purchase allowance can be critical in sustaining scientific excellence during the emergency period.

The social and behavioral sciences face a considerably different challenge. Whereas the principal, immediate problem in the mathematical, physical, and biological sciences is to sustain a tradition of excellence, the social and behavioral sciences in the FSU have been debilitated by decades of subjugation to ideological imperatives. Western colleagues therefore face the problem of **developing** a respected, self-sustaining community in those disciplines, rather than **sustaining** already acknowledged excellence. Thus, for the social and behavioral sciences, the most effective form of direct aid could be medium- to long-term visits to Western institutions for both junior and senior scientists that would permit them to grasp the "culture" of independent scholarly research in those disciplines.

Despite the precise form it takes, the overriding principle of direct aid programs is to bypass inefficient existing bureaucratic structures and provide aid to working scientists themselves based on some type of competitive, peer-review process.

This paper will explore the background of the current emergency for science in the FSU and existing and potential approaches for solving problems. It will recommend a specific actions that, with some fine tuning, could be applicable to disciplines beyond the mathematical and physical sciences. The paper will also seek to examine the immediate and longer term needs of the scientific community in the FSU in the context of the ultimate objective of achieving self-management with an investigator-initiated peer-review system.

The reader is alerted to the fact that this paper concentrates on the Russian Federation since the majority of FSU scientists are located in that country. However, large and important scientific groups are found throughout the FSU, particularly in the Western states, and it will be important to develop an awareness of the special needs and circumstances of each of them. The scope of this paper is unfortunately far too limited to take into account the many important details which differentiate the successor states from one another.

1. Background:

The overriding principle of direct aid programs cannot be stated too often: *to bypass the inefficient bureaucratic structures of the Academy, the institutes, and those few universities that conduct viable research, and provide aid directly to working scientists themselves, based on some type of competitive, peer-review process.* An important corollary principle is *reliance on personal and professional relationships rather than institutional ties to develop the mechanisms for soliciting, evaluating and administering aid.* If, on the contrary, assistance is funneled through the directorates of the Academy, the institutes, or the universities, most funds will be dissipated in preserving the existing bureaucracies.

It is important to note, however, that in physics, not all of the research institutes in the Russian Federation are managed and controlled by the Academy. The Institute for Theoretical and Experimental Physics in Moscow, for example, is a branch of the Ministry of Atomic Energy. Despite some exceptions, the institutes have traditionally functioned as isolated units, often in competition with one another.

While many of the successor states of the Soviet Union have been slow to reform the apparatus of centralized science management by the Academy and ministries, Ukraine put into effect an investigator-initiated peer-review program modeled on those in the West.

Personal trust is the currency for all direct aid transactions. Nonetheless, the APS and our colleagues in the FSU find institutional affiliations both viable and desirable since the most productive work is centered there. However, the extent to which such affiliations can be relied on differs according to discipline. In the case of mathematics, academic failure and social corruption--usually manifest in exclusionary ethnic and anti-semitic policies--have made the institutional and university departments unsuitable as vehicles for transformation and renewal. Thus, the American Mathematical Society (AMS) seeks to couple its aid programs to promoting the development of new mathematical institutions.

There is the further problem of infrastructure integrity. For if there is no heat or light and if the walls and roofing fall into disrepair, science is still endangered. Even more important, such essential central services as libraries and telecommunications are rapidly failing. These problems are addressed at greater length in the accompanying paper on Infrastructural Issues by Gerson Sher.

1.1 Dimensions of the Problem (Programmatic and Contextual)--

1.1.1 Libraries--Adequate technical libraries with current copies of world scientific literature are obviously essential to the work of scientists in the FSU. The accompanying paper by Gerson Sher includes a description of the special needs of physicists in the FSU, and on American Physical Society (APS) programs to help meet those needs on an emergency basis. A possible strategy for longer-term maintenance of scientific libraries appears in Section 3.1.2.

1.1.2 Computer-moderated telecommunications--Next to libraries, a high priority need for scientists in the FSU is for adequate telecommunications capabilities. Recommendations for short-term solutions is considered in Section 3.1.5. The accompanying paper by Sher explores the broader problem of telecommunications in the FSU, including experiences of the APS in dealing with individual scientists. It also proposes several possible short- and long-term solutions to the telecommunications problem.

1.1.3 Salaries, Research Funds, and the Brain Drain--Salaries are low and paid intermittently. Monthly wages range from 2,500 to 10,000 rubles (\$6 to \$25 based on exchange rates prevailing in February 1993). Physicists working at some institutions in Moscow have voluntarily foresworn monthly payments in order to make funds available to colleagues in regions of Russia distant from the capital. The collapse of the ruble, low and intermittent salaries, and a crumbling scientific infrastructure, have driven scientists at all levels to leave their posts, sometimes temporarily, often permanently. Up to 10 percent of the elite scientists from the major physics institutes have emigrated to Western Europe and the United States, and many of those remaining are forced to travel constantly to continue their work and to obtain sufficient hard currency to meet their domestic needs.

Some institutes, such as the renowned Landau Institute in Chernogolovka, almost ceased to be viable owing to the emigration of many senior scientists. Fortunately, that particular institute has been reinvigorated by a newly appointed director, Vladimir Zakharov, who also holds an appointment in the Department of Mathematics at the University of Arizona.

Funds for equipment, journals, and consumables are non-existent, doing great injury to experimental physics. Those younger scientists who cannot easily emigrate are often forced to seek employment in other sectors of the fledgling market economies. This "internal" brain-drain is of great concern to many senior scientists since they see the loss of their best junior associates as threatening the future of FSU science. There is no appreciation within the scientific

community for the role that these "displaced" physicists play in the transformation of FSU society.

A growing problem is the loss of technicians and artisans. FSU institutes have always had to rely on manpower to make up for deficiencies in commercial equipment availability and services. This has accelerated the decline in institutional infrastructure as technical support staff has been lost. At the Institute for Theoretical and Experimental Physics in Moscow, for example, there is only one plumber left to service the needs of a staff of 2,500.

The decline in experimental particle physics has been underway for the past 20 years and has accelerated precipitously over the past decade. Major projects have failed or been abandoned and such facilities as the Serpukhov accelerator are all but forsaken.

In Ukraine, where the situation has developed somewhat differently, 1.5 billion "coupons" (approximately 2.5 million dollars) have been allocated thus far to investigator-initiated peer-reviewed proposals; a sum equivalent to the resources provided by the Ukrainian Academy for the support of research institutes and universities. A ministerial officer, Serhey Ryabchenko (Chairman of the State Committee for Science and Technology in Ukraine), is administering this program and has agreed to provide matching funds to the laboratories of APS grant recipients, similar to an agreement reached with Deputy Premier Boris Saltykov in Russia.

1.1.4 Heterogeneity and Isolation within the Scientific Community--The physics community has two major components: the Academy and Ministry Institutes (which are the homes of the elite physicists) and the universities. Most of the significant research is done in the institutes, and both the Academy and government ministries have traditionally provided the resources needed for these scientists to establish and maintain communications among themselves. The universities have been responsible for training large numbers of students and have, in effect, become teaching "factories." The faculties have focussed on teaching and have traditionally done a credible job at the undergraduate level. But, lacking a high-quality research environment, the best graduate students must be recruited into the institutes. Thus, the universities are weak and reside well outside the mainstream of elite physics research.

Industrial research is also weak, and in some critical specialties, nonexistent. The exception is military research which had been isolated and pampered by the *ancien regime*. Many institutes were so self-contained that there was little interaction between them and, in some cases, open competition prevented scientific collaboration.

The second tier physics communities (those primarily associated with the universities and smaller, less well endowed institutes) have turned to a multiplicity of competing, would-be professional societies to satisfy their needs and ambitions. In Russia alone there is the Russian Physical Society, the Moscow Physical Society, the St. Petersburg Physical Society, the Nizhny Novgorod (Gorky) Physical Society, and numerous others. Some of these organizations view their role as finding commercial partners for technology transfer schemes. And while the

Russian Physical Society is attempting to unify the regional and urban societies, there is both resistance and suspicion.

In some of the other republics, however, the organization of such societies has met with some success. In Ukraine, for example, a significant portion of the physics community has rallied to the Ukrainian Physical Society, in large part because science in Ukraine became specialized under the Soviet Government with most of the resources and basic research institutes located in Russia. Thus, there is closer association among university and institute physicists, with much good science done in the universities. Nonetheless, there are centrifugal forces at work in some countries where ethnic and other rivalries disrupt unity among scientists. Particular concern has been expressed at conditions in the Baltics where government policies appear aimed at excluding ethnic Russians and other minorities. There have been examples of brutal repression in some of the Central Asian republics.

1.1.5 The Academy, The Ministries and The Government Circus--Russian government actions may be promulgated by parliament or decreed by the President. But they remain moot unless "enacted," a process as mysterious as it is rare. It is clear that the apparatus of government, the bureaucracies, are elephantine labyrinths which swallow resources while mandating programs.

Thus, for example, the telecommunications ministry has established corporate bodies that extort resources from commercial and academic ventures alike--often turning a blind eye to regulations prescribing cost limits--without regard to the consequences for Russian science.

In mid-1992, the Ministry of Science, Technology and Higher Education requested that external assistance to Russian science be exempt from taxes. But it was not until well after Presidential and Parliamentary action that the Finance Ministry agreed to support this policy, and only with some reluctance and then somewhat ambiguously.

Nor is this characteristic only of Russia. Similar problems plague programs in each of the republics. Negotiations with ministers and even deputy premiers are usually inconclusive, and in the current political climate, somewhat dubious since changes of regime (which must be regarded as inevitable) will almost certainly be followed by the abrogation of old policies. In Russia, where much of the discredited Soviet bureaucratic apparatus remains intact, even ministerial policies can languish in the netherworld of administrative indifference or outright opposition.

Nonetheless, some of the new leadership recognizes the need for structural change and have pursued policies which directly attack the power and prerogatives of the Academy and the ministries. In Ukraine as in Russia, government policy has been enunciated in support of science and technology with senior cabinet officials assigned to coordinating programs: Saltykov in Moscow and Ryabchenko in Kiev.

1.1.6 Inflation, Shortages, and The Less-Than-Perfect Banking Industry--The collapse of the ruble has been alluded to earlier and the lack of funds has led to shortages of consumables. The scarcity of paper and other resources has resulted in an almost complete breakdown of scientific publishing with the subsequent disappearance of new textbooks, journals and bulletins. Many scientific communities have turned to commercial publishers in the West and have obtained little support or encouragement. Publishers often ask for total distribution and copyrights in exchange for a few hundred printed volumes. In addition, the decline of the scientific enterprise has threatened those important FSU publications whose English translations have an international audience. Attempts to transfer funds in support of these and other activities have been frustrated by antiquated or nonexistent banking facilities and ambiguous tax laws, a problem which hampers the wider effort to support scientists. Many groups in the West have taken the expedient route of bringing cash into the FSU and physically distributing it to the recipients. More extensive distribution schemes are hampered by confiscatory fees, cumbersome procedures and regulations and uncertainty about the status of intellectual property rights. Some individuals and institutions have attempted to circumvent these problems by acquiring Western bank accounts.

1.1.7 The Collapse of Shipping and Mailing--In many parts of the FSU, mail and parcel shipment are unreliable. While this is not true for a number of the smaller republics, the problem is particularly acute in Russia. Some foundations have established facilities for occasional bulk shipments, but needed mail and journal shipments often disappear into the postal machinery.

