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The Application of Spectral Unmixing Technology for Lunar Regolith*

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Abstract Spectral unmixing technology has been developed to solve mixing pixel problem, the linear mixing model is more successful to this day. But when applied to the lunar regolith, it would have two limitations: the nonlinerity of intimate mixture and the error caused by the lack of endmember spectra. As to the former, simpled multiple scattering model based on Hapke's theory is developed to improve the linearity of intimate mixture and reduce computational complexity; as to the latter, Modified Linear Mixing Model (MLMM) is advanced to compensate for the error in endmember spectra. The motheds are test by the simulated lunar soils' spectra data gained from the Relab, the experimental result display their good performances.

Keywords Spectral unmixing technology; Lunar regolith; Modified Linear Mixing Model (MLMM); Single Scattering Albedo(SSA)

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0 Introducation

Lunar exploration plan in China has been brought into effect. In order to accomplish the mission which detects useful materials and compositions in lunar surface applying fourier transform imaging spectrometer and x-ray/γ-ray spectrometer, spectral unmixing technology[1] was developed for mixing pixels problem caused by low spatial resolution.

Spectral unmixing technology is a hot topic around the world, and many methods and models have been developed for it, which can be grouped under two heads: areal (or "checkerboard") mixing and intimate (or "salt-and-pepper")[2,3] mixing of endmember materials according to the spectral mixture systematics. The former assumed that the reflectance spectrum of a mixture is a linear combination of the EndMember Spectrum (EMS)[2~4], while the later is well known to be a nonlinear problem[2].

For the lunar regolith, because of Space weathering[5~7] such as micrometeorite bombardment, solar wind particle impact, flare or cosmic ray irradiation, or impact melt implantation from larger events, it should be thought of as intimate mixture of endmember materials[1,2,4]. So the non-linear mixing model more accurately predicts abundances for the Moon's surface and is more appropriate for most lunar science questions. While to the date there are many difficults in solution of the non-linear problem, and the model is too complex. According to Hapke's theory[5,7~9], the mixing system are predicted to be linear if the reflectance spectra are converted to single scattering albedo[2,7~9].

1 Conversion reflectance spectrum to Single Scattering Albedo (SSA)

Multiple scattering models[9] can provide approximate solutions to the conversion, through which the reflectance spectrum could be converted to the SSA, and the problem would be linearized[2]. One such model is the semiempirical Hapke's model. Applications of the Hapke's model to quantitative analysis of laboratory mineral intimate mixtures give abundances estimates better than 10% if an estimate of the particle sizes of the respective mixture's components are known[6,9].

1.1 Hapke's theory

Hapke (1981) derived a model for dimensionless particles which has principally been applied to soil data. The model was

$$\rho(\theta_i,\theta_v,\varphi)=\frac{\omega}{4}\frac{1}{\mu_v+\mu_i}\{[1+B(\xi)]P(g,\xi)+H(\mu_i,\omega)H(\mu_v,\omega)-1\} \qquad (1)$$

where θ_i is the angle of incident light, θ_v is the angle of emergent light, φ is the phase angle, ω is the average particle single scattering albedo, and μ_0 is cosine of incidence θ_i, θ_v is cosine of emittance so

$$\mu_i=\cos\theta_i \quad \mu_v=\cos\theta_v$$

$B(\xi)$ is a backscattering function that accounts for the hotspot effect

$$B(\xi)=\frac{B_0}{1+\left(\frac{1}{h}\right)\tan\left(\frac{\xi}{2}\right)} \qquad (2)$$

where h is the width of the hot spot, ξ is the

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angle between the sun and view vectors. B_0 is the magnitude or amplitude of the hotspot

$$B_0=\frac{S(0)}{\omega p(0,\xi)} \tag{3}$$

where $S(0)$ defines the magnitude of the "hotspot".

$P(g,\xi)$ is the phase function for the particle collection with asymmetry g

$$P(g,\xi)=\frac{1-g^2}{[1+g^2-2g\cos(\pi-\xi)]^{1.5}} \tag{4}$$

$H(x,\omega)$ is a function to account for multiple scattering

$$H(x,\omega)=\frac{1+2x}{1+2x\sqrt{(1-\omega)}} \tag{5}$$

Where x is taken place of by the μ_i and μ_v in the equation (1).

1.2 Simpled formula

Hapke's model has too many parameters to operate in numerical computing. But the equations could be simplied by the following assumption

1) By photometric normalization[6,7], the data could be normalized to an $i=30°$ and $e=0°$ observation geometry. Then $\mu_i=0.5$, $\mu_v=1$ and $\xi=30°$.

2) For the dark material, and the light materials are less than 75 μm, the backscattering effect can be negligible[7]. So $B(\xi)$ can be taken as 0 for lunar regolith.

