NASA-CR-200526

Final Report for NCC2-5084

"Analysis of Near-IR to Mid-IR Imaging and Spectroscopic Data of Mars, the Moon, and Selected Asteroids"

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Introduction

This final report will address research carried out by Dr. James F. Bell, Dr. Yvonne J. Pendleton of NASA Ames Research Center, and Dr. John B. Adams of the University of Washington. The work was done under contract NCC2-5084 during the period of August 1, 1994 to July 31, 1995.

The intent of this research, described in our JRI proposal, was twofold: (1) To develop efficient data reduction and analysis techniques for large multispectral and hyperspectral planetary data sets; and (2) To perform analyses and interpretations of near-IR and mid-IR planetary imaging spectroscopic data sets using the techniques that we developed.

Much progress was made on developing computational algorithms and identifying data reduction procedures for a number of different types of data sets. Progress on data analysis and interpretation was also made, and our results on Mars and the Moon have been reported in several research papers. In this report we present a summary of our final results on data reduction and analysis technique development, analysis of Mars near-IR spectra, and analysis of lunar mid-IR spectra. We also made progress on the reduction and calibration of near-IR asteroid reflectance spectra (*Cruikshank et al.,* 1995), however the detailed results of that research are still tentative and so are not reported here.

Data Reduction and Analysis Technique Development

As part of this research interchange project, we developed a suite of FORTRAN programs for use specifically on the reduction, calibration, and analysis of computationally-large planetary imaging and spectroscopy data sets. Because of the large sizes of imaging spectroscopic data sets as compared to traditional spectroscopy data sets, new techniques are needed in order to calibrate and interpret the data in a semi-automatic way so that the many thousands of measurements can be interpreted in a reasonable amount of time. Programs were written to perform the following:

(a) Instrumental corrections. Several image processing procedures have become standard steps in the reduction of imaging data sets. These include removal of bias or instrumental offset level from the data, and correction for pixel-to-pixel nonuniformities, commonly known as flatfielding.

Less common, but also potentially important, is a possible correction for instrumental nonlinearity (*e.g., McCaughrean*, 1989). Assuming that all of the appropriate calibration images have been obtained, most of these corrections can be applied without supervision by the user with the programs that we have developed. This is possible because the software checks to make sure that the appropriate wavelengths and/or exposure times are being dealt with for each step of the reduction. The automation of these instrumental correction procedures saves a substantial amount of time, especially when dealing with many thousands of images.

(b) Image registration. Registration involves accurate alignment of images at multiple wavelengths to form a 3-dimensional data set (spatial × spatial × spectral; an image "cube"), so that a spectrum can be obtained by simply extracting data through the spectral axis of the cube. In practice, this can be a tedious and rather subjective process, the result of which depends critically on the patience and experience of the user. We have developed several automated registration schemes that can be applied to large data sets to achieve a first-order registration quite rapidly. These schemes involve calculation of quantitative statistics (differences, ratios, correlations, and covariance matrices) between the image to be registered and the base image being used as the reference. An iterative search procedure is used to overlay the image to the base image, compute relational statistics, then shift the image slightly, and re-compute the statistics to see if a better fit has been obtained. An entire image cube can be registered to a base image this way, or each band in the cube can be sequentially registered to the next. The process proceeds without user supervision. After finishing, the user can "movie" through the registered images to verify the performance of the automated routine. Typically, the automated results need some fine-tuning by the user, but the automation of the initial step has saved a substantial amount of time compared to starting from scratch.

(c) Calibration. Calibration involves the process of transforming a raw data set into absolute units such as flux, radiance factor, or reflectance (*e.g., Hapke*, 1981; *Roush et al.*, 1992). This is achieved by using near-simultaneous observations of a well-known calibration source, such as a standard star for planetary science applications. Our software assists in the calibration exercise by automatically calculating the spectral shape and absolute flux of a star given its magnitude and spectral class. The program can then automatically divide the shape of the solar spectrum from the resulting flux-calibrated planetary image, or ratio the derived flux to that expected from a perfect Lambertian reflector viewed at the same geometry, to derive the relative reflectance or radiance factor values for the data set. These calibrated data units can then be used to compare the data with other telescopic, spacecraft, and laboratory measurements that have also been calibrated to the same units.

