**IMPROVED SCHEME OF MODIFIED GAUSSIAN DECONVOLUTION FOR REFLECTANCE SPECTRA OF LUNAR SOILS.** T. Hiroi, C. M. Pieters, and S. K. Noble, Dept. of Geological Sciences, Brown University, Providence, RI 02912, U. S. A. (takahiro_hiroi@brown.edu).

Our initial scheme for deconvolving reflectance spectra of lunar soils [1] using the modified Gaussian approach [2, 3, 4] has been reevaluated and improved. Instead of removing a double-linear continuum as in our previous study, a new form of continuum has been developed along with a semi-automatic method for selection of initial parameters, and the continuum parameters have been optimized together with modified Gaussian parameters at the same time. This new approach, which also constrains band strength to be negative, is the first attempt of deconvolving reflectance spectra of lunar materials with simultaneous optimization of all the parameters.

## 1. Introduction

Lunar soils have special characteristics that result from "space weathering" as the original rock powders are exposed to the space environment such as the solar wind and micrometeorite bombardments [*e.g.*, 5]. As a lunar soil matures, the near-infrared reflectance spectrum typically becomes redder and diagnostic absorption bands become shallower. Accurately modeling the lunar "red" continuum with superimposed absorption bands has been a challenge for analyzing lunar soil spectra with quantitative methods such as the modified Gaussian model [2, 3, 4]. In our previous approach [1], the basic properties of the modified Gaussian model for diagnostic absorption bands was combined with a double-linear modification of the straight-line continuum removal method traditionally used for lunar soils and the combined method was applied to the analysis of lunar soil spectra. Initial results were promising [6], but the relative strength of weak bands was not believed to be reliable.

## 2. Spectral Data

Laboratory reflectance spectra of lunar soils are measured relative to halon at 30° incidence and 0° emergence angles. The reflectance values are corrected for the absolute reflectance values of halon. The soil used as an example here, 12030 (20-44 μm fraction), is one of a suite of samples included in a study of lunar mare soils [6, 7].

## 3. Deconvolution Method

The modified Gaussian model deconvolution calculations usually use modified Gaussians (Gaussians in the wavelength space) and the 1st-order polynomials in the wavenumber space in order to express the continuum background of natural log reflectance spectrum (approximate absorbance spectrum) [2, 3, 4, 8]. Initial values are selected and the optimized continuum and band parameters are fit results. As described in [2], modified Gaussians are added as necessary for the best convergence so that the fitting error becomes the same level with the measurement error of the spectrum. Our program for lunar soils is written based on the modified Gaussian model (MGM) algorithm presented in [2] and a nonlinear inverse problem solution [9]. The MGM general algorithm is publicly available in [4].

*__Continuum__:* In order to give the continuum shape more flexibility to fit the characteristic spectral slope of lunar soils and yet to keep stability in optimizing both the continuum parameters and modified Gaussian parameters, we have developed the following continuum formula:

$$C(\lambda) = c_{-1}/\lambda + c_0 + c_1\lambda \qquad (1)$$

where $\lambda$ indicates wavelength, $C(\lambda)$ the continuum function, and $c_{-1}$, $c_0$, and $c_1$ are constants. Note that Eq. (1) is a superset of the conventional continuum shape which includes only the 1st and 2nd terms, suggesting this new continuum form is applicable to materials other than lunar soils. Also, because $C(\lambda)$ is most likely to be monotonous, free of any maximum or minimum point, they are unlikely to invade characteristic features of absorption bands which are intended to be expressed by modified Gaussians.

*__Initial Values__:* In order to make it easy to supply initial values for the continuum parameters and the modified Gaussian strengths, a double-linear tangential continuum in the reflectance space as in our previous study [1] was used. Three initial parameters of our new continuum in Eq. (1) were determined so that the continuum passes two contact points around 0.75 and 2.6 μm and a point in the middle of two contact points around 1.5 μm defined by the double-linear continuum. The initial center and width of each modified Gaussian are given by the user. The program estimates the initial strength by subtracting the double-linear continuum from the natural log reflectance at the center wavelength.

*__Solution Constraint__:* Values are also presented for the expected range each continuum and modified Gaussian parameter can vary in the fitting process. Because this constraint is put based on statistical distribution, it is still possible that the program tries to use values beyond the range specified by the given standard deviation. Therefore, in order to prevent the band strengths from becoming positive, the modified Gaussian formula has been modified as follows:

$$\ln R(\lambda) \approx C(\lambda) - \Sigma h_i^2 \exp[-\{(\lambda-\mu_i)/\sigma_i\}^2/2] \qquad (2)$$

where $R(\lambda)$ indicates reflectance spectrum, and $\mu_i$, $\sigma_i$, and $-h_i^2$ indicate the center, width, and strength of the $i$-th band, respectively. In this scheme, whether $h$

value is positive or negative, the band strength $-h^2$ remains negative. Width is usually expressed in terms of the full width at half maximum (FWHM):

$$\text{FWHM} = 2(2\ln 2)^{1/2}\sigma \approx 2.35482\,\sigma \qquad (3)$$

## 4. Deconvolution Result

Shown in Fig. 1 is an application of the above method to a laboratory spectrum of lunar soil 12030 (20-44 µm). Shown in Fig. 1a are the initial condition of the continuum, modified Gaussians, and error spectrum. The initial continuum and absorption band parameters are listed in Table 1. Once the measured reflectance spectrum is given, by specifying the standard deviation of all the parameters (within parentheses in Table 1), and the initial band centers and widths, the program can estimate the initial continuum parameters and band strengths and start the optimization process.