3) The particles on the surface of the lunar regolith are assumed to be larger than the wavelength of light and thus the single particle phase function $P(g,\xi)$ could be equal to 1[6,7,9].

Then

$$\rho(\theta_i,\theta_v,\varphi)=\frac{\omega}{4}\ \frac{1}{\mu_v+\mu_i}\{H(\mu_i,\omega)H(\mu_v,\omega)\}=$$
$$\frac{\omega}{4}\cdot\frac{1}{0.5+1}\{\frac{2}{1+\sqrt{1-\omega}}\cdot\frac{3}{1+2\sqrt{1-\omega}}\} \tag{6}$$

And get the resolution of ω as follow

$$\omega=1-\left(\frac{1-\boldsymbol{R}}{1+2\boldsymbol{R}}\right)^2 \tag{7}$$

where $\boldsymbol{R}=\rho(\theta_i,\theta_v,\varphi)$ is reflectance spectrum we get.

While Ronald G. Resmini[9] get ω as follow.

$$\omega=1-$$
$$\left(\frac{[(\mu_i+\mu_v)^2\boldsymbol{R}^2+(1+4\mu_v\mu_i\boldsymbol{R})(1-\boldsymbol{R})]^{0.5}-(\mu_v+\mu_i)\boldsymbol{R}}{1+4\mu_v\mu_i\boldsymbol{R}}\right)^2 \tag{8}$$

where $\boldsymbol{R}$ is the same to the equation of (7).

2 Linear mixing model

2.1 Traditional Linear Mixing Model (TLMM)

Assume there are c types of ground covers and n spectral bands at hand. In general, assuming $n \geqslant c$ to meet the condition of identifiability, a column vector $x=[x_l,\cdots,x_n]'$ is used to denote the spectrum of mixed ground covers in a pixel which have n spectral bands, and a column vector $f=[f_l,\cdots,f_c]'$ is used to denote the proportions of area within each pixel occupied by each of the c types of ground covers. Thus, the model can be scribed as follow

$$\boldsymbol{Mf}=\boldsymbol{x}+\boldsymbol{e} \tag{9}$$

where each column of $\boldsymbol{M}$ is the EMS corresponding to a specific ground cover class; $\boldsymbol{e}$ is an observation error vector representing deviation from the ideal spectral feature vector due to measurement error and error incurred during transmission of the image data from the sensor to the database.

Others, error vector $\boldsymbol{e}$ subject to the following conditions

$\|\boldsymbol{e}\|^2$ is minimized

So the spectral unmixing problem can be figured out by restriction least-squares (RLS) method[3,10].

2.2 Modified Linear Mixing Model (MLMM)

TLMM gets good result when EMS are known beforehand. When it is applied to the moon's surface, there would be another limitation brought by the lack of EMS of lunar materials.

Of course, this limitation can be solved by many methods[3]. One of the most widely used approaches is to find substitute with the purest spectra from the current data cube through some automatic endmember extraction motheds[12,13]. But the EMS by the means mentioned above are noised as well as the Mixing Spectrum (MS), which would cause serious error applying TLMM directly. Thus MLMM is adopted, described by the equations

$$(\boldsymbol{M}+\boldsymbol{E})f=x+e \tag{10}$$

where $\boldsymbol{M}$ $\boldsymbol{f}$ $\boldsymbol{x}$ $\boldsymbol{e}$ are the same to the equation of (9). Difference from TLMM, the noise matrix $\boldsymbol{E}$ is added to endmembers matrix $\boldsymbol{M}$, and error matrix subject to the conditions that $\|\boldsymbol{E}\mid\boldsymbol{e}\|^2$ is minimized. And the issue could be thought of as a total restriction least-squares (TRLS) problem[3,11]. According to the application, the problem can be simpled, which has been described detailedly in the paper[3].

3 Experimental result

3.1 Data acquisition

On the lunar surface, lunar soil is the most ubiquitous. So the study of the regolith are concentrated in lunar soil composed by particulates.

Here, the particulates data are obtained from the " RELAB Public Spectroscopy Database ". Those samples are made by Johnson Space Center to analysis the spectral characteristic of the lunar soil. All data are measured in the same condition, detailed information of the data is shown in Table . 1 and Table. 2.

