

Calibration for the Estimation of Weight Fractions using non-linear Spectral Unmixing. N. Mengewein, A. Grumpe, D. Rommel and C. Wöhler Image Analysis Group, TU Dortmund, 44227 Dortmund, Germany ({natascha.mengewein | arne.grumpe | daniela.rommel}@tu-dortmund.de).

Introduction: Spectral unmixing has been applied to a variety of scientific scenarios, e.g. remotely sensed spectral data of the lunar surface [e.g. 1, 2, 3]. Commonly, the spectral reflectance is modelled as a linear combination of base spectra, i.e. spectral endmembers.

According to [4, p. 283ff.] the linear combination is invalid for intimate mixtures, e.g. mixtures where the light is scattered at particles of different material before it reaches the sensor. The resulting non-linear unmixing scenario, however, may be linearised if the single-scattering albedo of the Hapke model [5] is unmixed.

The resulting mixing coefficients are sometimes interpreted as weight fractions. This interpretation, however, is invalid as we will discuss in this study. We furthermore present an approach to quantify the weight and the mol fractions of the endmember minerals.

Mixture model: According to [4, p. 283], the single-scattering albedo of the mixture is a weighted sum of the endmember single-scattering albedos, i.e.

$$w_{\text{mix}} = \frac{\sum_i N_i \sigma_i Q_{e_i} w_i}{\sum_i N_i \sigma_i Q_{e_i}}$$

where w denotes the single-scattering albedo, N_i , σ_i and Q_{e_i} are the amount of particles, the average particle cross-section and the average extinction coefficient, literally the average darkness of a particle, of the i -th endmember, respectively. In this study we assume a constant grain size for all particles and thus eliminate σ_i . Notably, the denominator acts as a normalisation factor. We collect the total amount of particles N_i and the extinction coefficient Q_{e_1} of the first endmember from both sums. Consequently, the amount of particles is conveniently expressed by the mol fractions n_i of the endmembers and the weights depend solely on the ratio $q_i = Q_{e_i}/Q_{e_1}$ of the endmember extinction coefficients:

$$w_{\text{mix}} = \frac{\sum_i n_i q_i w_i}{\sum_i n_i q_i}$$

The absolute value of the extinction coefficient is not important and consequently, we set the extinction coefficient of the darkest mineral, i.e. ilmenite, to a value of one and estimate the ratio of each endmember with respect to the darkest one.

Dataset and calibration procedure: In this study we use the endmember catalog of [6] comprised of an ilmenite, an olivine, a diallagite, an eulite, an augite, an enstatite and two different labradorites. Initially, a

smoothing spline [7] is applied to all measured reflectance spectra. Single scattering albedos are then obtained by a minimisation of the squared difference between the measured and the modeled reflectance spectra. The remaining parameters of the Hapke model [5] are adopted from [8]. The wavelength range is limited from 750 to 1750 nm due to low signal to noise ratios in the upper and lower wavelength ranges.

In order to estimate the extinction coefficient ratios, we create a mixture of each endmember with ilmenite using a weight fraction of 50 wt%, respectively. We compute the mixing coefficients of the single-scattering albedos using a linear least-squares optimisation with a sum-to-one constraint, i.e. the sum of the coefficients is enforced to a value of one. We then convert the weight fractions to mol fractions and solve the mixing equation for the unknown extinction coefficient ratio. The molar mass of each endmember, respectively, and the resulting extinction coefficient ratios are shown in Tab. 1. The extinction coefficient ratios are in very good agreement with the observed spectral brightness, i.e. the bright minerals enstatite and labradorite show small values.

Mineral	Molar mass [g/mol]	Q_{e_i}/Q_{e_1} Ratio
Ilmenite	54.576	1.0000
Enstatite	28.784	0.2803
Olivine	27.641	0.3307
Labradorite 1	29.239	0.0242
Labradorite 2	29.374	0.1684
Augite	31.234	0.4678
Diallagite	30.901	0.4357
Eulite	39.021	0.4762

Table 1 Molar mass and extinction coefficient ratios of the endmembers

Evaluation: The evaluation is based on mixtures that were not included in the calibration: First, a mixture of ilmenite and diallagite with different weight fractions. Second, a mixture of enstatite and labradorite 2 which are an extreme case and on the opposite end of the brightness scale compared to ilmenite. Third, a mixture of augite, enstatite and labradorite 2. In this study we are interested in the accuracy of the method and thus assume the endmembers of the mixture to be known a-priori. The reflectance spectra of the mixtures and their modelled counterparts are shown in Fig. 1.