(d) Analysis. Finally, our software package provides the ability to perform some first-order data analysis steps on reduced and calibrated planetary imaging spectroscopic data sets. These analyses include band ratios, band depth maps, simple linear unmixing (*Adams et al.*, 1993), principal components analysis, and traditional spectrum extraction and analysis. Most of these are modifications of standardized procedures that have been developed previously by others; however, we improved a few of the procedures for specific application to planetary imaging spectroscopy data sets. For example, band depth, $D_{\lambda b}$, is traditionally defined as (*e.g., Clark and Roush*, 1984):

$$D_{\lambda b} = \frac{R_{\lambda 1} + R_{\lambda 2} - 2R_{\lambda b}}{R_{\lambda 1} + R_{\lambda 2}} \tag{1}$$

where the out-of-band reflectance values are $R_{\lambda 1}$ and $R_{\lambda 2}$, and the in-band value is $R_{\lambda b}$. We developed an algorithm for situations where the absolute reflectance may not be known, for example in situations where standard star data could not be obtained in association with a particular data set. In that case, rather than discard the data as useless, most of the information can be salvaged by defining a relative band depth, $RBD_{\lambda b}$, as:

$$RBD_{\lambda_b} = 1 - \left\{ \frac{(I_{\lambda_b} / \bar{I}_{\lambda_b})}{[(1-f)\,(I_{\lambda_1} / \bar{I}_{\lambda_1}) + f\,(I_{\lambda_2} / \bar{I}_{\lambda_2})]} \right\} \tag{2}$$

where the I's represent uncalibrated images at wavelengths $\lambda_1 < \lambda_b < \lambda_2$, $\bar{I}$ is the whole-disk average value at each wavelength, and $f = (\lambda_b - \lambda_1) / (\lambda_2 - \lambda_1)$. The denominator in (2) represents the local continuum level at λ_b and is derived from a linear fit between images obtained at wavelengths on either side of the absorption band being mapped. The use of an accurate local continuum level in the definition of RBD is similar to the technique of *Crowley et al.* (1989), however, our use of image ratios within the RBD calculation is, to the best of our knowledge, unique.

Interpretation of Mars Near-IR Data

Many of the above techniques were utilized in the analysis of a large Mars spectroscopic data set obtained during the 1993 opposition from Mauna Kea Observatory in Hawaii. New moderate resolution (R = 300 to 370) reflectance spectra of Mars were obtained during the 1993 opposition from Mauna Kea Observatory using the UKIRT CGS4 spectrometer by *Bell et al.* (1994). Fifty spectra of different surface regions and a number of standard star spectra were obtained in the 2.04 to 2.44 μm wavelength region. Using techniques developed under this JRI program, the spectra underwent an absolute calibration scheme using standard star spectra and assumptions about the continuum flux of the Sun. Both flux ($W/cm^2/\mu m$) and radiance factor (observed flux / expected Lambertian flux) spectra were derived. The absolutely-calibrated spectra exhibited a point-to-point precision of from 1.1% to 2.8% depending on the brightness of the region observed. The errors on the absolute flux are from 7 to 11% (1σ) and on the radiance factor values the errors are from 9 to 12%, assuming a 5% uncertainty in the absolute flux distribution of the Sun.

A radiative transfer model (*Pollack et al.,* 1990, 1993) was used to compute atmospheric transmission spectra for Mars and the Earth in order to simulate the contributions of these atmospheres in our observed data. Also, we examined the Space Shuttle ATMOS instrument solar spectrum in the near-IR to try to identify absorption features in the spectrum of the Sun that could be misinterpreted as Mars features.