Table. 1 The detailed information of the MS

MS	Data name	EM Proportion/(%)			Size/μm	Measure	Spectrometer	SourceAngle	DetectAngle
		Olv	Opx	Anorth	Min/Max	Date		/(°)	/(°)
XC3	XT-CMP-033	66.7	16.7	16.7	45/75	17-Jun-91	BD-VNIR	30	0
XC4	XT-CMP-034	16.7	66.7	16.7	45/75	17-Jun-91	BD-VNIR	30	0
XC5	XT-CMP-035	16.7	16.7	66.7	45/75	17-Jun-91	BD-VNIR	30	0
XC6	XT-CMP-036	33.3	33.3	33.3	45/75	17-Jun-91	BD-VNIR	30	0
XC7	XT-CMP-037	16.7	41.7	41.7	45/75	17-Jun-91	BD-VNIR	30	0
XC8	XT-CMP-038	41.7	16.7	41.7	45/75	17-Jun-91	BD-VNIR	30	0
XC9	XT-CMP-039	41.7	41.7	16.7	45/75	17-Jun-91	BD-VNIR	30	0

Table. 2 The detailed information of the MS

EMS	Data name	Mineral Name	Size/μm Min/Max	Measure Date	Spectrometer	SourceAngle /(°)	DetectAngle /(°)
Olv	PO-CMP-081-C	Olivine	45/75	17-Jun-91	BD-VNIR	30	0
Opx	PE-CMP-041-C	Orthopyroxene	45/75	17-Jun-91	BD-VNIR	30	0
Anorth	PA-CMP-060-C	Anorthite	45/75	06-Jun-91	BD-VNIR	30	0

3.2 Process step

Because of the limitation of the experimental condition, only the numerial computing with the data was operated and compared with information coming from Relab. The processes being followed:

1) MS: are taken from the spectra of lunar soils simulated by intimate mixing minerals. The detailed information is given in Table. 1.

EMS: are taken from the spectra of simulated samples' compositions displayed in Table. 2.

2) Reflectance Spectrum + TLMM Result: because of the existence of systematic error, MS has errors in itself, so MS is regarded as the "$\boldsymbol{x}+\boldsymbol{e}$" , and EMS as the "$\boldsymbol{M}$" of equation (9), and the problem is solved by RLS.

3) SSA1+MLMM Result: MS and EMS are thought as REFLECTANCE SPECTRUM, converted to SSA by the equation(7) at first, then regard MS as the "$\boldsymbol{x}+\boldsymbol{e}$" , and EMS as the "$\boldsymbol{M}+\boldsymbol{E}$" of equation (10), and solved by TRLS.

4) SSA2+MLMM Result: the same as step 3) except applying equation (8) to convert REFLECTANCE SPECTRUM to SSA.

3.3 Result

In Table. 3, results of three methods are displayed, besides, the Root-Mean-Square (RMS) error are computed according to the real proportions shown in Table. 1.

Table. 3 Comparison of result and error of three methods

MS	Reflectance Spectrum+TLMM result	RMS	SSA1+MLMM Result	RMS	SSA2+MLMM Result	RMS
XC3	54.9% 39.7% 5.4%	0.278	66.3% 16.9% 16.9%	0.012	66.5% 14.1% 19.3%	0.039
XC4	12.1% 83.6% 4.3%	0.215	16.5% 67.2% 16.4%	0.006	16.6% 63.9% 19.5%	0.040
XC5	20.9% 38.0% 41.1%	0.336	15.2% 15.2% 69.6%	0.036	13.8% 12.2% 74.1%	0.091
XC6	28.0% 58.8% 13.2%	0.329	32.5% 33.3% 34.2%	0.012	31.9% 29.6% 38.5%	0.065
XC7	15.0% 66.0% 19.1%	0.332	16.4% 40.7% 42.9%	0.016	15.5% 36.5%48.0%	0.083
XC8	40.4% 38.7% 20.9%	0.303	39.4% 15.9% 44.6%	0.038	38.0% 13.1% 49.0%	0.089
XC9	31.3% 65.8% 2.9%	0.297	41.9% 42.3% 15.8%	0.011	42.0% 38.9% 19.1%	0.037

4 Conclusion

From Table. 3, the multiple scattering model solves the linearization of intimate mixture spectral unmixing nonlinear problem, and gives abundances estimates better than 10%. The experiential formula derived form the model here gives a better result. In addition, the MLMM is adopted to eliminate the limitation of lack of pure endmember spectrum. It is demonstrated that the "SSA1 + MLMM" could resolve perfectly the non-linear problem of the intimate material mixing spectrum, which provide a good method for the study of compositions' abundance of lunar regolith.

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用于月球风化层遥感的光谱分离技术研究

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摘　要　为了解决混合像元问题,发展了一门新的技术——光谱分离技术,线形混合模型是目前应用最成功的方法,但是当应用到月球风化层遥感时,其存在两个内在的缺陷:一是由于充分混合引起的非线性,二是纯光谱的不“纯”性.对于第一个缺陷,从Hapke理论出发,充分考虑了数据的特点,大大简化多重散射模型来提高充分混合的线形性,同时降低了原模型计算的复杂度;对于后一个问题,提出用修正线形混合模型来弥补“纯”光谱中的误差.该方法通过Relab数据库中的模拟月壤的光谱数据进行了验证,试验结果表明,这种方法具有很好的性能.

关键词　光谱分离技术;月球风化层;修正的线形混合模型;单次反照率

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