DECONVOLUTION OF REFLECTANCE SPECTRA USING NONLINEAR LEAST SQUARES CURVE FITTING: APPLICATION TO MARTIAN METEORITES. Mario Parente[1] and Janice L. Bishop[2], [1]Stanford University, Packard Engineering Building, 350 Serra Mall, Stanford CA, 94305. cyberey@stanford.edu, [2]SETI Institute / NASA-Ames Research Center, Mountain View, CA 94043.

Introduction: We present a spectral deconvolution technique and model based on the description of electronic transition absorption bands in continuum-removed spectra. The model differs from the standard gaussian modeling in the way the continuum is removed. An improved nonlinear curve fitting algorithm is used to fit the model to the data. The approach represents also an alternative to the MGM model [1] and results in suitable deconvolution of the highly overlapping bands in martian meteorites.

Samples: Two meteorites have been selected for study here: Allan Hills 84001 and Elephant Moraine 79001. Allan Hills 84001 (ALH84001), is primarily orthopyroxene [e.g 2]. Minor olivine is also present [3]. Reflectance spectra of this meteorite clearly show the presence of orthopyroxene [4]. Elephant Moraine 79001 (EETA 79001) is a unique shergottite containing two different igneous lithologies (labeled A and B). Lithology B contains both low-Ca pyroxene (pigeonite) and high-Ca pyroxene (augite) with some maskelynite [5]. Lithology A is made up of a basaltic host similar to lithology B containing crystals of olivine and orthopyroxene [e.g. 6].

Development of the Algorithm: Spectral deconvolution is a particular type of nonlinear curve fitting problem in which we try to fit a nonlinear model to the data. gaussian [e.g. 7, 8] or modified gaussian [1] models have been used for spectral deconvolution. We chose to model the electronic transition absorption bands with gaussians and we fitted a linear combination of those to a continuum – removed version of the original spectra.

Continuum Removal: One technique we propose removes the complete upper convex hull from the spectra. We use this approach when we do not want to treat absorption bands individually because some of the minerals of interest show features that are considered diagnostic if taken in pairs (e.g. pyroxene).

The continuum removal is performed by subtraction in log reflectance, unlike a similar technique in [7] and [8] in which the operation is carried out by division in reflectance. We choose the log domain because we find that in reflectance the effect of artifacts produced by the removal process is more evident.

In cases where the continuum removal procedure creates spurious bands in the spectrum (for the high convexity of the convex hull) we make use of an alternative approach in which the user is free to choose the anchor points (the tangential points) on the spectral curve and then the algorithm fits user defined functions between these points.

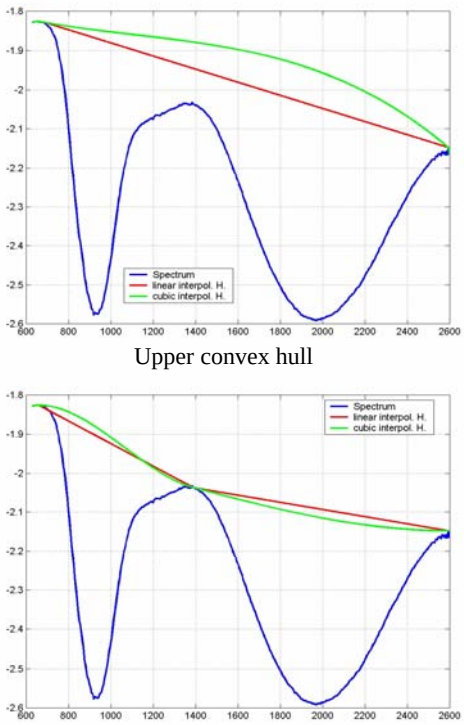

Figure 1: Example of the two types of continuum removal for the spectrum of ALH84001.

Figure 1 represents the two methods for continuum removal explained above: the red curve is a linear function fitted to the anchor points (of the convex hull or chosen by the user) of the spectrum, while the green curve is a higher order (smoother) fitting function.

The usual alternative to the continuum removal is to model the continuum as a straight line in the wavenumber scale and to fit it along with the gaussian bands as in [1]. In such models the bands are added to the continuum in the log reflectance. We claim that this practice is equivalent to superimposing a tangent continuum to them and that the use of gaussians in the wavelength domain for our wavelength range is justified [9].

Fitting Procedure: We use two algorithms to perform nonlinear least square curve fitting: the popular Levenberg-Marquardt algorithm [10], [11] and the Trust Region interior-reflective Newton method [12]. These algorithms are explained in somewhat more detail in [9]. Our formulation chooses between the two depending on the size of the problem.