1.2 Existing Short-Term APS Programs--

Programs devised by the American Physical Society (APS), American Astronomical Society (AAS), and the American Mathematical Society (AMS), fall into two categories: short- and intermediate-term, both of which are geared to an ultimate goal of creating a self-sufficient, investigator-initiated, peer-review system of science self-management. This objective is obviously dependent upon the economic and political recovery of each nation. For the most part, the programs of these learned societies are constructed around short-term needs since they do not have the resources (nor the ambition) to tackle longer term goals except in an abstract, preparatory way; for example, by studying the objectives, structures, organization and operations of longer-term programs with a view to advising other institutions on how to develop and administer such programs.

The APS short-term emergency program consists of the distribution of back-issues of journals directly to institutions and libraries, the provision of limited resources for the repair or replacement of small pieces of equipment, the awarding of scholarships and small grants to exceptional researchers, the sponsorship of colleagues in the FSU as Matching Members by APS members and other organizations so that they may receive literature subscriptions, support for regional summer and winter schools for both researchers and graduate students, travel support to FSU enable colleagues to participate in major meetings and the organization of advisory

committees in the republics to serve as conduits for information, and program management. Several of these components of the program are discussed in more detail in Sections 2.3 and 2.4

The program is financed from APS funds, donations from our members (who have thus far provided more than \$100,000), and from funds and services provided by foundations. In particular, the Alfred P. Sloan Foundation awarded a matching grant of \$100,000 in support of the appeal for donations from APS members. The Soros Foundations have provided an additional \$525,000 to supplement the APS small grants and fellowship programs. The Meyer Foundation has made an award of \$100,000 to be disbursed as emergency grants. The National Science Foundation (NSF) has awarded the APS a two-year \$100,000 grant in support of summer schools and workshops, journal distribution, and administrative travel. Some urgent literature shipments have been supported by a joint American Academy of Arts and Sciences -- United Parcel Service program.

We are currently negotiating with other foundations for additional funds and we are preparing to collaborate (or have entered into collaboration informally) with the American Mathematical Society, the American Astronomical Society, the American Association for the Advancement of Science, the American Academy of Arts and Sciences, the European Physical Society and other institutions such as the University of California, which is providing funds for collaborative research with Russian institutional laboratories.

Information essential to the APS program has been provided by knowledgeable colleagues who have extensive experience and wide contacts in the FSU, and from expatriate colleagues currently resident in the United States, especially through the instrumentality of a major forum of expatriate colleagues, distinguished senior scientists, government officers and foundation representatives, held on April 22, 1992, in conjunction with the annual Washington, DC, meeting of the APS.

We also met with our European Physical Society (EPS) colleagues in Budapest May 25-27, 1992, and in Amsterdam October 1-2, for EPS-APS workshops on the Crisis in Basic Science in East-Central Europe and the Republics of the Former Soviet Union. We have agreed to participate in a series of coordinated actions in communications, regional self-help, support of libraries, peer review, centers of excellence, data bases, equipment distribution, and summer schools and workshops. We have also tentatively agreed to join with the European physics community in supporting a UNESCO-UNDP initiative aimed at strengthening the universities in East Central Europe and which will rely on grants from various development banks.

We conservatively estimate that of the approximately 2,000 grant and fellowship applications (representing more than 5,000 scientists) which the APS's Moscow committee has received, 80 percent merit support on the basis of scientific excellence and competence. This would require resources in excess of \$2 million per year (for Russia alone -- \$3 million per year taking into account all of the republics), excluding all expenditures for journals, equipment, consumables and travel (assuming average disbursements of \$500 for the year for each recipient). Our present resources of \$800,000 can accommodate no more than 640 group applications--from all

republics (on average there are 2½ physicists per application)--of the estimated 1,600 which merit awards.

The advent of such *ad hoc* programs has had an immediate, enormous impact on both the morale of our colleagues in the FSU and on their governments. Thus, with these funds and with Russian commitments to support basic science, we may be able to hold the core of the mathematical and physical sciences together during the current emergency period.

2. The APS in Action:

2.1 Early Actions--In the beginning of March, 1992, in response to growing concern about the crisis in basic science in the Republics of the former Soviet Union, APS President Ernest M. Henley asked William Blanpied (National Science Foundation), then Chair of the APS Committee on International Scientific Affairs, to chair an *ad hoc* Task Force on the crisis. The Task Force consists of Kurt Gottfried (Cornell), Herman Feshbach (past APS President, MIT), George Gamota (MITRE Corporation), Anthony Fainberg (Office of Technology Assessment), Pierre Hohenberg (AT&T Bell Labs), Herbert Berk (University of Texas), Yuri Orlov (originally a Task Force member and now advisor, Cornell) and Lev Okun (advisor, Institute for Theoretical and Experimental Physics, Moscow) with Henley serving *ex-officio* and Irving Lerch (APS Director of International Scientific Affairs, New York University) as APS Liaison Officer. Staff liaison and administrative support is provided by Amy Halsted of APS. Many of the Task Force members have extensive personal and professional associations in the FSU or have broad experience in international scientific affairs.

At the same time, Henley sent letters to D. Allan Bromley, Assistant to the President for Science and Technology, and Walter Massey, Director of the National Science Foundation, recommending immediate action to supplement NSF grants to support collaboration with colleagues in the FSU and to find additional funds for new programs.

By the end of March, the Task Force had recommended two immediate steps: the distribution of surplus issues of complete annual sets of *Physical Review*, *Reviews of Modern Physics* and other journals to responsible physicists in the USSR who will assure their access by colleagues throughout the Republics, and a Presidential appeal distributed by e-mail, limited bulk mailing (to APS Fellows and Department Chairmen of Ph.D. granting institutions), and as news announcements in *Physics Today* and *APS News*.

2.2 Journals--Our programs to provide APS journals to physics libraries in the FSU are discussed in the accompanying paper by Gerson Sher on Infrastructural Issues.

2.3 Development of International Schools and Workshops in the Republics of the former Soviet Union--Many of the elite institutions of the former Soviet Academy developed an extraordinary educational system that discovered and nurtured scientific talent and promoted a unique intellectual culture of physics. This is particularly true of the Lebedev, Ioffe and Landau institutes, for example. The opportunity of the moment is to open these unique schools

to the world by providing for the exchange of faculty, the recruitment of students from the region and the United States and the development of regional and international summer schools and workshops. The program was begun in 1991 with the St. Petersburg High-Energy Summer School (supported, in part, from the 1992 NSF award to APS). The St. Petersburg Nuclear Physics Institute has organized an international winter school in theoretical physics which took place at the end of January, 1993 and which was attended by 10 carefully selected US graduate students. It consisted of intensive lectures and seminars. In addition, several other republics, notably Ukraine, are seeking to establish their own regional summer schools and workshops. The APS program is supporting the establishment of one summer school in Ukraine and one in Russia and one winter school at the St. Petersburg Nuclear Physics Institute. The Ukraine program will develop a series of workshops which would eventually lead to the organization of "Gordon-like" annual conferences.

Faculty exchanges are made by agreement between the local institutes and cooperating US institutions. Similarly, in all these schools FSU and US counterpart institutions coordinate among themselves the selection of participants, both students and lecturers.

2.4 Small grants and fellowships--Policy and oversight for the APS small grants and fellowships program is provided by the Task Force appointed by President Henley in March 1992 (see Section 2.1) and is administered by the Society's Office of International Scientific Affairs. Initial policy guidelines were developed in Washington, DC on April 22, 1992, as described in Section 2.1. Subsequently, a US-FSU advisory committee was established to support the deliberations of the Task Force, and national advisory committees were organized in Moscow, Tallinn, Kiev, Tbilisi, Yerevan and Vilnius. Efforts continue to organize committees in the other republics.

2.4.1 The function of the FSU national advisory committees is to solicit emergency grant proposals from small groups, to organize disciplinary and, if necessary, regional subcommittees to assist in the evaluation of proposals, and to perform a preliminary evaluation of the submissions to assure accuracy and determine relative merit. Appropriate proposals are then forwarded to the Task Force, which forwards them for ranking to review panels in the appropriate APS disciplinary Divisions. The Task Force then determines how which proposals should be funded on the basis of these rankings. No proposal recommended by a national committee has yet to be declined. Rather, those not immediately funded are being held for further review pending a determination of available resources. This procedure has been adopted on the grounds that provision of funds based on a competitive, peer-reviewed process is very new -- and very unsettling -- to most FSU scientists.

Funds are provided on the basis of \$500 per group member per year, with groups not exceeding six physicists; it is anticipated that many awards will be extended beyond the first year. Where group leaders have access to hard currency and significant travel support, they are excluded from receiving emergency funds but are encouraged to apply for assistance on behalf of the group itself. By encouraging distinguished senior physicists to apply for support on behalf of their lesser known co-workers, the APS seeks to assure that the best physics is represented in the

application process. Funds may be used by the recipients as they see fit so long as they continue their scientific work. They are asked to prepare an article for submission to an appropriate peer-reviewed journal -- within one year for theorists and two years for experimentalists.

2.4.2 The disciplinary Divisions and Topical Groups of APS are encouraged to develop their own system of advisory committees and panels to promote their own scientific interests. For example, the Laser Science Topical Group (LSTG) has organized laser science advisory subcommittees to work inside the FSU with their respective national advisory committees to solicit and review proposals. In addition, the LSTG uses its own review panels to critically appraise proposals forwarded by the national advisory committees to the Task Force. The LSTG also raises funds in support of the general APS program.

2.4.3 Oversight is provided by 1) the Task Force which is responsible to the APS President, 2) the APS Executive Board which reviews expenditures and 3) the APS Council which approves program parameters and funding levels recommended by the Task Force.

2.4.4 As of December 31, 1992, 179 group awards totalling \$223,500 have been transferred for disbursement to Russia and Ukraine. Fifty group awards totalling \$42,000 are awaiting transfer to Armenia, Belarus, Estonia and Ukraine pending verification of the setting up of personal dollar accounts for the recipients in these countries. In addition, \$9,600 was provided as travel grants to 8 physicists to enable them to attend the International Atomic Energy Agency (IAEA) Fusion Physics Conference in Würzburg in September. These account for a total commitment of \$275,100 and we are currently processing an equal number of grants. In addition, \$15,000 has been set aside to finance travel to the FSU to facilitate organizational and administrative functions.

2.4.5 In June, 1992, Herman Feshbach, a former APS President and member of the Task Force, and Irving Lerch met with Deputy Premier Boris Saltykov to negotiate tax exemption for grants of funds, equipment and journals. In addition, and with the assistance of the Moscow Advisory Committee, Saltykov was encouraged to provide matching funds to the small laboratories of the grant recipients. The purpose was to insure Russian government participation in the program and to assure that those technicians and scientists associated with award winners (but who were not members of the research group) benefitted. Thus, the program provides funds to those who do the research and payments completely bypass bureaucratic structures. Tax exemption was presumably formalized by the Finance Ministry in October, although documents attesting to this have not yet been received. However, all disbursements are made under the presumption of tax exemption and statements to this effect are issued to each recipient. In December, Task Force advisor Yuri Orlov went to Russia to review the status and operations of the program, to advise the Moscow Committee on their activities, and to give guidance and counsel to the Task Force concerning needed changes. In Ukraine, a member of the APS Task Force, George Gamota (Mitre Corporation), met with Serhey Ryabchenko (see 1.1.3), Pavel Kislyi (Head of the Supreme Rada of Ukraine) and I. Yuhnovskii (First Deputy Prime Minister) to explore different aspects of the APS program. In

general, there was agreement on tax exemption for stipends and on matching funds to the laboratories of grant recipients.

2.4.6 Disbursements are currently arranged through the Soros Foundation offices in each country. Funds are transferred by APS to a holding bank in Finland and are subsequently transferred into dollar accounts in the names of individual recipients in local banks by Soros Foundation officers. The national advisory committees and Soros Foundation officers are notified of the names of the award winners and letters of disbursement are sent to the national advisory committees for distribution. The committees, foundation officers, and recipients coordinate with each other to arrange for the pickup of funds. No funds are given to the national advisory committees for disbursement. Recipients sign bank receipts which are returned to the APS Office of International Scientific Affairs.