Shown in Fig. 1b are the optimized continuum, modified Gaussians, and residual error spectrum after 20 iterations. The root mean square deviation (RMSD) is 0.0034. Optimized parameters are listed in Table 2. All the noticeable features on the measured spectrum such as absorption bands, shoulders, and inflections were expressed by this combination of our new continuum and modified Gaussians. Compared with our previous attempt [1, 6] using a double-linear tangential continuum, this new approach appears to be more reasonable and flexible in that the continuum has one more adjustable parameter and all the continuum and modified Gaussian parameters are optimized at the same time. A new scheme in Eq. (2) to prevent a positive band strengths seems to be working very effectively in our other test calculations involving much weaker bands than shown in Fig. 1 [10].

**Table 1. Initial continuum and absorption band parameters for lunar soil 12030 (20-44 µm).**

| *Initial Continuum Parameters* | | | |
|---|---|---|---|
| $c_{-1}$ (µm)* | $c_0$* | $c_1$ (µm$^{-1}$)* | |
| -0.1984 (0.1) | -1.7768 (0.1) | 0.2072 (0.1) | |
| *Initial Absorption Band Parameters* | | | |
| No. | Center (µm) | FWHM (µm) | Strength* |
| 1 | 0.96 (0.1) | 0.22 (0.22) | -0.333 (0.10) |
| 2 | 1.20 (0.1) | 0.38 (0.38) | -0.087 (0.04) |
| 3 | 2.07 (0.1) | 0.73 (0.73) | -0.132 (0.68) |
| 4 | 0.45 (0.1) | 0.50 (0.50) | -0.245 (0.10) |
| 5 | 0.30 (0.1) | 0.13 (0.13) | -0.767 (0.10) |

Parameters with * are given automatically by the program. Number in parenthesis indicates standard deviation of the expected solution.

**Table 2. Optimized continuum and absorption band parameters for lunar soil 12030 (20-44 µm).**

| *Optimized Continuum Parameters* | | | |
|---|---|---|---|
| $c_{-1}$ (µm) | $c_0$ | $c_1$ (µm$^{-1}$) | |
| -0.1781 | -1.5586 | 0.1483 | |
| *Optimized Absorption Band Parameters* | | | |
| No. | Center (µm) | FWHM (µm) | Strength |
| 1 | 0.956 | 0.219 | -0.3653 |
| 2 | 1.183 | 0.458 | -0.2229 |
| 3 | 2.034 | 0.897 | -0.2355 |
| 4 | 0.350 | 0.684 | -0.3990 |
| 5 | 0.296 | 0.117 | -0.3758 |

## 5. Summary

A modified Gaussian deconvolution of reflectance spectra of lunar soils using a new form of continuum has been shown to be possible.

**Acknowledgments:** Reflectance spectra of lunar soils were measured at RELAB (Brown University), a multiuser facility supported by NASA grant NAG5-3871.

**References:** [1] Hiroi T. and Pieters C. M. (1998) *LPS XXIX*, No. 1253. [2] Sunshine J. M. et al. (1990) *JGR.95*, 6955-6966. [3] Sunshine J. M. and Pieters C. M. (1993) *JGR 8*, 9075-9087. [4] Sunshine et al. (1999) *LPS XXX*, No. 1306 (http://www.planetary.brown.edu/mgm/). [5] Pieters C. M. et al. (1993) *JGR 98*, 20817-20824. [6] Pieters C. M. et al. (1998) *LPS XXIX*, No. 1827. [7] Taylor L. A. et al. (1998) *LPS XXIX*, No. 1160; Taylor L. A. et al. (2000) *LPS XXXI*, this vol. [8] Hiroi T. et al. (1996) *Icarus 119*, 202-208. [9] Tarantola A. and Valette B. (1982) *Rev. Geophys. Space Phys. 20*, 219-232. [10] Noble K. et al. (2000) *LPS XXXI*, this vol.

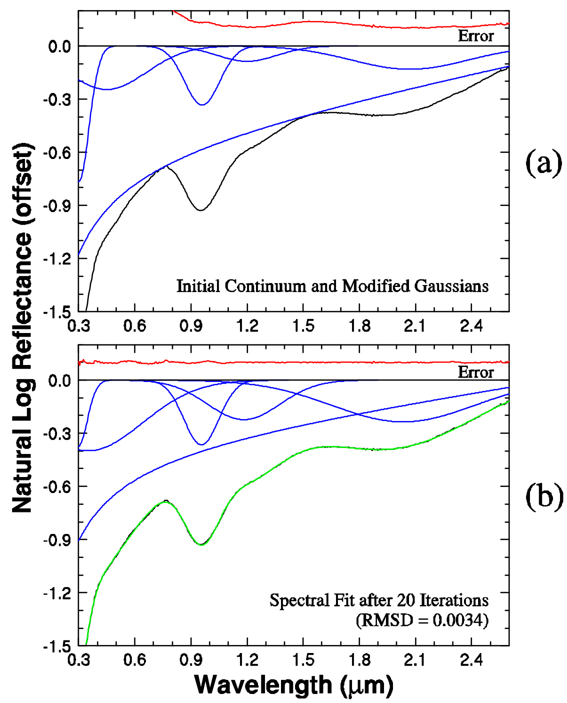


Fig. 1. Initial and optimized continuum and modified Gaussians in deconvolving reflectance spectrum of lunar soil 12030 (20-44 µm). Residual error spectrum is shown in the top of each plot with an offset for clarify.