Results and Discussion: The model enabled detection of individual bands due to electronic transitions that are typically difficult to resolve with other methods because they overlap. The evidence of pyroxene is inferred by identifying the diagnostic absorption bands around 1000 nm and 2000 nm. The algorithm also provides a simple way to infer abundances of pyroxene endmembers in a sample.

The ratio of the relative areas of the low-Ca and high-Ca pyroxene bands in the 1000 nm region is similar to the same quantity in the 2000 nm region. It has been suggested that those quantities are proportional to the ratio of abundances of low-Ca and high-Ca pyroxene in the mixture [13].

An example of the deconvolution results for a spectrum of a particulate sample of lithology B of the EETA 79001 meteorite are shown in Figure 2. We can clearly see the two pyroxene bands in the 1 and 2 μm regions and an additional band near 1.15 μm. The results obtained in terms of abundances, band centers and areas for the two pyroxenes in this sample are in accordance with previous studies [5, 14].

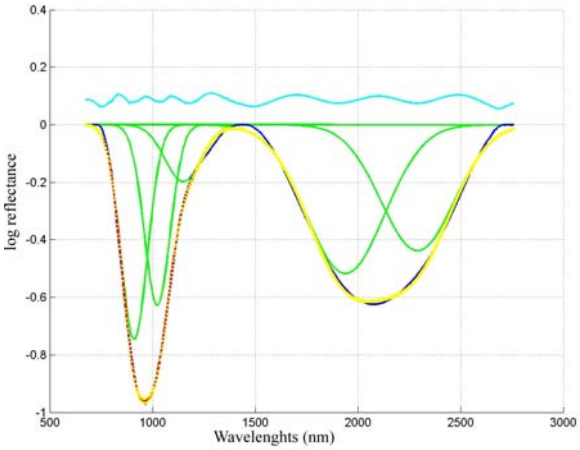

Figure 2: deconvolution result for the continuum-removed EETA 79001 lith. B powder; red: spectrum, green: gaussian bands, blue: fit, yellow: confidence level on fit, light blue: rms error.

The evidence of olivine could be inferred indirectly by evaluating the postion of the band near 1.2 μm. This measure is justified by experimental comparison of meteorite spectra with and without olivine content. Although basaltic glass and some feldspars also exhibit electronic absorptions in the 1 μm region and can contribute to a minor shoulder superimposed around 1.1-1.2 μm to the usual pyroxene mixture spectrum, their effect is usually very mild [e.g.15,16]. The effect of olivine on creating such a shoulder on pyroxene spectra is somewhat more pronounced [16] and tends to shift the position of the 3rd band towards 1.25 μm.

The deconvolution results of the spectrum of a particulate sample of EETA 79001, lithology A, are shown in Figure 3. Here the 3rd band is shifted toward longer wavelengths which is consistent with the presence of olivine.

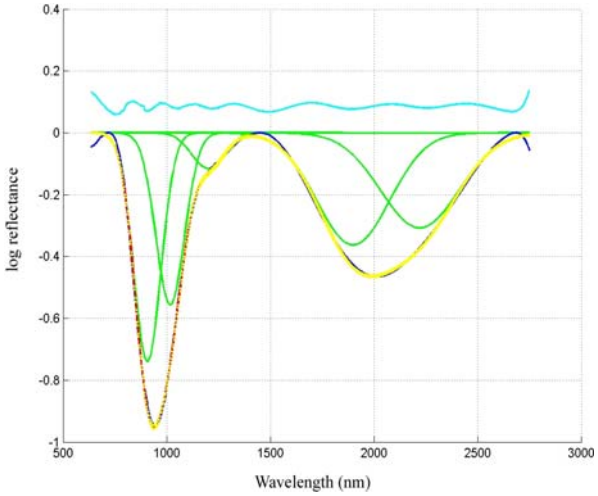

Figure 3: deconvolution result for the continuum-removed EETA lith. A powder .

Applications to Mars: MGM absorption band modeling has been employed for identification of pyroxene and olivine in OMEGA data of Mars [17]. We are in the process of applying our gaussian deconvolution model to samples containing both mafic minerals and alteration minerals and plan to use this in the future as well for analysis of OMEGA and CRISM spectra. Martian meteorites are an ideal set of samples for testing this new spectral analysis tool because the mineralogy of these samples has been well characterized.

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