2.4.7 Program review is the shared responsibility of the national advisory committees and the Task Force. The national advisory committee will request work reports from experimentalists after the first year and pre-prints of manuscripts from theorists after their first year and from experimentalists after their second year.

2.4.8 Lists of awards and program evaluations are made public and given to funding agencies and other societies (in order to detect multiple awards, program bias and other problems).

3. Action Plan (recommended actions listed in order of priority): While most recommendations will be sufficiently general to apply to any number of programs, a few should be addressed to the International Science Foundation for the Former Soviet Union (ISFFSU) Board, or to a consortium of funding agencies, where appropriate. While a few recommendations overlap those contained in the accompanying papers on Infrastructural Issues by Gerson Sher and on The Global Scientific Heritage of the FSU by Robert Hoffman, Douglas Siegel-Causey, and John Moore, we can discover no serious inconsistencies among those recommendations.

3.1 Emergency Short-Term Programs--

3.1.1 Organization--Each scientific community, presumably through its learned societies, academies and, perhaps, with foundation and government funding, should seek to organize coordinating and advisory committees nationally, internationally and within each of the successor states of the FSU. The purpose of these committees should be to develop plans, mechanisms, procedures and principles for the development of assistance programs. **It should be a clearly stated objective of all efforts that the purpose of such aid is not to pursue an imperial program to acquire cheap talent for the benefit of the West, but to make it possible for each scientific community to survive the current crisis so that each will contribute to the recovery of their nation. This policy is in the best tradition of free and open inquiry and exchange and benefits all mankind.**

3.1.2 Library support²--The APS program provides only limited numbers of APS publications. While these journals are important to the FSU physics community, there is urgent need for other US, European and Japanese research and archival publications. The need is far too great to be addressed by any single, existing funding agency, since it is estimated that this would cost from \$12-\$13 million/year for Russia alone.

A possible strategy is as follows: 1) select several central institutional libraries in each nation capable of assuring the circulation of all journals, 2) survey all journals available in these libraries in 1990, 1991 and 1992 to determine which back-issues are needed, 3) determine the minimum number of issues needed to promote wide availability (to include photocopying of relevant issues where necessary). The selected institutional libraries will be charged with distributing copies to outlying institutional and university regional libraries to assure wide accessibility to all communities. Such a program is estimated to require an expenditure of approximately \$4 million over 2 years for the physical and life sciences.

3.1.2.1 A title survey for all physics journals, total numbers of copies, by discipline, for each academy library in each republic was made for 1991 and 1992. A similar survey is currently underway in the Russian Academy Library for the Natural Sciences in Moscow (and in institutional and university libraries in some of the sciences). The numbers of multiple copies needed is part of this survey.

3.1.2.2 Representatives of the European Physical Society have initiated negotiations with European publishers to secure discount subscriptions³. The APS position is that back issues of physics journals (both U.S. and foreign) should be provided free and that all current and future subscriptions should be provided at the "runoff" or "last copy" price, approximately 10% of the library subscription price. The final cost will obviously determine the total numbers of journals to be purchased. Our European colleagues have negotiated a price of approximately 800,000 ECU for all physics journals which represents 50% of the institutional library subscription price. This is most certainly too high and will be negotiated further.

3.1.2.3 We recommend that a consortium of foundations provide support of not more than \$4 million over a two-year period to replace as many journal issues as possible in select institutional and university libraries for the natural sciences in the FSU. (If additional funds are needed, a multidisciplinary panel would return with a fully substantiated request.) We further recommend that a multidisciplinary commission be established to negotiate with European and US commercial publishers an appropriate fee for the provision of all scientific journals. These negotiations should include access to electronic databases.

²See also recommendations in the accompanying paper on Infrastructural Issues by Gerson Sher.

³Unlike the situation in the United States where the principal physics journals are published by the APS and American Institute of Physics (AIP), the most important European physics journals are published commercially and are considerably more expensive than their U.S. equivalents.

3.1.3 Emergency Grants and Fellowships--Several learned societies in the United States have demonstrated their capability to organize committees of distinguished in the FSU for the purpose of developing and managing programs in support of scientific activities. A central objective is to introduce self-management as an efficient means to allocate resources based on investigator-initiated peer-review mechanisms. This process should be expanded and supported by major government and non-government funding programs. There may be cases where some communities in some countries are not sufficiently well organized to insure rapid notification, solicitation and processing of proposals. In such a case, an automated system of soliciting and grading incoming applications may be undertaken, with emphasis placed upon publication records and research associations. **We propose that the learned societies be provided with sufficient funds to continue existing emergency grants program, and that learned societies that seek to establish new programs based on local self-management and peer review be provided adequate support for that purpose. Such actions will conserve total available resources and assure the survival of the nascent "bottom-up" approach in the FSU. It will also facilitate the organization and development of intermediate and longer-range programs. As expert panels and site teams are organized to implement reviews for longer-term programs, the learned societies should be relied upon to provide lists of qualified nominees for panels and committees.**

3.1.4 Emergency travel to attend international meetings--The distinguished Russian physicist Lev Okun, who chairs the APS Moscow Committee, has emphasized that funding agencies should take note of the need to provide travel funds for FSU scientists to attend meetings in the West at which they have been invited to make presentations. **In view of the fact that the learned societies organize a significant proportion of scientific meetings and actively participate in others, it is proposed that the societies coordinate their requests for such travel support in order to insure against multiple awards. It is recommended that participating societies consider the question of the appropriate size of these awards. (The APS's supplementary FSU travel grants have varied from \$750 to \$1,200 depending on the support provided by the conference organizers and sponsors).**

3.1.5 Computer Moderated Telecommunications⁴--Numerous proposals have been made and several programs implemented to provide needed computer telecommunications support to the scientific community in the FSU. Thus far, the APS has concentrated on Russia and Ukraine. Among scientific disciplines, the communications capabilities of the physics community are generally most advanced, with the highest capacity enjoyed by the particle physics community. But these capabilities are wholly inadequate and are threatened by numerous problems. It is urgent that approximately \$3 million be made available over a two year period to arrest the decline in computer moderated telecommunications and to extend these capabilities to the whole of the scientific community. The immediate need is to provide secure and reliable connections with the Moscow scientific community and to develop the network to include all other regions within the Russian Federation. Support for telecommunications facilities within the other republics should be coordinated with other providers within the international community. **We recommend that a consortium of donors be asked to set aside**

⁴See also the accompanying paper on Infrastructural Issues by Gerson Sher.

no more than \$3 million over a two-year period as emergency funds to purchase needed equipment and provide operating costs to expand telecommunications within Russia. Working out details for the use of those funds should be a high priority for the first six months of 1993. An immediate allocation of approximately \$170,000 will be needed to provide satellite capacity through the ground link at either the Institute for Space Research in Moscow or the new station installed at the Russian Academy Presidium. With respect to the other successor states, funding should be set aside to provide computers, servers, modems, optical disk readers, and other suitable equipment to help scientists exploit existing facilities.

3.1.6 Alerting the Scientific Communities--To alert all of the scientific communities in the FSU to the existence, criteria, and form for requesting support under emergency and longer duration programs, it is recommended that the journal *Argumentii i Facti* should be used (along with other suitable publications). Forms for emergency grant applications to include information for grant proposals may be published and widely distributed (circulation is 26 million). The various FSU scientific communities, their advisory boards and review panels will subsequently be provided with the forms and information needed to guide applicants through the process of applying for funds. The use of journals or other communications means will not be adequate as the physics community learned at the inception of its program. **It is recommended that the editors of *Argumentii i Facti* and/or other suitable broad-distribution media be requested to make their journals available as preliminary fora for alerting the Russian community to the existence and requirements for all aid programs. It will be important to find equivalent organs for contacting scientists in the other republics.**

3.1.7 Information Clearing House--It is urgent that the February 9 conference discuss mechanism and means to publicize grants, to insure that resources are not dissipated in multiple awards. **We recommend that an open, accessible mechanism be established for tracking and managing awards and that this mechanism include disbursements made by other foundations, learned societies, governmental and international programs.**

3.1.8 Promoting Collegial and Institutional Collaboration--It is important to consider promoting international collaboration through the exchange of faculty and junior research staff. **Funds should be allocated to provide sufficient resources to support joint Western-FSU institutional and university appointments, the routine, short-duration exchange of key scientists and to continue the development and support of regional schools and workshops in the nations of the FSU.**

3.2 Intermediate and Longer-Term Programs--Intermediate and longer range programs should shift their focus away from the stipend and subsistence support that characterizes most emergency programs to the actual support of research and related professional activity. This will make possible provision of increased support for experimental research than has been available through most emergency programs, since the small funds available have been of disproportionate value to theorists. Grants to individual scientists must also address the issue of "overhead" or infrastructure support. But to avoid the obvious complication of contributing to a corrupt or

ineffectual bureaucracy, it will be necessary to impose strict fiduciary restraints on all such aid and to monitor grants with appropriate tracking mechanisms and performance requirements.

3.2.1 Endowed Professorships--Scholars of international stature and outstanding achievement usually reside in the Academy institutes, although many have university associations. It would strengthen university programs to name distinguished scholars to endowed chairs with a view toward bridging the gap between the great research institutions and the universities.

3.2.2 Postdoctoral Fellowships--It will be important to establish postdoctoral fellowships to be awarded for a two-year period, with the possibility of an extension for a third year if funds are available. Each two-year fellowship should consist of a stipend and a conference travel allowance.

3.2.3 Independent Investigator Awards--Such investigator awards will provide salary support for independent junior and middle-level investigators, equivalent to assistant and associate professorships in the United States.

3.2.4 Research Grants--Research grants should be awarded, on the basis of competitive peer review, to investigators heading leading research programs. Each grant should be funded for a period of two years, with the possibility of an extension for a third year contingent on satisfactory progress and if adequate funds are available. The levels of support will vary with discipline, institution, group size, and needs. However, grants should be sufficiently large to support the work of independent groups and laboratories. Allowable costs should include salaries, supplies, essential small equipment, travel, communication and other allowable needs. Support of the principal investigator's graduate students should be an important element of the budget. An institutional allowance or overhead should be provided from the grant based on demonstrated costs. The overhead rates may not exceed 15 percent and should be negotiated with each institution after careful review of the efficiency of administration and management.

INFRASTRUCTURAL ISSUES

Background Paper

by

Gerson S. Sher⁵

prepared for

SUSTAINING EXCELLENCE IN SCIENCE AND ENGINEERING IN THE FORMER SOVIET UNION

A Conference

February 9, 1993
National Academy of Sciences

1. Introduction

Individual scientific and engineering researchers are of course the single most important asset of any nation's research enterprise. But these researchers work within a system of supporting relationships and facilities - the infrastructure - that defines in many ways the limits of their productive capabilities. In a broad sense, the scientific infrastructure consists of the buildings in which scientists work, the means by which they acquire and share information, the systems that produce new scientists, and the means by which the research community coordinates its efforts with other sectors of society. The extent to which these factors are important may vary from field to field; experimental equipment, for example, is generally less important for mathematicians than for engineers. But there are many needs that are common to the health of all fields, such as the need for free and efficient scientific communication. When these support systems fail, not only does science suffer but the most able and enterprising researchers find it increasingly compelling to move their work to other, more supportive environments.

⁵The author is indebted to Dr. Steven Goldstein, Ms. Sandra Burns, and Dr. Kenneth Gordon for their important contributions to this paper. Several sections of a draft paper on Direct Aid to Scientists by Irving Lerch and William Blanpied have also been incorporated. The views expressed in this paper are those of the author and do not necessarily represent those of the National Science Foundation or the U.S. Government.

