

SPECTROPHOTOMETRIC ANALYSIS OF LUNAR SURFACE MATERIALS: A NEW TECHNIQUE FOR THE QUANTITATIVE DETERMINATION OF GEOCHEMICAL COMPONENTS

R. Jaumann, L. Kamp and G. Neukum, DFVLR Oberpfaffenhofen, Inst. for Optoelectronics, Planetary Remote Sensing Section, 8031 Wessling, FRG

An analysis technique, based on spectral reflectance measurements, for calculating the concentrations of geochemical components in lunar materials has been developed. This new technique makes use of a principal component analysis and a multiple regression analysis in order to quantify the geochemical and mineralogical information recorded in a lunar reflectance spectrum.

Spectral reflectance measurements (UV to near IR) of lunar soils are dominantly influenced by the mean geochemical elements of soil composition. Charge transfer transition and crystal-field transition of some of the ions of these elements (particularly elements of the first transition series Fe, Ti, Mn, Cr) cause distinct absorptions whereas other mineralogically dominant ions like Si, Al, Mg, Ca are responsible for the general shape of the reflectance curve as well as for the overall brightness of the spectrum.

The spectral characteristics (0.4-2.5 μ m) of lunar soil samples have been investigated in order to determine the relationship between the measured reflectance and the geochemical composition of lunar materials. For this purpose we reexamined laboratory measurements from J.B. Adams and C.M. Pieters (1,2) and applied a principal component analysis to these data. The principal component analysis transforms a reflectance spectrum of dependent variables \vec{r} into a principal component spectrum \vec{p} , which is located in a n-dimensional factor space (the dimension is given by the primary eigenvalues (3)) of independent axes. The columns of the transformation matrix Q are eigenvectors and the vector elements of the eigenvectors a weighting factors for the measured reflectance values. These independent factors (eigenvectors) correspond to the basic mineralogical and physical sources affecting a lunar reflectance spectrum (4). Thus, the spectra of the eigenvectors (eigenvector elements vs. wavelength) are determined by the dominant signatures of primary mineralogical and physical parameters defining a reflectance spectrum (Fig.1).

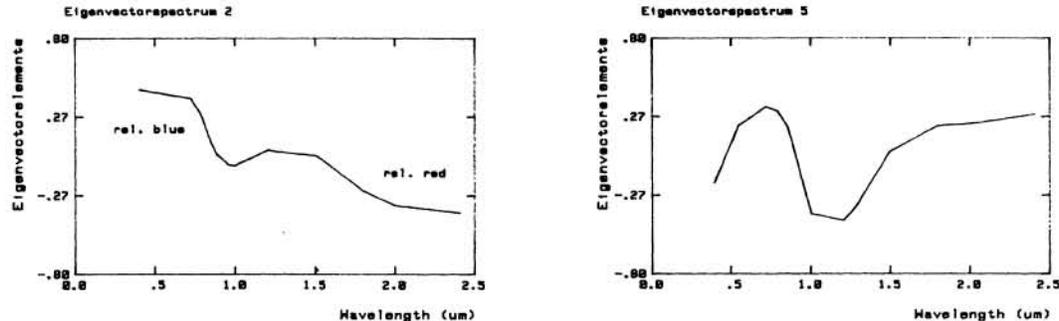


Figure 1. Spectra of two eigenvectors. The spectrum of eigenvector 2 describes the relative reddening of a lunar reflectance spectrum, which is dependent on the agglutinate and glass content in a soil. The agglutinate content itself is again dependent on the maturation state of the soil, therefore the second principal component could be understood as a complex function of the glass content and the particle size distribution in the soil. The shape of the spectrum of eigenvector 5 is similar to the spectral signature of the mineral olivine, and the fifth principal component can be explained as a function of the abundance of this mineral.

Therefore eigenvector spectra can be used to interpret each principal component in terms of wavelength dependent mineralogical or physical parameters.

In the same way as lunar minerals are build up by geochemical components (a geochemical component is expressed as the oxide of an element), we found the principal components to be linearly correlated to the lunar mean geochemical components (FeO, TiO₂, SiO₂, Al₂O₃, MgO, CaO, MnO) and an agglutinate and glass component. For the less abundant (< 1wt%) geochemical components - except for MnO - no linear correlation could be identified on the used database, but these less abundant geochemical components may be connected

to the principal components by a higher order correlation. Thus each principal component could be understood as a linear combination (linear model) of the mean geochemical components and the agglutinate component and vice versa. A multiple regression analysis connects the principal components to geochemical composition. The combination of both analysis methods (principal component analysis and multiple regression analysis) produces spectral calibration coefficients \bar{C} which relate the measured spectrum \bar{r} directly to the geochemical composition \bar{g} ,

$$\bar{g} = \bar{C} \bar{r},$$

whereby important aspects of the physical state of a soil (particle size distribution, glass content) are taken into consideration by these eigenvectors, which are primarily dependent on physical parameters. The calibration matrix \bar{C} is the matrix product of the principal component transformation matrix \bar{Q} and the matrix of the regression coefficients.

In order to test our new analysis technique we divided the chemically and spectrally analysed lunar soil samples in two data sets. The first data set was used for calculating the calibration coefficients. In the next step these calibration coefficients were applied to the independent second data set, which was not involved in the calibration coefficient determination in order to calculate the concentration of the mean geochemical components. The estimation error for the calculated concentration of a certain geochemical component in the independent data set is comparable to the error of the multiple regression analysis (Tab.1) for the same geochemical component, and therefore the determination of the calibration coefficients is sufficient to calculate the mean geochemical composition of lunar samples using spectral reflectance measurements. Thus, the assumption of a linear model is well justified.

	FeO	TiO ₂	SiO ₂	Al ₂ O ₃	MgO	CaO	MnO	Agg
$\sigma(r)$	1.3	1.5	1.9	2.5	2.1	1.0	0.05	3.7
$\sigma(i)$	1.4	1.6	1.9	2.6	2.2	1.1	0.05	4.1

Table 1. Comparison of the accuracy of the spectrophotometric analysis involving two independent data sets. $\sigma(r)$ = error of the multiple regression analysis for a certain geochemical component (wt%); $\sigma(i)$ = estimation error of the calculated concentration for a certain geochemical component in the independent data set; Agg = agglutinates.

The calibration coefficients can also be combined with high-precision remotely sensed data of the Moon for calculating the mean geochemical composition of real lunar surface elements (5). Remotely sensed data can also be used for verifying the spectrophotometric analysis technique (5).

Once the chemical composition has been estimated, the average mineralogical composition of a surface element can be calculated based on the chemical composition of lunar norm minerals (typically lunar olivine, pyroxene, plagioclase and ilmenite (6)) according to the formula:

$$\bar{m} = \bar{N} \bar{g},$$

where \bar{m} is the concentration of the above minerals in a certain sample, \bar{g} is the geochemical composition of the sample; the matrix \bar{N} defines the geochemical composition of the norm minerals.

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