Using various spectrum analysis techniques, eleven narrow absorption features were detected in the Mars spectra. Five were attributed all or in part to Mars atmospheric CO_2 or CO [2.052, 2.114, 2.150, 2.331, and 2.357 μm]. Four others were interpreted as evidence for telluric (H_2O, CH_4) or possibly solar/stellar spectral contamination [2.315, 2.385, 2.412, and 2.432 μm]. Weak bands at 2.278 and 2.296 μm may have mineralogic origins, although a solar contribution could not be excluded. Two of the atmospheric bands [2.331 and 2.357 μm] appear to have widths and depths that are consistent with additional, non-atmospheric absorptions, although a residual solar contribution at these wavelengths also could not be entirely ruled out.

Analysis of the *Bell et al.* (1994) data provide no conclusive identification of the mineralogy responsible for the absorption features detected on Mars. However, examination of terrestrial spectral libraries and previous high spectral resolution mineral studies indicates that the most likely origin of these features is either CO_3^{2-}, HCO_3^-, SO_4^{2-}, or HSO_4^- anions in framework silicates or (Fe, Mg)–OH bonds in sheet silicates. If the latter is correct, then an explanation for the extremely narrow widths of the cation–OH features in the Mars spectra as compared to terrestrial minerals must be devised.

Interpretation of Lunar Mid-IR Data

We also utilized many of the new reduction and analysis procedures described above in a preliminary examination of new imaging spectroscopic data of the Moon obtained at mid-infrared wavelengths from the NASA Kuiper Airborne Observatory (*Bell et al.*, 1995). The observations were conducted during a 30-minute KAO observing leg in October 1993. The data were obtained by J.D. Bregman (NASA/Ames) and D.M. Rank (U.C. Santa Cruz) using a new KAO facility camera based on a 128×128 Si:Ga array and LHe dewar (*Bregman et al.* 1995). The images were obtained in a 30 degree longitude by 15 degree latitude region of the southwestern limb near the craters Schickard, Baade, and Inghirami. Images of this region in 71 wavelengths between 5.0 and 7.0 μm were obtained through a 1.5% CVF.

Because of the exploratory nature of the observations, it was not possible to obtain enough data for a complete and rigorous calibration of the images. Thus, utilizing many of the relative calibration techniques discussed above, we devised a bootstrap relative calibration scheme that allowed analysis of the compositional variability within the scene and that allowed us to assess the general detectability of lunar rocks and minerals in the mid-IR. We performed the "standard" data reduction steps using dark and flatfield images obtained in the lab shortly after the observing run. The images were then spatially co-registered automatically and fine-tuned by hand to within 0.5 pixel. The average spectrum of all the regions of the Moon imaged was determined, and then the final image cube (128×128×71) was generated by dividing this average spectrum from the original data. The resulting image cube cannot be directly compared to laboratory spectra, but it does allow relative spatial variations to be detected and the wavelengths of these variations can be directly associated with the wavelengths of features seen in laboratory rock and mineral spectra.

The KAO mid-IR images and spectra have undergone only a preliminary analysis at this time. Clearly, there is a wealth of detail in the data shown above that needs to be examined using techniques such as those that we have devised for this JRI project. However, these exploratory observations and the analyses done so far show that the lunar surface is detectably heterogeneous at mid-IR wavelengths, which is encouraging for possible future, more detailed KAO and spacecraft mid-IR imaging observations.

Summary

This JRI research project has concentrated on the development of data reduction and analysis techniques for planetary science applications. The emphasis has been on maximizing the ease of interpretation of computationally large datasets, using many traditional analysis techniques as well as new techniques explicitly modified for imaging spectroscopic data sets. This project has led to the publication of several research papers on lunar and Martian surface composition, as well as preliminary results on the interpretation of spectra of several asteroids.

Acknowledgments

This research effort would not have been possible without the initial guidance, support, and expertise of Dr. James B. Pollack, who passed away in mid-1994. We are extremely grateful to Ames technical monitor Dr. Yvonne J. Pendleton for her advice and support with this research project. We also thank Ames scientists Dr. Jeff N. Cuzzi, Dr. Robert M. Haberle, and Dr. Ted L. Roush for their wisdom and guidance. Finally, we thank Ginger Vogler for doing a masterful job of setting up and administering this grant on the University of Washington end. Funds for the support of this research have been allocated by the NASA Ames Research Center, Moffett Field, CA, under Joint Research Interchange No. NCC2-5084.

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