The infrastructural crisis of science in the former Soviet Union (FSU) is of vast proportions, the catastrophic product of a combination of seventy years of enforced isolation, a legacy of centralized management and political control, and more recently political upheaval and economic chaos. Buildings are falling into disrepair, laboratory equipment is not just obsolescent but archaic, basic supplies and materials are virtually nonexistent, computing is for the most part primitive and spotty, telephone lines are unreliable. Access to any research resource requiring hard currency - supplies, publications, international telecommunications, journals - is beyond reach to all but the most privileged or those fortunate enough to have good contacts in the West. It is true that these commodities had for decades been severely restricted in the Soviet scientific community and rationed according to a system of privilege and political influence, rather than scientific merit. However at present the shortage of these goods is particularly acute because foreign currency, which was held by at least some elite institutions under the old system such as the military and the Academy of Sciences, has all but vanished. In no other area of scientific life is the evidence of the ravages of the new "golden curtain" more evident than here.

The dimensions of the problem in the FSU are indeed so enormous that no assistance effort can possibly "solve" it. It may legitimately be questioned whether it is the proper role of foreign assistance efforts to make major resource allocation decisions in lieu of the domestic capability to do so in the host country, including support for large-scale facilities and projects. The financial scope of the problem alone is overwhelming and beyond the capabilities of any potential donor. But even if available funding were unlimited, the collapse of the old structures for managing resource allocation, and the urgent need to develop more effective frameworks and systems in their place in the midst of a crisis situation, will limit the long-term effectiveness of any assistance effort unless it simultaneously attempts to address the financial needs *as well as* the system in which they exist.

At the same time, many of the infrastructural needs mentioned above are so basic and inexpensive, by Western standards, that even very small amounts of money strategically placed can provide tremendous leverage. Some needs are so critical to the functioning of a modern scientific community that making even a small dent in them may have a disproportionately large impact. Additionally, while some needs can easily be met at the level of support to individual investigators, others shared resources - such as telecommunication networks, journals, etc. - must be dealt with at a more general level if their use is to be reasonably efficient. Not all the problems are financial - in some cases, for example, policy issues such as export controls are involved.

Finally, it should be stressed that addressing this category of needs is not of importance only to the FSU scientific community. The world scientific community will also be a major beneficiary because the abilities of FSU scientists and engineers to communicate their findings, to be informed about developments abroad, to travel, and to identify new talent, are essential to ending the isolation of the FSU from the rest of the world, and that of the world from the extraordinary richness of FSU science and engineering.

This discussion paper focuses on four major issue areas: electronic communications, scientific literature, travel to international scientific meetings, and linkages between the research

community and other sectors of society (education and industry). Each of these issues relates to the broad theme of *scientific communication*, which is an essential element of the scientific environment that has a profound impact on the very ability to function as part of a larger scientific community. It was indeed the extremely stifling quality of scientific communication that characterized the Soviet scientific establishment in the past.

Today, the scientists of the FSU are in danger of falling into even further isolation from world science than in the past because of the legacy of control, economic disruption, the collapse of internal library and other information systems, and rapid technological advances in international communications. Yet these same advances may now make it possible for many FSU scientists who might otherwise seriously contemplate emigration to consider, instead, a situation in which living in the FSU and working as a member of the world scientific community are not mutually incompatible concepts. It is in the interest not only of FSU science but also the world scientific community to ensure as vigorous a flow of information as possible in both directions and that the isolation suffered by Soviet science in the past cannot be reimposed.

2. Electronic Communications

2.1 Background

Computer networking with access to the Global Internet, with over 1.1 million attached computers in about 50 countries, is no longer a frill but an essential need for research and higher education. Interactive computer networking permits the user to do the same things on a computer located half way around the world as could be done on a computer in the next room, providing that there is enough transmission capacity in the connecting networks. This includes exchanges of electronic mail, retrieval of information on demand from data bases, exchanges of documents and other files, remote execution of programs, multimedia conferencing among colleagues in several locations, etc. It also permits remote use of specialized computing and experimental resources, such as computers, telescopes and particle accelerators. Computer networking is thus a basic enabler of research, education, development and business activities. It is a "force multiplier" because it can enhance the effectiveness of users many-fold.

The gap between networking "haves" and "have-nots" is growing as the Internet continues to grow exponentially. Those who have access are enabled to do more and more with the networks, leaving those who do not have access further behind. This phenomenon can be observed world-wide. The FSU is especially vulnerable because it is starting from such a rudimentary position in terms of availability and quality of telecommunications systems, hardware, etc.

Access to computer networks is particularly important for domestic use when other means of communication are of questionable reliability or availability. Electronic mail often gets through when voice phone does not, for example, and it is less sensitive to time-of-day constraints because the addressee need not be present when the mail is delivered to the target machine.

Also, special error correction helps the electronic mail and transferred files get through circuits full of noise that would render speech unintelligible.

Computer networking can provide substitutes for scarce or non-existent local materials, equipment or bibliographic reference materials by permitting participation in work groups in other places of the world. Remote participation in the field of high energy physics is already well known to the FSU and their collaborations with western laboratories. But collaborations in other fields, from oceanography to medicine can also provide meaningful participation for otherwise isolated and resource-poor investigators.

Computer networks also contribute to political stability. They also help maintain communities of interest in the face of shortages and other adversities, including political upheaval. By making it possible for people with common interests to share experiences and information, global communities of interest are spawned and supported by literally thousands of special mail lists, bulletin boards and "news groups." The growth of such communities helps ensure that the recent political and other changes in the FSU will be irreversible.

2.2 Current Situation of FSU Computer Networking

Several joint ventures with western companies provide international electronic mail and file transfer service. But, there is little or no interactive service beyond major cities or internationally because the infrastructure is scarce or non-existent, and what does exist is very expensive. The commercial services are priced far beyond the reach of state-sponsored institutes and schools, and tend to be affordable by profitable domestic businesses or local affiliates of western enterprises.

The scientific community in the FSU is served--for the most part--by two organizations: Soviet Union European Academic and Research Network/For Research, Engineering and Education NETwork (SUEARN/FREENET) and RELCOM. SUEARN/FREENET is the FSU partner of EARN and BITNET, respectively, with FREENET running under the TCP/IP protocol used by Internet. It is based on aging mainframe computers (produced in the USSR and related to old IBM designs) and is unreliable. In addition, the expansion of the user base has been slow. Most of the Moscow-St. Petersburg-Novosibirsk physics community is served by the commercial network, RELCOM, which is based on networked small machines employing the UUCP connection to Internet in Finland. The unreliability of the telephone net slows message delivery considerably, delaying transmission from 2 to 4 days. But most important, RELCOM costs are rapidly rising, making it impossible for institutions to maintain their connections.

Real-time access to the academic computing networks in both Europe and the United States is almost nonexistent thus locking FSU users out of the more important abstract and textual databases (and there has been little, if any, distribution of CD ROM subscription disks to compensate this deficiency). For the Russian physics community, there is some relief in the existence of two dedicated lines, one from DESY (Hamburg) and one from CERN. However, these are low-capacity lines (unsuited to real-time database access or high-speed data transfers)

which are routed through Moscow switching stations and, as a result, connections are not reliable. Communications with some of the other republics, notably Ukraine, Georgia, the Baltic States and Armenia are usually good because the communities are small and concentrated. In particular, two direct lines are being laid which will connect Ukraine with Western Europe. The Scandinavian countries have nurtured a special relationship with the Baltic States and have subsidized direct and satellite connections.

Commercial services, including RELCOM, SPRINT and others have not been compelled to provide special fee schedules to the scientific community in Russia because the total volume of traffic is insignificant compared to commercial users. However, a new user group, RELCOM Academic and Research Network (RELARN) has been established in an effort to develop the non-commercial use of existing facilities and to seek resources to implement a networking plan to serve their members. There has been some movement towards coordination between RELARN and SUERN/FREENET users but a coherent set of proposals has yet to be developed.

The lack of reliable connections between Moscow and Western Europe, Japan and North America, and a reliable distribution network within the republics, remain major problems. It is clear that telecommunications needs and requirements differ from country to country and that any approach should be based on a decentralized system tailored to regional needs.

Research and academic networking in state-supported institutions was at best spotty up to a few months ago, and may be much worse off now as a result of large increases in telecommunications tariffs by the Russian state telephone monopoly. So far, the research and academic community have been unable to convince the telecommunications monopoly to provide special discounted rates for their not-for-profit sector.

Both telecommunications infrastructure and modern equipment to attach to what does exist are said to be sorely lacking. There are at least two levels of phone system services available for sale to the general public: the ordinary service which is said to be of very poor technical quality, and the ISKRA 2 phone system of former special government bureaus which can be purchased at much higher rates. Many western telecommunications companies are said to be queuing to invest and build infrastructure in the FSU, but progress is slow. Only the very lowest speed circuits can be leased for international connections, thus limiting what FSU researchers could do to the most basic of computer networking capabilities (e-mail, modest file transfer, submission of batch computing jobs). But even these limited capabilities can help to bind them to the global community and lessen the debilitating effects of isolation and deprivation.

Western government research organizations, including the U.S. Department of Energy and NASA, are working on a number of possibilities for limited networking connections to specific laboratories in the FSU, principally Russia. NSF is funding the purchase of e-mail terminals as part of its cooperative research grants and it is examining possibilities for connectivity in support of the general research and academic communities. However, U.S. government restrictions on access by FSU countries to U.S. federally-supported networks remains an important constraint. In addition, the Carnegie Corporation of New York has funded a study

of the current status of telecommunications and requirements for international connectivity in the former Soviet Union and that study is nearing completion.

2.3 Opportunities for High-Leverage Intervention

2.3.1 General:

- provide technology, promote speedy export licensing, and obtain permission to route FSU interactive traffic in U.S. Federal networks;
- influence Russian telecommunications policy-makers to provide affordable services for research and academic communities;
- install an interoperable, standard telecommunications plant to increase both domestic and international connectivity options.

2.3.2 High-Leverage Steps for Donors:

- find incentives for FSU institutions to prioritize affordable telecommunications services for research and academic communities;
- finance high-visibility demonstrations of practical solutions. These might require large startup investments (~\$1 million) and high sustaining contributions for limited period (several hundred \$K annually). Such projects might also entail matching or in-kind contributions from the FSU States - maybe a way to accomplish the preceding task!
- bring FSU telecommunication decision-makers to western countries to educate them as to the need for, and benefits from, computer networking;
- energize and support competing service providers that might help to drive down prices;

2.2.3 Steps for Professional Societies, Universities, and Other Institutions:

- provide low-cost packages of basic computer equipment suitable to function as e-mail terminals - PC's, modems - to as broad a range of FSU partners as possible, with special attention to institutions in FSU cities outside Moscow and St. Petersburg and to universities;
- develop and share lists of e-mail addresses of the U.S. science and engineering communities with FSU colleagues. Develop electronic bulletin boards to facilitate long-distance discussion, both internationally and within the FSU;
- offer remote access to scientific databases at reduced cost.

3. Scientific Literature

The attached paper by Sandra Burns of the AAAS entitled, "The Distribution of Scientific Journals in the Former Soviet Union," is a report on a feasibility study conducted by AAAS for the MacArthur Foundation concerning the distribution of Western scientific journals to the FSU. The original purpose of the study was to examine the feasibility of instituting a program to reinstate lapsed journal subscriptions. However, it was found that this approach was impractical for a variety of reasons to carry out through a single, central effort; as a result, AAAS has resorted to focusing on several central scientific libraries in Russia, Ukraine, and Belarus. The paper also describes other efforts of professional societies, including the American Astronomical Society (with partial support from the Sloan Foundation), the American Institute of Physics and the American Physical Society, the Sabre Foundation, the American Chemical Society, the American Psychological Association, and the AAAS in this area.

