

SPECTRAL MODELING OF PLANETARY ANALOGUES, PRELIMINARY RESULTS. L. Pompilio¹, G. Pedrazzi², M. A. Craig³, M. Sgavetti¹, and E. A. Cloutis³, ¹Department of Earth Sciences, University of Parma, V. Usberti 157/A 43100 Parma, Italy; loredana.pompilio@unipr.it, ²Department of Public Health, University of Parma, V. Volturmo 43100 parma, Italy, ³Department of Geography, University of Winnipeg, 515 Portage Ave., Winnipeg, MB, Canada R3B 2E9.

Introduction: A major problem in mapping spectroscopy is to identify the composition of the mineral mixtures occurring at the planet surface, which could have particulate texture and solid surface appearance as well. The fitting techniques so far applied to model reflectance spectra of minerals and mixtures ground on the superposition of Gaussian-like absorption bands [1, 2, 3] or modified Gaussians [4, 5, 6, 7] to some kind of continuum. Nevertheless, although the absorption process can be fairly assumed as a normal distribution of light path lengths around a central wavelength [4], the absorption band shape can deviate from Gaussian-like due to a number of effects. Impurities, accessory minerals, spectrally neutral phases, glass and saturation phenomena [8] all concur to distort the Gaussian-like shape of absorption bands and are very common in rock spectroscopy.

Here we test a new decomposition algorithm (Exponential Gaussian Optimization, EGO) able to model band saturation, overlapping absorptions, effects due to sample impurities and neutral substances better than the most common decomposition techniques so far used in the VNIR range. The main objectives of our efforts are to: 1) test and validate a fitting model which includes band saturation and asymmetry effects; 2) parametrically define a threshold between symmetric and asymmetric Gaussian-like profiles; 3) build a basic approach for modeling the complex spectra of rocks.

Experimental approach: We use an increasing-complexity approach aimed at modeling the nature of spectral complexity. Therefore, we evaluate the performances and reliability of both MGM (Modified Gaussian Model [4]) and EGO fitting techniques. In order to increase complexity and evaluate the effects of different variables on spectra, we use the following materials: a) Orthopyroxenes PYX023 (6.36% Fe²⁺ as FeO) and PYX032 (23.65% Fe²⁺ as FeO) crushed and dry sieved to obtain 5 different grain size splits (<45, 45-90, 90-250, 250-500 and 500-1000 μm); b) Orthopyroxenes PYX023 and PYX032 (45-90 μm) mixed with a bright neutral material (BaSO₄); c) Orthopyroxene PYX032 mixed with clinopyroxene PYX017 with different average grain size (<45 and 90-180 μm).

The measurements have been acquired relative to spectralon with an Analytical Spectral Device (ASD) FieldSpec Pro HR field portable spectrophotometer at

the University of Winnipeg. Spectral range investigated is between 0.35 and 2.50 μm; i=30°, e=0°; spectral resolution is fixed at 2-7 nm with a 1 nm spectral sampling interval; high STN ratio results by averaging about 1000 measurements.

In order to better constrain the processes causing absorption of VNIR light, pyroxene band I (near 1.0 μm) has been isolated and fitted using up to two EGOs and alternatively one or more parameters locked. The results of modeling have been statistically evaluated and compared using the standard error of the estimate, coefficient of determination R², adjusted coefficient of determination R²_{adj}, Akaike's Information Criterion and correlation matrixes.

Mathematical approach: EGO takes into account non-Gaussianity of spectral absorptions due to the superposition of multiple components and saturation effects. Therefore, it is able to model peak asymmetry and flattening (fig. 1). When saturation effects and the occurrence of small amounts of different materials become spectrally relevant, the band shape is no longer a Gaussian and the fitting process becomes a very complicated task. To solve this trouble, as a first approximation, we start modeling via a slight modification of the basic Gaussian function that implies to change the Gaussian profile and symmetry and preserve some relevant parameters. The EGO profile moves from these considerations. It is summarized in equation below:

$$EGO(\lambda) = -\frac{s}{1 - e^{-\frac{1}{2}t}} \left\{ 1 - e^{-\frac{1}{2} \left[te^{-\frac{1}{2} \left(\frac{\lambda - \mu}{\sigma + k(\lambda - \mu)} \right)^2} \right]} \right\}$$

where s , μ and σ are band intensity, center and width, respectively. t allows band flattening to be modeled and k accounts for band asymmetry (fig. 1). It can be demonstrated that the EGO profile becomes a Gaussian by keeping $k = 0$ and t very close to 0.

Results and discussion: Based on statistics, we found that EGO generally returns *best fit* models. This is not surprising in that EGOs include 2 more parameters than Gaussians and this justifies the better performances. Now the question is: are these additional parameters related to any spectral effect or simply mathematical artifacts?