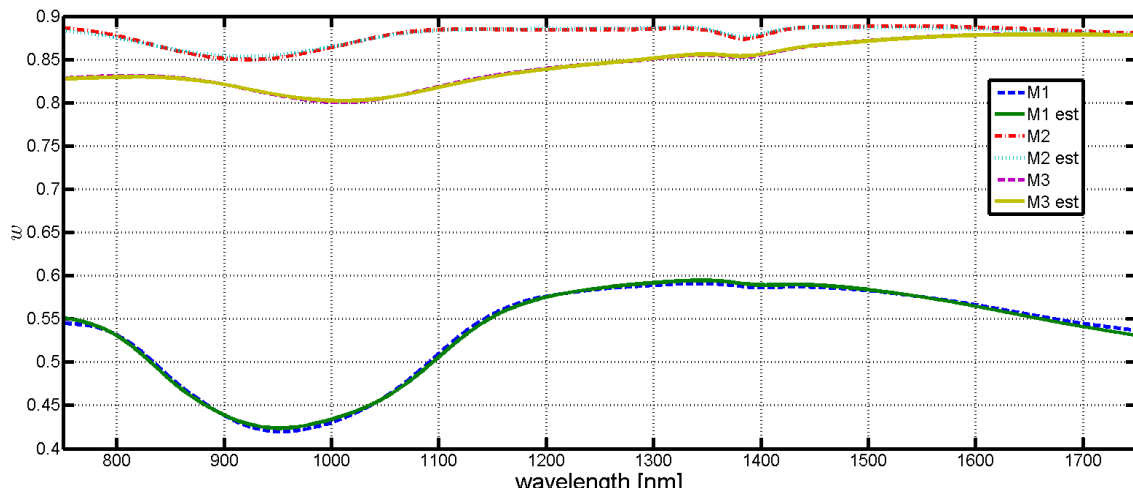


Figure 1 Single scattering albedo spectra of the mixtures. The dark M1 mixtures is comprised of ilmenite and diallagite. The enstatite labradorite 2 mixture (M2) shows the largest single scattering albedo values. The triple mixture M3 contains augite, enstatite and labradorite 2. The linear mixtures of the single scattering albedos of the endmembers are denoted by M1 est, M2 est and M3 est, respectively. All artificial mixtures are in very good agreement with physical mixtures.

The mixing coefficients of the c_i Hapke model are again computed using the linear least-squares optimisation with a sum-to-one constraint. From the ratio

$$\frac{c_i}{c_j} = \frac{n_i q_i}{n_j q_j}$$

of the i -th and j -th coefficient and the constraint that all fractions sum to one follows that the mol fraction of the i -th endmember amounts to

$$n_i = \frac{1}{\sum_j \frac{c_j q_i}{c_i q_j}}$$

The obtained mol fractions are converted to weight fractions using the molar masses from Tab. 1.

Tab. 2 summarises the weight fractions, the mixing coefficients and the estimated weight fractions. In all cases the mixing coefficients show deviations from the true weight fractions. This is especially pronounced in the presence of ilmenite. The estimated weight fractions are in good agreement with the true weight fractions. However, there is a larger residual inaccuracy for the brighter mixtures that do not contain ilmenite.

Mixture	Mineral	wt% (true)	c_i	wt% (est)
M1	Ilmenite	20	0.46	17
	Diallagite	80	0.54	83
M2	Entatite	70	0.86	79
	Labradorite 2	30	0.14	21
M3	Augite	20	0.21	10
	Entstatite	30	0.43	38
	Labradorite 2	50	0.36	52

Table 2 Summary of the mixtures. The true and estimated wt% values are in good agreement while the mixing coefficients show larger inaccuracies if ilmenite is present.

Conclusion: In this study we propose a new calibration procedure for spectral unmixing algorithms using the Hapke model. The computed extinction coefficient ratios are applied to three distinct mixtures and show promising results. The estimated weight fractions are close to the true weight fractions and thus, in contrast to the mixing coefficients, have a physical interpretation. Future work will contain more calibration measurements and a further assessment of the accuracy on a wider range of mixtures.

References: [1] Mustard, J. F. and Pieters, C. (1989) *Journal of Geophysical Research*, 94(B10), 13619-13634. [2] Keshava, N. and Mustard, J. F. (2002) *IEEE Signal Processing Magazine*, 44-57. [3] Dhingra D. et al. (2011), *Lunar and Planetary Science Conference*, abstract 2431. [4] Hapke, B. (2012) *Theory of Reflectance and Emittance Spectroscopy* 2nd Edition, Cambridge University Press. [5] Hapke, B. (2002) *Icarus*, 157, 523-534. [6] Rommel, D. et al. (2014) *Proc. Europ. Lunar Symp.*, 95-96. [7] Marsland, S. (2009) *Machine Learning: An Algorithmic Perspective*, CRC Press. [8] Warell, J. (2004) *Icarus* 167, 271-286.