Prior to the collapse of the USSR, state operations such as *Mezh Kniga* negotiated directly with scientific publishers to provide archival and research journals to Academy, university and institute libraries. Thus, most scientific publishers had no knowledge of who received their publications. This was true for both learned society publishers such as the American Physical Society and the commercial science publishers. For APS, over a two-year period, institutional journal subscriptions dropped from 428 in 1990 to essentially 0 in 1992. In cataloguing all research and archival journal subscription needs in physics for the academy libraries of the natural sciences in Belarus, Armenia, Kyrgyzstan, Kazakhstan, Estonia, Azerbaijan, Latvia, Lithuania, Tajikistan, Uzbekistan, Ukraine, Georgia and Russia, we find almost all West European journal subscriptions lapsed, with 365 titles missing from the Russian Academy library alone. Institutional and university libraries are equally bereft, although the problem is mitigated by subsidized personal subscriptions.

In response to the decline in institutional library subscriptions, the APS has responded with a continuously increasing number of Matching Memberships. The APS Matching Membership program provides memberships for physicists in currency-poor countries, with costs being shared between APS and a U.S. sponsor. Such members (and/or their sponsors) can subscribe to APS journals at member rates. Twenty of these Matching Memberships for the FSU are sponsored by the American Institute of Physics and consist of the Russian editors of AIP publications. Numerous APS members and NSF funds sponsor more than 200 in the western republics.

The American Academy of Arts and Sciences has received a grant from the United Parcel Service (UPS) for air shipment of journals to the FSU. The program was targeted at Russia and will probably not continue. By means of this program, the APS has shipped complete yearly sets of *Physical Review* and *Reviews of Modern Physics* to key institutions in Moscow, St. Petersburg, Novosibirsk, Tallinn, Vilnius, Kiev, Yerevan, Tbilisi. These will be made broadly available throughout the FSU. This distribution program supplements the Matching Membership subscriptions which target individual colleagues for receipt of specific journals.

The Soros Foundation has--and the MacArthur Foundation is expected to have soon--offices in the Republics. The APS has an agreement with the Soros Foundation to use their offices as

shipping destinations for equipment and journals and is using their banking facilities for the disbursement of funds. In some areas, this will enable the APS to avoid some of the current tax and import duties levied on incoming funds and equipment. The problem has been raised with UN, UNESCO and IAEA officials in an effort to determine whether the UN system can provide a solution as well. UN and UNDP offices are being set up in Moscow, Kiev and Minsk, and we may use these facilities for the disbursement of hard currency, if needed.

An inexpensive method for shipping journals and equipment into the Baltic States, the republics and East-Central Europe is managed by the Sabre and Brother's Brother Foundations. They send bulk shipments by surface transport 4 times each year at a cost of 35 cents per pound from warehouses on the eastern seaboard.

The above referenced study of this issue by Burns, as well as the experiences of the APS, suggest the following generalizations which may be used to guide the thinking of donors and professional societies in devising responses:

3.1 General Issues

- Mail and other distribution systems have broken down in the FSU, both internally and externally. The unreliability of delivery systems for hard-copy publications increases the importance of other communications technologies, especially electronic.
- The disarray in the postal system even further isolates researchers in remote regions (i.e., outside Moscow and St. Petersburg) and in the non-Russian republics. Special attention should be given to ensuring that these locations are included in programs to address these issues.
- The holdings of university libraries are significantly weaker than those of Academy of Sciences organizations. Linkages need to be established between these facilities and special attention should be devoted to university libraries.
- Technologies such as CD-ROM for making available large amounts of information would be very effective; however, the appropriate hardware must also be purchased and put in place.
- The collapse of communications with the FSU, and of journal subscription lists within the FSU has generated a need for directories of FSU scientific institutions and individuals. In this respect the assistance of FSU partners and support recipients would be extremely valuable.

3.2 Steps for Donors

- Make grants to professional societies to fund journal subscriptions and CD-ROM databases to libraries, institutes, and universities and to subsidize remote access to scientific databases such as MEDLINE;
- Support procurement and installation of CD-ROM equipment in selected FSU S&T facilities.

3.3 Steps for Others

- Create programs by professional societies to solicit membership contributions for journal subsidies;
- Subsidize subscriptions by individual U.S. scientists participating in cooperative activities.

4. Travel to Scientific Meetings

Closely related to the issue of access to scientific literature is that of participation in scientific meetings; both are central to the flow of information in the scientific professions. Yet participation of Soviet scientists in meetings held abroad, a rare enough phenomenon before the fall of the Soviet Union as a result of political controls, has now become even more problematic because of the drastic devaluation of the ruble and the total financial inaccessibility of international travel to all but a very few. The inability to participate in such meetings compounds the isolation of FSU scientists and denies them a means of keeping current in their field that most scientists elsewhere in the world take for granted. The presence of scientists from the FSU at such meetings is of value not only to them but also to the discipline as a whole which is otherwise deprived of timely information about important developments in the field taking place in FSU laboratories.

Little systematic information is available on the extent to which special support has been available to FSU scientists and engineers wishing to travel to scientific meetings in the United States. Some meeting sponsors have been able to reduce or eliminate registration fees for FSU guests, but defraying their travel and subsistence costs is usually beyond the capacity of societies or organizers. FSU visitors participating in independently sponsored cooperative activities sponsored by NSF, NAS, or other programs, have often been able to take advantage of their stay to attend major scientific meetings, but cooperative programs do not generally fund participation in such meetings as a sole objective.

4.1 Possible Steps:

- A portion of membership contributions collected by professional societies in support of FSU scientists might be set aside in a special fund for support of FSU

scientists attending professional meetings sponsored by the society or in its discipline.

- Foundations and other organizations might consider requests from professional societies for support of special assistance for FSU scientists seeking to attend scientific meetings.

(In both of the above cases, mechanisms would have to be devised to disseminate information about such opportunities to FSU scientists and to filter and select requests for assistance.)

- Consideration might be given to siting certain smaller meetings in the FSU, either as bilateral workshops or special sections of society activities.
- Grants programs for support to individual FSU scientists should include support for travel to international scientific meetings as a key component. The creation of a well-provided-for but still isolated scientific community would only repeat past problems.

5. Linkages with Other Sectors

Just as the linkages between the scientific research enterprise of any country with that of the world scientific community are important to the health of both, the linkages of that country's effort within its own society are of critical importance to its ability to sustain itself and to attract internal and external resources for its long-term development. While FSU emergency S&T relief efforts may properly devote the greater part of their attention to support of individual researchers and their immediate needs (including the infrastructural needs described above), they must also do so with the knowledge that these efforts are of only limited duration. Unless emergency relief programs also devote some effort to addressing the underlying problems of the FSU R&D establishment, their medium- and long-term impact may be only superficial or worse once the outside supporters leave the scene and the policy-makers and researchers of the FSU are left to work out where to go from there.

Of special concern are the linkages with education and industrial development. These are central to the health of any nation's scientific enterprise. One of the hallmarks of the Soviet Union's S&T organization and policy for sixty years were the gaps between the research sector - particularly its elite establishment in the Academy of Sciences system - and education, on the one hand, and industry on the other. The roots of this arrangement are complex with their origins deep in the history of the Stalin Revolution of the 1930's, but their result was an artificial - and deliberate - separation of these sectors, a separation so profound and even enforced that in any other society it would be seen as an extreme handicap to the health of science and technology. Indeed the history of Soviet S&T policy consisted largely of a series of largely unsuccessful efforts to redress the inefficiency and waste imposed by this basic structural arrangement, brought about more by political exigency than by scientific or economic rationality.

The preferential access to resources of researchers and institutions in the Academy system, as compared with university and industrial research laboratories, has been remarked upon widely by visitors.⁶ There is a temptation to draw from this comparison the overly simplistic conclusion that assistance efforts should go primarily to leading institutions and researchers in the Academy system and that the universities can be dealt with later. And of course support should go only to the best people and facilities. But support for university science must not be neglected by assistance programs, because it is essential to the long-term health of the research enterprise to have a healthy pipeline of young scientists and engineers. While it perhaps cannot be the goal of such programs to create new educational institutions (although some foundations have done just that elsewhere in Eastern Europe), it is appropriate and important for them to make special efforts to seek out and support deserving research groups in universities and to give priority to activities that are characterized by partnerships among researchers from the Academy and university sectors.

Much the same can be said of the industrial R&D sphere. Here, the profound disjunction between the relatively high-quality basic research carried out in Academy institutes and the poor in-house capability of industrial ministries to innovate is widely perceived as a key source of Soviet technological backwardness. There is also no doubt that there are researchers and laboratories of very high quality in the industrial sector, in many cases the beneficiaries of military R&D funding that has now all but disappeared. But these researchers typically have limited understanding of the cycle of turning ideas into technologies and products in a competitive market environment, and a key element in learning these skills is to build close ties with the academic research sector, on the one hand, and with the consumers of the technology on the other. Again, while assistance efforts cannot create these structures outright, they can judiciously promote their growth by offering special incentives to potential grantees to build these linkages into their activities from the beginning.

To address these concerns, special priority should be given to programs that support:

- High-quality researchers at university institutions, with special allowances for instrumentation.
- Activities that involve young investigators, graduate students, and undergraduates.
- Activities that involve cooperation between academy, university, and/or industrial laboratories.
- High-quality applied research with potential industrial or commercial application, with linkage where possible to implementing organizations such as commercial enterprises.

⁶To be sure, there are important exceptions. One educational institution often cited as being of exceptional quality in terms of research and linkages to other sectors is the Moscow Physico-Technical Institute (MFTI). Another exception is the entire area of defense-related production, which had been well endowed. The fact, however, that these examples are exceptional (and arguably irrelevant, in terms of the military-industrial complex now that defense R&D funding is virtually nonexistent) and not typical simply illustrates the problem.

- Assistance in implementing training opportunities (e.g., workshops, internships) in university administration and commercial application, S&T marketing, intellectual property rights, and technology transfer.

In addition, the following steps should be taken:

- Ensure that information about all funding opportunities is broadly disseminated among and within the FSU university community.
- In any information dissemination program, make use of U.S. corporations and foundations currently active in the FSU.
- Make effective use of the expertise of U.S. government agencies involved in supporting and conducting industrially oriented research and technology development in the U.S.
- Assist FSU successor states in the development of technology policy, including topics such as the government role in technology development, methods of transferring technology from research laboratories into commercial products, and strategies for obtaining technology from other countries and arranging joint ventures with other FSU successor states.
- Especially in applied and industrial research, include U.S. researchers - universities, government laboratories, or corporations - as active partners for improved leverage and research performance.

INFRASTRUCTURAL ISSUES

Appendix

**THE DISTRIBUTION OF SCIENTIFIC JOURNALS IN THE
FORMER SOVIET UNION**

Feasibility Study Seminar Report

Sandra M. Burns

November 1992

INTRODUCTION

The economic situation in what was formerly a 15-republic Soviet Union is dismal, making it extremely difficult for scientists to conduct research and to keep abreast of the latest developments in their respective fields. One vital link with the world scientific community involves foreign scientific journals, yet the formerly Soviet scientific community has not been able to renew subscriptions in recent years due to the shortage of hard currency. This could have dire consequences for scientists in the FSU, just emerging from decades of isolation, and already facing problems ranging from unemployment, to scarcity of research material, to food shortages. The journals problem is particularly acute for younger FSU researchers attempting to publish results of their work in prestigious international journals in their respective fields. Their lack of access to western journals means that they have no examples of articles selected for publication nor a complete picture of what journals exist to which they could submit manuscripts. More importantly, it is crucial that researchers keep abreast of research results elsewhere in the world. If the serious lack of journals continues, the survival of the FSU scientific community is in jeopardy, and it could take years for FSU science to recover.