Pyroxene separates. Band flattening is evident in spectra as the average grain size of the powdered split

increases. Data confirm that the width is approximately constant for PYX023, whereas a slight increase (~40 nm) is observed for the more Fe-rich PYX032 with average grain size (fig.2). Band depths reaches a maximum between 45-90 and 90-250 μm average size for PYX032 and PYX023, respectively and then decrease for larger grain sizes, as already observed [9 and references therein]. Similar pattern is followed by t ; k slightly decreases when grain size increases.

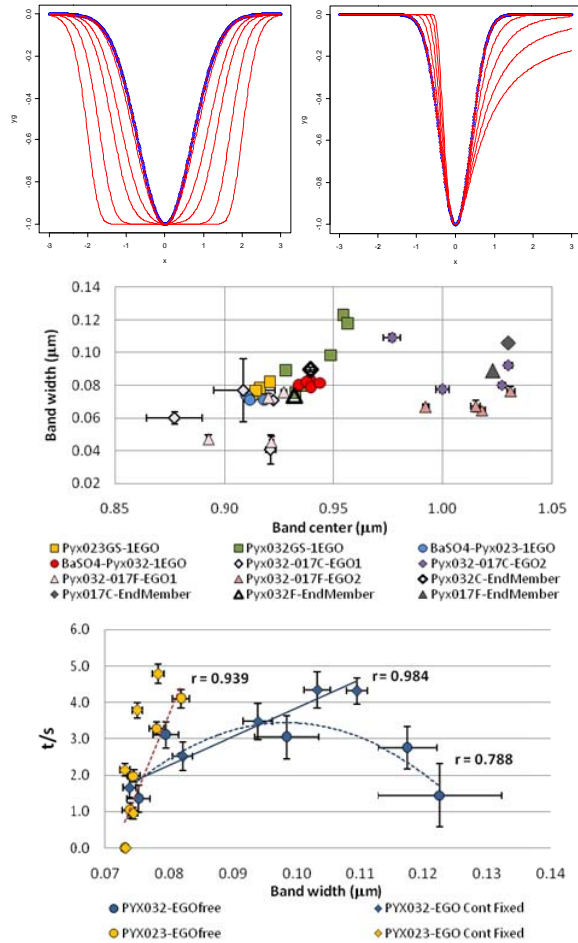
Pyroxene/BaSO₄ mixtures. Statistically, EGO performs better than 1 or 2 modified Gaussians. Band widths remain constant for each mixture. Band flattening at high amounts of the neutral is only apparent. Band depth decreases for increasing amounts of BaSO₄ regularly, but not linearly, as expected [10]. k does not show perceptible variations and is very small.

Ortho/Clinopyroxene mixtures. Models with 2 EGOs return the best statistics. Band widths and centers shift toward lower values as compared to the end-members and the uncertainty increases (fig. 2). k is quite high compared to previous models and shows approximately symmetric variations around the single EGO models, in opposite directions. t is around 0 in the finer mixture models and for clinopyroxene band in the coarser. Band depths of overlapping EGOs show opposite behavior, but they cannot be unambiguously related to relative concentrations in the mixtures.

These results show that: 1) Band saturation, as modeled by EGO, produces band broadening (much more evident for more Fe-rich PYX032) and t/s ratio increase (fig. 3). Linear trends result for PYX023 and PYX032 models with free parameters and continua tangent to the band ends, respectively. When all the parameters are free to change, deviation from linearity occurs in the more Fe-rich PYX032 models, thus suggesting some caution in the fitting procedure. 2) Dilution with a neutral bright material (BaSO₄) preserves the absorption band shape, thus marking a completely different effect from saturation. 3) Overlapping bands develop non-Gaussian profiles which are very hard to model. k has shown to be suitable for modeling band asymmetry due to impurities or accessory phases with as low concentrations as to be detectable. Nevertheless, it loses magnitude as the band broaden. It suggests there could be a threshold value between EGO and additional Gaussian curves.

Conclusion: Gaussian and MGM decomposition techniques have been extensively used so far to model spectra of mafic minerals, mixtures and unknown data from remote. EGO algorithm has the potential to become a very powerful tool for absorption band modeling, both electronic and vibrational. In addition, the open source software policy adopted for code develop-

ing and the opportunity to switch to a Gaussian profile when saturation and asymmetry are negligible effects makes it very versatile and fascinating. We strongly believe that EGO could be employed as spectral modeling tool after proper validation using high purity samples, dark neutrals, glass and rocks as targets.



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Figure 1: EGO simulations (red line). Left) s , μ , and σ are: -1, 0, 0.7, respectively, $k = 0$; from the Gaussian (blue dots) t is: 1, 5, 10, 30, 100. Right) s , μ , and σ are: -1, 0, 0.4, respectively, $t = 0.001$; from the Gaussian k is: 0.001, 0.01, 0.1, 0.2, 0.3, 0.4. **Figures 2-3:** Some fitting results. Confidence limits at 0.05 level are reported.

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