Absorption Band Modeling in Reflectance Spectra: Availability of the Modified Gaussian Model. J. M. Sunshine[1] (sunshinej@saic.com), C. M. Pieters[2] (pieters@mare.geo.brown.edu), S. F. Pratt[2] and K. S. McNaron-Brown[2], [1]Advanced Technology Applications Division, Science Applications International Corporation, 4501 Daly Drive, Chantilly, VA 20151, [2]Department of Geological Sciences, Brown University, Providence, RI 02912.

Introduction: The Modified Gaussian Model (MGM), a physically based description of electronic transition absorption bands in spectra, is now more readily available for use by all interested colleagues. In order to facilitate compatibility with as wide a range of computer systems as possible, the MGM code has been translated from FORTRAN and HP graphics language to two different platform independent sets of code written in IDL and MATLAB. All three versions of the MGM code will be available (starting no later than 3/1/99) from the RELAB website maintained by the Brown University's Department of Geological Sciences (*www.planetary.brown.edu*).

The Modified Gaussian Model (MGM): The MGM, originally developed by Sunshine *et al.* [1], is a method for accurately resolving spectra into their physical components, constituent absorption bands. The modeled absorption bands can then be used to infer compositions and amounts of co-existing phases. One of the major strengths of the MGM is that the derived absorption bands are determined directly from measured spectra. Unlike other methods, MGM modeling does not rely on pre-determined assumptions about the spectral constituents, nor does it require the direct use of terrestrial samples or meteorites as spectral analogs. The MGM approach is thus particularly well suited for analysis of remote spectra.

The MGM is a refinement of the Gaussian model used previously by many investigators [e.g. 2-6]. Modified Gaussian distributions, by adhering more closely to the physical processes involved in electronic transition absorptions, are the first accurate mathematical description for the shape of isolated absorption bands [1,7]. Under the MGM spectra are modeled as sums of absorption bands, each represented by a modified Gaussian distribution, superimposed onto baseline curves, or continua. Each absorption is described by three model parameters; a band center, width and strength. Similarly, continua, which are typically modeled as straight lines in energy, are characterized by two additional model parameters, a slope and an offset. It should be noted that unlike other approaches [e.g., 3, 8], under the MGM continua are neither predetermined nor fixed to be tangent to spectra and thus, like the absorption bands, are free to move based on the data. All MGM modeling is carried out in the physically based units of natural log reflectance and energy but, for convenience, is typically displayed as a function of wavelength. Further details of the mathematics of the MGM can be found in Sunshine *et al.* [1] and Sunshine and Pieters [7].

Since the MGM centers around an accurate model of electronic transition absorptions, it is not merely a mathematical description, but rather a physically based model of reflectance spectra. Thus, results derived with the MGM can confidently be used to infer composition. The MGM has been shown to accurately resolve individual absorption bands in laboratory spectra and has been used to quantify variations in absorption bands as a function of composition in the spectra of pyroxene mixtures [7, 9], olivines [10], and actinolites [11]. The MGM has also been successfully used to analyze spectra of the surface of Mars collected with the ISM spectrometer [12, 13]. These studies have provided key compositional links between the surface of Mars and laboratory studies of the SNC meteorites. In addition, the MGM has made it possible to quantitatively estimate the composition of olivine in olivine-rich asteroids [14], to compare spectra of HED meteorites with those of Vesta-like asteroids [15], and to quantify and help interpret minor absorptions in spectra of S-asteroids [16].

Using the MGM: As described by Sunshine *et al.* and Sunshine and Pieters [1, 8], the MGM uses a non-linear least squares inversion based on the stochastic technique of Tarantola and Valette [17]. A startup file is used to begin MGM modeling. This file includes: stopping criteria (a minimum residual error threshold and a minimum change in residual error: typically 0.002 and 1.0E-05, respectively), the number of absorption bands, and initial estimates for all model parameters, including those defining the continuum. In addition, because the MGM uses a stochastic inversion approach, initial uncertainties for each model parameter must also be included (expressed as 95% (two sigma) confidence limits). Two examples of starting model parameters, final model parameters, and plots of MGM results are shown in Figures 1 and 2.

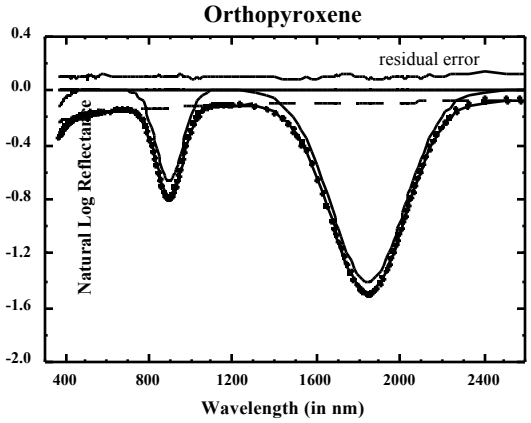
FORTRAN, IDL, and MATLAB Codes: In its original form, the MGM code is written in FORTRAN 77 and uses HP plotter language for graphics. In addition, it exclusively reads and writes spectra in a RELAB internal binary file format. The FORTRAN version of the MGM therefore unfortunately runs only on DEC VMS machines with Tektronix screen emulation, is compatible only with HP printers, and requires that data be in RELAB specific formats. Although the MGM has always been available to any investigators who requested it, these constraints have significantly hindered its use. In an effort to make the MGM more readily useable, the code has been re-written in both IDL (Interactive Data Language by Research Systems, Inc.) and MATLAB (The Mathworks, Inc.). Both the IDL and MATLAB versions input and output simple ASCII files, use built-in capabilities for graphics, and

can be run on numerous computer platforms. We are hopeful that the availability of all three versions will allow the MGM to be used by all interested investigators to support their research needs.