The US scientific community is well aware of the threat to FSU science, and has convened several meetings in an effort to identify problem areas and compare notes about specific steps being taken to assist colleagues in the FSU. Examples of such sessions include the March 3, 1992 meeting at the National Academy of Sciences on "The Future of Basic Research in the FSU"; the August 13, 1992 session at the White House Office of Science and Technology Policy, part of planning for an Autumn 1992 meeting between Presidential Science Adviser D. Allan Bromley and Russian Deputy Premier Boris Saltykov; and an October 28, 1992 meeting convened by the American Academy of Arts and Sciences, "Saving Soviet Science." Time and again, the need for journals and for financial support of researchers are at the top of the lists of priorities emanating from these meetings.

In light of this, and with the support of the MacArthur Foundation, AAAS recently completed a feasibility study to determine how best to address the situation. The original plan was to identify journals subscriptions, going to the FSU from AAAS affiliates, which had lapsed due to the shortage of hard currency in the FSU, and then determine the cost of reinstating the lapsed subscriptions. This turned out to be problematic, however, for a number of reasons, as reflected in the results of the initial feasibility study funded by MacArthur.

FEASIBILITY STUDY

Launched by AAAS in early 1992, the feasibility study had two major components: a survey of publishing societies; and a study of library and research facilities in the FSU. Many requests to AAAS for journals were generated by the contacts made through the feasibility study and by a short article appearing in the newspaper *TRUD* via Voice of America reporting on our efforts to secure journals for FSU researchers.

The Survey

To conduct the survey, AAAS sent questionnaires to 16 affiliated societies, requesting information on the journals they publish and trends in subscriptions going to the FSU in recent years. Through this survey, AAAS aimed to accomplish several tasks:

- identify societies most likely to have subscriptions going to FSU;
- determine the number of subscriptions going annually to the FSU;
- ascertain the cost involved given the number of subscriptions;
- get a break down of institutions and individuals to whom the journals are addressed;
- determine the publishing societies' willingness to continue the subscriptions at cost for two years;
- examine other journals projects underway, to avoid the duplication of efforts.

The results of the survey indicated that it would be both very difficult and quite costly for any one funding organization to attempt to reinstate current and recently lapsed journal subscriptions for several different societies and associations. In fact, in the course of conducting this study it became apparent that several factors complicate a journals project of this magnitude, three of which deserve special attention.

- First, precise information on journal recipients in the FSU republics was kept at a Soviet institution, *Myezhkniga*, a central governmental organization in Moscow through which all foreign book and journal orders were processed in the former Union. The US scientific societies had no access information as they often used subscription services to fulfill journal subscriptions foreign recipients. With the breakup of the USSR, *Myezhkniga (MK)* underwent a major transition, losing its hard currency accounts in the process, and reports are that remaining staff members at *MK* are attempting to enter the business world, offering to sell various types of information on the FSU. Accurately identifying former recipients of the US journal subscriptions would therefore amount to an immense, if not impossible, task.
- Second, given the breakup of the USSR, distribution channels used previously, including surface mail and air mail, are no longer viable and new reliable ones must be found. The situation is particularly bad for distributing materials through Moscow to non-Russian republics.
- Third, since the majority of those subscribers we have been able to identify were individuals, not libraries or institutes, reinstating these subscriptions ultimately would have a minimal effect on FSU science since the journals would only be targeted to a small segment of the FSU research community.

For these and other reasons, rather than attempting to reinstate the journal subscriptions, we have devised an alternative approach to make select journals available at major scientific libraries which are accessible to the majority of researchers in Russia, Ukraine, and Belarus.

Library and Research Facilities

During the feasibility study, the AAAS project director made site visits to Russia, Ukraine, and Belarus where she met with researchers, librarians, administrators, government officials, and university representatives. As is well known, the situation for scientists is extremely difficult, especially since individual research institutes are in flux, as supplies and salary support dwindle. Discussions revealed that the scientific community as a whole is well-acquainted with the several science and technology (S&T) libraries for different sectors of the research community located in major cities. These generally include a library affiliated with the Academy of Sciences, a public S&T library, and a university library. The main Academy of Sciences library also maintains smaller branches throughout the city, primarily at research institutes. There is also a library affiliated with the Academy of Medical Sciences in each of the former USSR republics.

All major libraries have a foreign acquisitions section headed by a director whose English language skills tend to be quite good. Library affiliates or branches also have a foreign acquisitions or journals librarian who works closely with the foreign acquisitions director at the main branch. This network of foreign acquisitions librarians will be an important component of the AAAS plan, as library personnel are very capable, would be cooperative in conducting the journals project, and are in an advantageous position to encourage equitable usage of journals.

AAAS has chosen to target four centers of scientific research: Moscow, St. Petersburg, Kiev, and Minsk. A sample of libraries to be involved in the AAAS project includes the following:

Library of Natural Sciences of the Russian Academy of Sciences/Moscow. The 300 institutes of the Russian Academy (RAN) look to the Library of Natural Sciences as the central source of fundamental scientific information. At one time, the library had 3,000 foreign journal subscriptions, but this has decreased to about 10% of that. The most recent journals on the shelves date from December 1991. The institution is only for Academy-related researchers, however, which is one reason AAAS believes it is important to work with university and other libraries as well.

Jakub Kolas Library for Science and Technology/Minsk. Most of the scientific material in Belarus is located at this library, affiliated with the Academy of Sciences in Belarus. University, Academy, and industry researchers utilize the library which formally subscribed to \$1.5 million of foreign journals, and also received 1,200 titles via international exchanges; this has decreased substantially. The library has devised a system of intra-library loans with its branches elsewhere in Minsk to facilitate the sharing of journals.

Moscow State University Library. Formally, the library had 1,500 titles of journals, and only about half as much hard currency for foreign subscriptions as other libraries. The library system at Moscow State consists of some 20 individual department libraries. University libraries in Minsk and Kiev face a similar lack of resources. The university system is clearly in poorer shape than the Academy system, and the university infrastructure would profit greatly from S&T assistance.

Each library is struggling to obtain journals in any way possible. One interesting alternative to foreign subscriptions does seem to have arisen -- some libraries are considering engaging the services of the Moscow-based enterprise "AS Plus." An advertisement for "AS Plus" obtained in Minsk indicates that the group offers to send photocopies of entire journals to libraries in former republics. Payment is made for three months only. Most of the library personnel with whom AAAS has been in contact expressed skepticism as to whether such a system would work, finding it potentially very costly and unreliable. They also had serious doubts as to the idea's viability given the severe shortage of paper in the FSU.

Related Journals Projects

The survey also revealed other US efforts underway to provide journals to FSU researchers, several of which complement the proposed AAAS effort. These include the following.

American Astronomical Society (AAS): The membership of AAS set up a program to provide journal subscriptions and support for small grants program. Funding came from personal donations in response to solicitation by electronic mail and the Society's Newsletter. By October 1992, contributions had reached \$54,000, which has been augmented by matching funds of \$70,000 from the Sloan Foundation. A shipment of journals has reached the FSU through a grant from the United Parcel Service to the American Academy of Arts and Sciences.

American Institute of Physics (AIP) and American Physical Society (APS): AIP has established two separate journal donation programs to the FSU. The first supplies US journals to the editors of the 20 Russian language physics journals with which AIP works. Each editor receives *Computers in Physics*, and two journals of the editor's choice from among all physics journals published by AIP and its Member Societies. In addition, AIP cosponsors with the American Physical Society (APS) memberships in the APS for all of the editors, which provide them with the monthly *Physics Today* as one of the benefits. Under the second program, 100 free subscriptions to AIP journals and magazines are sent to other scientists in the FSU.

Sabre Foundation: Under the Sabre Foundation's "Scientific Assistance Project," books and journals solicited from scholarly publishers in the US and abroad are distributed to targeted libraries in Eastern Europe and in the former Soviet republics. Within the FSU,

Sabre has had most extensive contacts in Ukraine, and in the Baltics; a Russia project is slated to begin by 1993.

American Chemical Society (ACS): ACS has earmarked \$30,000 to support journals for the FSU over three years. Recipients will arrange for overseas shipment. ACS has provided 800 kg. of back issues, shipped to Moscow, for distribution to research institutes via a special Aeroflight, in cooperation with the Science Office of the Russian Embassy in Washington, D.C.

American Psychological Association (APA): APA provides 57 institutional subscriptions to the FSU on a complimentary basis. APA also sends back issues of psychological journals and books to Estonia and Novosibirsk, and plans to earmark some journals for the FSU under its program to provide journals to developing countries.

American Association for the Advancement of Science (AAAS): The AAAS Board of Directors voted unanimously to send 20 subscriptions to *Science* to several FSU republics, at the Association's expense. At the same time, recipients are being contacted to verify the subscription information, to confirm receipt of the magazine, and to inquire as to its use and how it is made accessible to researchers.

The major obstacles cited in all of these endeavors include the need to find a reliable delivery system as well as to avoid the perception of the journals as "charity" by both the recipients and by the membership of participating US societies.

THE GLOBAL SCIENTIFIC HERITAGE OF THE FSU

Background Paper

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Foreword

The global scientific heritage of the former Soviet Union is both historical and contemporary. It includes the great scientific traditions outlined in the first part of this paper as well as unique and irreplaceable collections of specimens, data, and documents. The paper does not pretend to be a systematic or comprehensive report on this heritage. Rather, its purpose is to suggest by illustration the importance of this heritage and to stimulate discussion and extension of the subject. It contains a number of concrete recommendations for action, but these mostly pertain to the specific examples given. The intent is to generate discussion that will produce more general recommendations and actions. One of these might be to develop a more comprehensive survey of the collections extant in the FSU so that a rational plan of action could be developed.

Historical Background

The scientific heritage of those republics formerly comprising the Soviet Union is inextricably bound to the history of imperial Russia. For three centuries, Russia has in various times and to various degrees dominated its neighbors militarily, politically, and culturally. This historical period seems now to be drawing to a close, but it forms the background of the development of modern science in the region. And since modern science grows out of, and in a broad sense is a part of a people's culture, we must consider the development of the scientific heritage as a part of the cultural heritage.

One must first note that early Russian culture developed within the context of Eastern orthodoxy -- theological dogma maintained a strong hold over Russian intellectual life, and western scientific thought was condemned; "the discoveries of Copernicus, for example, were labelled.. 'satanical craft'..." (Vucinich 1956).

The emperor Peter I provided the catalyst to initiate change in the rigidly conservative culture of Russia. Having personally experienced western attitudes and accomplishments during his youthful years of travel in western Europe, Peter the Great planted western traditions and institutions in Russian ground. In 1724 he called for the establishment of a scientific forum in the western style, and the next year the Imperial Academy of Sciences was founded. Although his personal interest in western science was initially mainly utilitarian, he came to value basic scientific research. However, the new academy was established not simply as a scientific research institute but was also to organize Russia's system of secondary and higher education. Peter died that same year, and since Russia did not have her own scholars, its first members were recruited from western Europe by his successors, in particular by Elizabeth and the two Catherine's (I and II). Among the most notable of these were the mathematicians Hermann Euler, the natural scientists Bernoulli and Bayer, and the philosopher Büllfinger.

For the first quarter century of its life, the Imperial Academy lacked a governing statute and was run directly from the imperial court. In 1747 it received from the empress Elizabeth a statute dividing it into the Academy proper and the university, and began to achieve a degree of stability.

The second half of the eighteenth century saw the members, although still predominantly western European in training, open their ranks to more native Russian scholars (Mikhail Lomonosov was named in 1741), including such eminent natural historians as Peter Pallas, who organized the first expeditions to study the geography, geology, biology, and ethnography of Siberia, which was now under Russian control.

