Quantifying Lunar Soil Composition with Partial Least Squares Modeling of Reflectance

L. Li

Department of Geology, Indiana University-Purdue University, IN46202-6815, USA (ll3@iupui.edu)

The surface chemical and mineral composition is important to understanding geological processes on the Moon throughout its evolution history. Optical remote sensing is the most efficient approach to obtaining lunar soil chemical and mineral composition in regional and global scales and this is commonly achieved by relating spectral characteristics of returned lunar soil samples to their constituents.

Partial least squares (PLS) and principal component regression (PCR) were applied to lunar highland and mare soil data characterized by the Lunar Soil Characterization Consortium (LSCC) for prediction of abundance of lunar soil chemistry and minerals. The goal of this study was to develop a tool for predicting the abundance of chemical and mineral constituents of lunar soils from reflectance data. To compensate the effects of nonlinearity due to multiple scattering on estimates of soil constituents, two approaches were separately pursued: (1) converting reflectance into single scattering albedo (SSA) via Hapke's radiative transfer model and assuming a linear relation of the abundance to SSA spectra, and (2) relate the chemical or mineral abundance to the score values of soil reflectance spectra via nonlinear functions. To determine the best model, the number of the optimal components for simultaneously estimating abundances of several soil chemicals or minerals was selected by using a cross validation procedure or a single cut off based spectral variations explained. The results from PLS and PCR were compared. The results from both PLS and PCR were improved by removing nonlinearity effects as compared to those without this compensation. Both PLS and PCR performed equally well in predicting chemical and mineral abundances when a cross validation was applied, but PLS used fewer number of components than PCR did. PCR always resulted in larger errors than PLS did in estimates of chemical and mineral abundances. While both PLS and PCR can be applied to lunar hyperspectral imagery (M3 mission) for compositional predictions, PLS should be preferred over PCR.

Keywords: Lunar soil; Reflectance; Single scattering albedo; multiple scattering; Partial least squares; Principal component regression.