References:

[1] Sunshine, Pieters, and Pratt, *JGR,*, 1990.
[2] Burns, *Am. Mineral.*, 1970.
[3] Clark and Roush, *JGR*, 1984.
[4] Gaffey, *Am. Mineral.*, 1986.
[5] McCord *et al.*, *JGR*, 1981.
[6] Roush and Singer, *JGR*, 1986.
[7] Sunshine and Pieters, *JGR,*, 1993.
[8] Gaffey *et al.*, *Icarus*, 1993.
[9] Sunshine, Pieters, and McFadden, *Icarus*, 1993.
[10] Sunshine and Pieters, *JGR,*, 1998.
[11] Mustard, *Amer. Mineral*, 1992.
[12] Mustard and Sunshine, *Science*, 1995.
[13] Mustard, *et al.*, *JGR*, 1997.
[14] Sunshine *et al.*, *LPSC 29th*, 1998.
[15] Hiroi *et al.*, *Icarus*, 1995.
[16] Hiroi, Vilas, and Sunshine, *Icarus*, 1996.
[17] Tarantola and Valette, *Rev. Geophys.*, 1982.

Fig. 1: MGM fit to a transmission spectrum of an orthopyroxene Crystal [1].



Starting Model Parameters for Orthopyroxene

Continuum (polynomial in energy):
Offset: 0.85 ± 10 Slope: -0.10E-05 ± 0.10E-3

Band	Center	FWHM	Strength
1	333 ± 10000	400 ±	-20. ± 100
2	1000 ± 200	250 ± 400	-1.0 ± 10
3	2000 ± 200	300 ± 400	-2.0 ± 10

Final Model Parameters for Orthopyroxene

Continuum (polynomial in energy):
Offset: 0.94 Slope: -5.57E-06

Band	Center	FWHM	Strength	Log Area
1	333.89	113.52	-0.15	-1.15
2	898.59	147.68	-0.66	-13.96
3	1845.36	416.05	-1.40	-46.18

Current RMS Error = 1.14 % after 8 iterations

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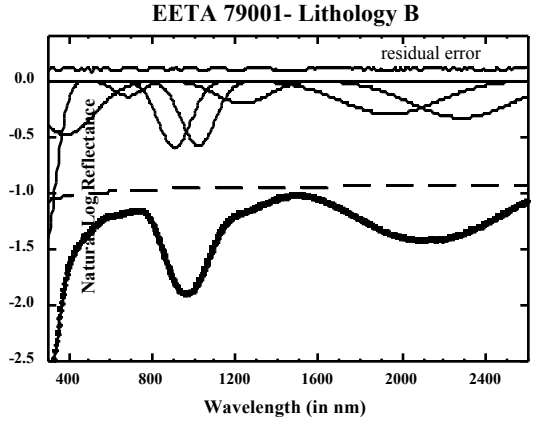
Fig. 2: MGM fit to the spectrum of Lithology B from the Elephant Moraine A79001 shergotty meteorite [3].



Starting Model Parameters for Lithology B

(based on MGM pyroxene mixtures results [2])

Continuum (polynomial in energy):
Offset: 0.47 ± 0.5 Slope: -0.12E-05 ± 0.10E-4

Band	Center	FWHM	Strength
1	284 ± 400	948 ± 600	-1.05 ± 300
2	403 ± 400	328 ± 400	-0.48 ± 100
3	662 ± 200	145 ± 400	-0.10 ± 20
4	908 ± 200	188 ± 200	-0.56± 20
5	1015 ± 200	193 ± 200	-0.51 ± 20
6	1148 ± 200	278 ± 200	-0.68 ± 20
7	1832 ± 300	560 ± 200	-0.53± 20
8	2266 ± 300	564 ± 200	-0.45± 20

Final Model Parameters for 79001 Lithology B

Continuum (polynomial in energy):
Offset: 0.40 Slope: -1.66E-06

Band	Center	FWHM	Strength	Log Area
1	285.54	131.32	-1.46	-16.88
2	387.59	330.91	-0.48	-24.96
3	684.33	162.85	-0.14	-4.85
4	908.94	184.89	-0.60	-23.50
5	1022.02	189.45	-0.58	-23.56
6	1233.79	300.18	-0.21	-13.17
7	1939.83	552.66	-0.30	-35.27
8	2282.63	569.08	-0.33	-36.55

Current RMS Error = 0.51% after 28 iterations