In the early years of the nineteenth century the Academy began to show some changes. It gradually began to relinquish its educational responsibilities to the growing universities, and its monopoly on scientific research was broken by the establishment of independent learned societies such as the Moscow Society for the Study of Nature, founded in 1805. At the same time, the Academy established, under the statute of 1803, departments of history, economic and political science, and Oriental studies. This was followed by a third statute (1836) which explicitly

relieved the Academy of any educational duties and proclaimed it to be the "primary scientific body of the Russian empire." Shortly thereafter, it absorbed the Imperial Russian Academy founded by Catherine the Great in 1783, thus absorbing language and literature into its domain. For nearly a century thereafter, the academy had three principal divisions: physical-mathematical sciences; Russian language and literature; and historical and political sciences and philology.

Throughout the remainder of the nineteenth century and into the twentieth, the Russian Academy of Sciences functioned much as did similar academies in western countries. Ties with those institutions were strengthened, foreign scholars elected to membership, and Russian scientists regularly studied in western laboratories. Nevertheless, in contrast to the increasing democratization seen in the west, the Russian Academy worked within a strong autocracy.

During this period as well there were striking parallels between scientific developments in the United States and Russia that were driven by similar historical events. The nineteenth century colonization and conquest of the American West was a partial reflection of the earlier, but continuing colonization and conquest of Siberia, Middle Asia, and finally the Caucasus region. In the vanguard of both of these efforts was scientific exploration directed by the Russian Academy, and in the United States by a combination of military expeditions and the newly founded Smithsonian Institution. This was of obviously great importance in shaping the study of the natural sciences in both countries, both of which developed strong traditions in these areas of science.

An essential element of those traditions was the collection and preservation of object of the natural world--specimens of individual animals and plants; samples of rocks, soils, and water--that could later be examined, described and analyzed in museums, herbaria or botanical gardens, or laboratories of research institutes. These objects constituted the concrete foundation of those biological and geological sciences that are as much historical as experimental in their natures, and as such the specimens are both essential and irreplaceable. Museums and associated institutions in Russia were founded early (Peter the Great's Kunstkamera, for example), and developed steadily under both imperial and Soviet patronage.

These collections include scientific specimens, rare publications, unpublished or nontraditional scientific resources (e.g., maps, notebooks and diaries, photographs) collected from times and regions now recognized as critical to understanding present-day problems such as global change, biodiversity, and environmental perturbation. They now constitute an important part of the world's scientific patrimony, but the holdings generally have been unknown to the international community.

The first World War and its aftermath created a watershed in Russian science that was not initially apparent. For the first decade after the October 1917 revolution, the new authorities, while asking the academy to undertake a variety of practical investigations and creating a series of new commissions, did not directly interfere in most cases with the internal functioning of the academy, which continued to be administered under the terms of the statute of 1836. All that

changed in 1927, when a series of organizational changes effectively Sovietized, and Bolshevikized, the academy by 1929. In that year occurred the first mass purge of the academy, to be followed by many others. This story has been told well and in great detail by a series of authors. It should be noted, however, that the traditions of Russian science that had been growing and maturing in the two centuries since the Imperial Academy of Sciences was established provided a resilient framework which could in many cases absorb the distorting stresses placed upon it by the Communists. That these stresses did sometime produce a breakdown in important areas of science is widely recognized -- politicization of genetics under Stalin, through the influence of Prezent and Lysenko is a well known tale -- but similar fates were accorded to applied mathematics and statistics, ecology and conservation (Weiner, 1988), and virtually all of the social sciences. Although driven underground, these sciences survived in the form of private seminars and in samizdat, only gradually emerging after Stalin's death.

The scientific communities that we see today in the republics of the former Soviet Union exhibit a range of health. The basic physical sciences are intellectually strong, as are what may be called the "field sciences," those natural sciences that depend upon direct observations of nature, such as the many branches of biology, geology, and geography, as well as the museums and similar institutions preserving the voucher specimens that validate these sciences. Genetics, and with it molecular biology, have made a remarkable recovery from Lysenkoism. The social sciences as a group remain more problematic. However, the infrastructure of most of these sciences is seriously deficient. At present, lack of adequate equipment, including computers, imposes great limitations, but simple items such as high quality microscope slides, alcohol to preserve specimens, and even such common supplies as paper are in short supply or absent. Coupled with this is the problem that the organization and direction of scientific research in most academy institutes and universities remains essentially unchanged since the collapse of the Soviet Union and the dismantling of the Communist Party. The vast majority of scientists are constrained by the existing bureaucracy and organization to continue almost as though the party still controlled the academy. In addition, and in some respects most important, FSU scientists are among those segments of society that have suffered most from the economic breakdown that is occurring in Russia and its sister republics. Rapid inflation has eaten away most of the buying power of scientific salaries, to the point that the average scientist must spend much of his time searching for life's necessities, or else earning money outside of his scientific profession.

Given this scientific heritage and those factors, both historical and economic, that now control the behavior of scientist in the FSU, what does this suggest concerning possible approaches to alleviating the afflictions of science? The following broad generalities might be considered:

1. Support those sciences that have been traditionally strong.
2. Encourage greater democratization of the academy system.
3. Encourage greater diversification in active research by those institutions that have traditionally conceded that role to the academy, such as universities and other public or private organizations.
4. Encourage collaborative research between FSU and western scientists, in order to foster democratization and diversification.

Evolutionary and Environmental Biology

More specific actions must be tailored by specialists to meet the needs of their particular disciplines. We speak here only for evolutionary and environmental biology, and particularly those fields that depend upon scientific collections of specimens and associated data from nature.

The number of such specimens in museum, herbarium, and institute collections in Russia and other republics of the former Soviet Union numbers in the millions. Unfortunately, estimates of collection size are available for only a few of the major institutions (Table 1). The largest is the collections of the Zoological Museum of the Academy of Sciences, which houses some tens of millions of animals; the largest plant collection is at the Komarov Institute of Botany--both are in St. Petersburg. In Moscow, the Zoological Museum of Moscow State University, and the Main Botanical Garden of the Academy are much smaller, but nonetheless of great significance. Other collections of major regional significance are located in Siberia, in the Far East, and in the several republics.

Some of the scientific collections were initiated for specific regional issues, such as documenting the history or biota of a particular autonomous region. In most case, however, the scientific tradition represented by the various Academies of Sciences controlling these collections has meant that scientific collections in the FSU, regardless of age, size, or locality, are of high scientific value and comparable to modern collections elsewhere. Such a claim cannot be made, for example, for many regional collections in the U.S., where data standards are minimal or lacking, or specimen preparation, maintenance, and storage are inadequate. Some of the regional scientific collections in the FSU comprise holdings of specimens and early publications unduplicated anywhere else, including the larger collections in Moscow and St. Petersburg.

Until recently, these collections have been carefully conserved by dedicated curators and scientists. Dedication is the watchword here -- during World War II, some scientists in the Zoological Museum in Leningrad refused to be evacuated from the besieged city and remained to protect the collections from destruction, and the devotion of the staff of the Vavilov Institute to their unique seed collections is legendary. By Western standards, some curatorial practices appear suboptimal; cardboard boxes are used to house bird and mammal specimens, rather than dust- and insect-proof metal cases, for example. These reflect economic realities, however, rather than lack of expertise. Similarly, most collections are housed in old buildings (in Moscow and St. Petersburg, some are 18th century in age), where temperature and humidity controls cannot be brought up to Western standards.

Nevertheless, those who have worked with the collections know that they remain generally in good shape, with properly recorded associated data. The new problem facing the scientists is that the basic level of support formerly available for building maintenance, heating, and for

Table 1. Biological Collections in the Former Soviet Union

INSTITUTION	SPECIMEN TYPE	GEOGRAPHIC COVERAGE	TOTAL NO. SPECIMENS	RISK ASSESSMENT
Moscow				
Main Botanical Garden	Plants	FSU	350,000	High
Moscow State University Museums	All	FSU	3,000,000	High
Central Helminthological Museum	Parasites	World	145,000	Moderate
St. Petersburg				
Komarov Botanical Institute	Plants	FSU	5,700,000	High
Vavilov Institute of Cultivars	Plants	World	236,000	High
Zoological Institute	Animals	World	20,000,000	High
Other Major Collections				
Acad. Sci. Collections, Alma-Ata	All	Kazakhstan	550,000	High
Acad. Sci. Collections, Baku	All	Asia	1,500,000	Moderate
Acad. Sci. Collections, Dushanbe	All	Asia	400,000	?
Acad. Sci. Collections, Frunze	All	Asia	600,000	Moderate
Acad. Sci. Collections, Kiev	All	Ukraine	2,500,000	?
Acad. Sci. Collections, Tashkent	All	Central Asia	1,900,000	?
Acad. Sci. Collections, Tbilisi	All	Georgia	2,700,000	High
Acad. Sci. Collections, Yerevan	All	Armenia	800,000	High
Centr. Sib. Acad.Sci., Novosibirsk	All	Siberia	950,000	Moderate
Inst. Biol. Prob. North, Magadan	All	Far East	650,000	High
Rostov-On-Don State Univ.	All	Volga	1,300,000	High
Tomsk Univ., Tomsk	All	Siberia	1,800,000	High
Other Collections				
Various localities	All	FSU	3,500,000	Mod - High
Total	All	World	45,000,000	Mod - High

essential preservatives such as alcohol, is no longer there. Temperature in buildings sometimes falls to 10° C or below, and some fluid-preserved specimens are slowly drying up, due to lack of sufficient funds. Important field research sites and scientific preserves (zapovednik) no longer can maintain staffs to patrol their territories, and poaching has become a very serious problem in many.

To address the most serious problems in this discipline; the following steps might be considered:

1. Identify those scientific collections of objects and data (including libraries) that are of international importance.
2. Establish small (2-4) teams of disciplinary specialists to visit those collections, to assess their current condition and urgent needs.
3. Prioritize, by importance and need, those institutions which should receive emergency assistance (funding, expertise).
4. Determine the safest and most efficient means of delivering the assistance, and ensuring that needed repairs, supplies, etc. are obtained.
5. Prepare for international publication descriptions and summaries of the prioritized institution collections, listing the scope and extent of the holdings, and the basis for status as international resources.
6. Support computerization of holdings and creation of accessible databases.

Parasitology

This discipline holds a unique and central position among the zoological sciences of the FSU. Contrary to what is regarded as a minor role in North America, parasitology in Russia has represented a far-reaching scientific discipline that has been the focus of intensive research, particularly over the past 70 years. The founder of contemporary Russian parasitology was K.I. Skrjabin, who was responsible for the emergence and diversification of helminthology and was the driving force that influenced the direction and stability of this science in the Soviet Union (Petrov et al. 1953; Ryzhikov et al. 1978). The contributions by Skrjabin were significant, resulting in the training of a substantial number of Soviet helminthologists (in excess of 500 scientists by Skrjabin alone), the organization of research centers, and the publication of an array of seminal monographs in helminth systematics. These latter have proven to be requisite for modern parasitological research, having no published counterparts in the western literature.

Initiated in the period 1920-1922, the Helminthological Department of the All Union Institute of Experimental Veterinary Science was to become in 1932 the All Union K.I. Skrjabin Institute of Helminthology (VGIS) in Moscow, the current site of the Central Helminthological Museum. Later in 1942, the Helminthological Laboratory of the USSR Academy of Sciences was founded. These institutions along with laboratories in Vladivostok, Kiev, St. Petersburg and elsewhere serve as repositories for some of the most diverse and irreplaceable helminth collections in the world, along with important research libraries and archives.

The formation of these institutes marked the beginning of full integration of parasitology and helminthology as a primary direction for research among many sections of the USSR Academy of Sciences and their affiliates scattered throughout the Soviet Republics. Coincidental with the earliest organization of these institutes, a series of All Union Helminthological Expeditions (now in excess of 350) were initiated in 1921. These resulted in the rapid and comprehensive elucidation of the helminthofauna of terrestrial, aquatic and marine vertebrates (and invertebrates) of the FSU by specifically trained teams, often under the guidance of Skrjabin. The All Union Expeditions fostered field collections across representative habitats and landforms of the FSU and were instrumental in the training of almost every major contemporary Russian helminthologist. The legacy of these synoptic explorations resides in an extensive and irreplaceable data base on the morphology, taxonomy, evolution and distribution of helminths not only within the borders of the FSU but of worldwide scope (Table 1). As a consequence, the helminth faunas among vertebrate hosts in the FSU are better understood than in any other comparable region of the world. Collections represent a source of unrivaled biogeographic, systematic and ecological information for hosts and parasites, and requisite components of any biodiversity research program.

Oceanography⁷

In the field of oceanography, according to NOAA, large quantities of irreplaceable data that are of great potential value to the world's scientists are in danger of being lost forever. For example, NOAA estimates that the volumes of bathythermographs and hydrocasts held by the Russian National Oceanographic Data Center are 30% and 50%, respectively, of the corresponding holdings in the U.S. These data frequently supplement U.S. holdings, since they are from areas where the U.S. has not collected data (e.g., water column data from FSU peripheral seas, the Arctic Ocean, the Indian Ocean, and the Southern Hemisphere. The data are considered to be of good quality, and to form the basis for fruitful collaborations between U.S. and Russian scientists. Table 2 reproduces a summary of oceanographic holdings in the FSU that was prepared by NOAA.

NOAA has developed a plan for a collaborative program with institutions of the FSU. The plan would:

1. Digitize large quantities of manuscript and atlas data into common formats;
2. Perform data continuity analyses;
3. Merge U.S. and FSU data to create a global database available without restriction to the international scientific community;
4. Reanalyze the merged database and recompute ocean climatologies.

The program would be carried out through one-to-one pairings of U.S. government organizations and FSU counterparts; the FSU organizations selected are the Russian National Oceanographic Data Center at Oboresk (physical oceanographic data), the Geological Institute of the Academy of Sciences in Moscow (bathymetric data), and the Arctic/Antarctic Research Institute in St.

⁷Based on material provided by NOAA.

Table 2. Estimated Oceanographic Data Holdings in the Former Soviet Union

INSTITUTE	DATA TYPE/ TIME COVERAGE	AREA OF COVERAGE	DATA VOLUME	ESTIMATED RISK LEVEL
Physical Oceanographic Data				
Russian NODC Obninsk	Hydrocasts (1900-1990)	Global	220,000 digitized	High to very high
	MBTs (1946-1991)	Global	260,000 undigitized 180,000 digitized 160,000 undigitized	
Murmansk Marine Biological Institute	Hydrocasts	Baltic, North Atlantic north of England	100,000 undigitized	High
Navy Ministry, St. Petersburg	MBTs (1940-1991)	Global	150,000 digitized 200,000 undigitized	Unknown
Arctic and Antarctic Research Institute, Vladivostok and Murmansk	Hydrocasts	Polar Regions, Sea of Okhotsk, Bering Sea	5,000 undigitized	Moderate
Fisheries Ministry, Vladivostok	Hydrocasts	North Pacific, Sea of Japan, Yellow Sea	100,000 undigitized	High
	MBTs (1946-1991)		50,000 undigitized	
Riga Institute National Academy of Science, Latvia	Hydrocasts	Global	140,000 undigitized	Moderate
Bathymetric Data				
VNII Okeanologiya, St. Petersburg	Single Beam Echosounder (1946-1989)	High Arctic	100,000 analog records 15,000 analog stations	High
	Multibeam echosounder (1986-1991)	North Atlantic	Unknown	High
Geologic Institute, Academy of Science, Moscow	Single beam echosounder (1946-1989)	Global, except high arctic	2 million miles analog tracklines	High
	Multibeam echosounder (1986-1991)	Global, except high arctic	20 million digital records Unknown analog records	Very high
Sea Ice Data				
Arctic and Antarctic Research Institute, Vladivostok and Murmansk	Sea ice analysis charts (1990-1991)	Polar regions	Unknown	Unknown

Petersburg (sea ice data). This program does not directly involve U.S. university researchers and may leave out Russian scientists who are not affiliated with the selected Russian organizations. Thus there may remain a significant role for private sector activity in the field of oceanographic data and research.

Seismology⁸

The FSU's collections of seismic data are also at risk. According to IRIS, seismic stations that have recorded data for decades are being shut down and archives of data will soon be destroyed. Not only would this mean the loss of data important for developing scientific for understanding earthquake propagation, it would result in inability of the former Soviet republics to monitor seismicity and to carry out coherent programs of earthquake hazard assessment. Furthermore, the station shutdowns threaten loss of coverage over a significant portion of the earth's surface, a development that would be disastrous for global seismology should it occur.

The problem in seismology has a particular geographic twist, since two of the most important threatened observing stations are in Kazakhstan and Tajikistan. In most other sciences, the key people and facilities are in Russia.

IRIS identifies three action items:

1. Maintain the infrastructure for seismological observations and research; rescue the data from threatened observing stations and ensure the survival of the "national" seismic network.
2. Coordinate and provide facilities for joint research projects (IRIS could provide the necessary facilities base for such a program).
3. Support key CIS scientists and key research programs, particularly those involving younger scientists who have not yet achieved international recognition.

The assessment of the problem with seismological data, the diagnosis of the problem, and the specific actions that would be appropriate may be a subject for further elaboration.

⁸Based on information provided by IRIS.

Glaciology⁹

The World Data Center A for Glaciology (WDC-A)¹⁰ has identified a number of targets for the rescue of environmental data. Snow cover data from 38 regions of the FSU are available in Obrinsk in rare hard copy reports from the 1930s to 1965 and in monthly publications since then. Besides snow cover data, the tabulations include data on depth, thickness of crust, snow water equivalent, snow topography, and snow type, as well as other atmospheric and surface data. These hardcopy records are rare and would provide validation of passive microwave observations. Digitization is needed.

A second data set consists of 69 published volumes inventorying 14 percent of the world's glaciers. These data are needed to complement and interpret available FSU data on glacier fluctuations, a key variable in the IPCC 90 and 92 reports. WDC-A also proposes to provide support for digitization of data from the Soviet North Pole manned stations on ice floes. A final effort involves the digitization of records from the Institute of Arctic and Antarctic Research in St. Petersburg, which includes sea ice data for the Eurasian Arctic and tables of surface and air reconnaissance of ice and snow conditions in the Arctic and Antarctic. These data are important to understanding the flows of polar sea ice.

In the non-Russian states, the Central Asian Regional Research Hydrometeorological Institute (SANIGMI) in Tashkent has extensive holdings on snow cover, avalanches, glaciers, and runoff in the mountains of Central Asia. They have maintained a glacier research station at 4000m on the Abramov Glacier in the Pamir-Altai Mountains since 1969. Extensive data sets exist at SANIGMI as a result of these activities. In addition, the other Asiatic republics (Kazakhstan, Kyrgyzstan, Tajikistan) have archived data at SANIGMI. There is concern now, however, that these states may discontinue archiving their data at SANIGMI and may even recall those which are there now.

Other Data Sets

The oceanographic, seismographic, and glaciological data sets briefly described here are merely examples, albeit important ones, of a wealth of data that is at risk in the former Soviet Union. These data are of great potential importance to scientific investigations throughout the world. Some previously unavailable data are now becoming open to scientists. Cataloguing the

⁹Based on information provided by the World Data Center A for Glaciology [Snow and Ice].

¹⁰The twelve World Data Centers (WDC's) of the International Council of Scientific Unions are a valuable source of scientific contacts between the United States and Russia. These centers have extensive experience, both in the past and in the present, in the exchange of geophysical and environmental data and scientific personnel between the United States and Russia, where companion World Data Centers are located. In some cases the contacts and exchanges date back to 1957 when the WDC system was founded to support data management activities of the International Geophysical Year. The scientific disciplines represented by the centers include oceanography, meteorology, glaciology, paleoclimatology, solar-terrestrial physics, marine geology and geophysics, rotation of the earth, rockets and satellites, solid earth geophysics, seismology, atmospheric trace gases, and remotely sensed land data. The U.S. National Academy of Sciences provides oversight of the WDC-A data centers through the Committee on Geophysical and Environmental Data. The Executive Secretary of the committee is Dr. Lorraine Wolfe (202-334-3368).

information and taking steps to rescue imperiled data sets are activities surely in the interests of the world's scientific communities and, ultimately, its peoples.

Mathematics¹¹

Mathematics presents a unique situation. Russian mathematicians, despite occasional opposition by the political authorities and central scientific organizations, have developed one of the world's most successful systems of mathematics education. The system is an orally transmitted cultural tradition, and its survival depends on the survival and continued activity of those who understand and practice it. According to the American Mathematical Society, the system includes the following components:

1. A pyramid of mathematical Olympiads for high school students, formerly culminating in the all-Union Olympiad.
2. "Mathematical Circles," held outside school hours under the guidance of research mathematicians, where high school students learn to solve problems.
3. Special high schools for mathematics and physics staffed by research mathematicians and university students as well as high school teachers.
4. A series of books, and the journal Quant, for high school students, written by research mathematicians.
5. A particular style of mathematical seminars at universities which mixes undergraduate teaching with research exposition in a unique way.

The organizations that developed this approach did so under adverse circumstances, without official support. They survived and even prospered in these circumstances, perhaps because the adverse conditions afforded them the aura and spirit akin to that of samizdat. In the process, they developed an independent, intellectually pure style.

Now, however, they are in danger, because their authors and practitioners are suffering the same deprivations as are other Russian scientists. Their disappearance would be a serious blow to world science. It would mean the loss of future top mathematicians, since the Russian system has produced a large number of such people. We would lose a source of important ideas for our own educational system. Finally, the Russian system produces an approach to mathematics whose practitioners are a source of mathematical ideas for the entire world.

Some aid programs have been launched in this area. The German Volkswagen Stiftung has started a program to help save the university seminars. The Mathematical Association of America is working to provide back issues of Quant for high school students. The AMS is providing support to individual research mathematicians through grants. But these programs are directed at individual segments of the Russian mathematics education system; a more systematic, holistic approach is thought to be needed.

¹¹Based on information provided by the American Mathematical Society.

The AMS makes the following recommendations for action in this matter:

1. Provide direct support for the mathematics Olympiads.
2. Provide modest pay for high school teachers who teach the "mathematical circles" and for university students who volunteer to teach in mathematical high schools.
3. Provide support for existing seminars for teachers.
4. Provide funds to support publication of mathematical books and journals.
5. Give direct support to mathematical researchers and University seminars.

In providing aid to Russian mathematics, the AMS makes several procedural recommendations,

1. Avoid using institutions that previously hindered the development of the instruction system to administer the funds.
2. Take steps to insure that aid provided to mathematics teachers does not cause resentment among teachers not so favored. Payment on an "overtime" basis for special work will alleviate this problem.
3. Do not attempt to interject American educational ideas into the program.

Conclusion

As used in this paper, the scientific heritage of the FSU refers to the collections of physical specimens -- plant and animal -- and of data from many fields of science, as well as to certain unique pedagogical techniques that have been developed over decades of experience. The paper does not cover the most important part of the heritage -- the talented and skilled scientists and engineers who live and work in the FSU. However, the collections and the techniques that are the focus of attention here represent a heritage of incalculable value to the world scientific community. Rescuing them from what seems to be almost certain serious damage or even total loss should be a matter of the highest priority.

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SUSTAINING EXCELLENCE IN SCIENCE AND ENGINEERING IN THE FORMER SOVIET UNION

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