LINEAR UNMIXING OF FINE PARTICULATE MATERIALS: IMPLICATIONS FOR COMPOSITIONAL ANALYSES OF PRIMITIVE ASTEROIDS

V. C. Lowry[1], K. L. Donaldson Hanna[1], H. Campins[1], N. Bowles[2], and V.E. Hamilton[3]

[1]University of Central Florida, Orlando, FL, USA, [2]University of Oxford, Oxford, UK, and [3]Southwest Research Institute, Boulder, CO, USA

Introduction

- Linear least squares (LLS) unmixing of thermal infrared (TIR) spectra is a fast and effective way to spectrally estimate the modal mineral abundances of laboratory samples and remotely-sensed surfaces to within 5% on average.[1]
- This technique has been applied to spectra of whole rocks, coarse particulates, meteorites, and the Martian surface to successfully determine modal abundances.[1, 2, 3]
- Using LLS allows one to deconvolve mixed spectra into areal percentages of each endmember with the underlying assumption that this then corresponds to the volume percentages.[1, 2, 3]
- In this study we investigate the effectiveness of a LLS unmixing approach to estimate mineral abundances for samples dominated by fine particulates (< 38 μm).
- **Results from this investigation have implications for the interpretation of TIR spectral observations of primitive asteroids that have a layer of fine particulate regolith.**

Model

- We used a weighted least squares (WLS) algorithm and a full spectral library of fine particulate pure minerals including Augite, Olivine, Enstatite, Calcite, Saponite, Magnetite, Troilite, Spinel, Pyrrhotite, Cronstedtite, and Albite to unmix spectra of a suite of fine particulate, primitive asteroid analogs[5].
- Using WLS, the residuals, the difference between model and spectra at each wavelength channel, are weighted by the square of the known uncertainty in the measurement at each wavelength corresponding to the diagonal entries of the covariance matrix. Thus, more precise measurements are weighted more heavily in the unmixing.
- We also applied a modified version of the WLS algorithm, which included a sum-to-one (STO) constraint based on a model by Heinz and Chang[7], to the spectral data.
- Unmixing was applied to the **Full Spectral Range** (2000 to 200 cm^{-1}) and a **Limited Spectral Range** (1050 to 800 cm^{-1}).

Conclusions

- For the ambient anhydrous mixture Natasha (Tables 1 & 2) and meteorites (Tables 3 & 4) the WLS and STO algorithms underestimated the abundances of the spectrally dominant mineral phases.
- Minor phases in Natasha and the meteorites (abundances ≤ 5%) were typically not modeled[1, 2, 3], and phases not present in the mixtures were selected (Tables 1-4), particularly phases that are spectrally flat and with low albedos (i.e., magnetite and pyrrhotite).
- We attribute this to the fact that terrestrial and extraterrestrial mineral end members included in the spectral library are not truly representative of the mineral phases present in the chondritic meteorites investigated here[5].
- Overall the RMS errors generally improved when the spectral range was limited to 1050 to 800 cm^{-1}.

Acknowledgements

Supported under NASA Cooperative Agreement 80NSSC19M0214 to the Center for Lunar and Asteroid Surface Science.

References

[1] Ramsey M. S. and Christensen P. R. (1998) *JGR, 103*, 577-596. [2] Hamilton V. E. and Christensen P. R. (2000) *JGR, 105*, 9717-9733. [3] Rogers A. D. and Aharonson O. (2008) *JGR, 113*,E06S14. [4] Hamilton V. E. et al. (2019) *Nature Astron., 3*, 332-340. [5] Donaldson Hanna K. L et al. (2019) *Icarus, 319*, 701-723. [6] Hamilton, V. E. et al. (1997) *JGR, 102*, 25,593- 25,603. [7] Heinz D. C. and Chang, C.-I. (2001) *IEEE Transactions on Geoscience and Remote Sensing, 39*, 529-545. [8] Moersch J. E. and Christensen P. R. (1995) *JGR, 100*, 7465-747. [9] Mustard J. F. and Hays J. E. (1997), *Icarus, 125*, 145-163.

Ambient Anhydrous Mixture Natasha

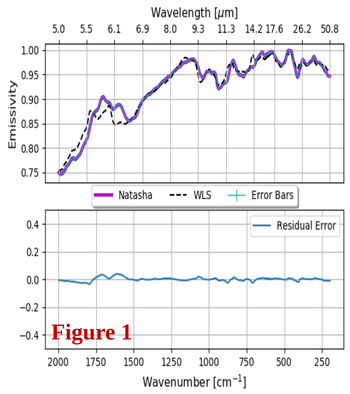

Figure 1. Ambient Anhydrous Mixture Natasha unmixed using the WLS algorithm in the **Full Spectral Range**

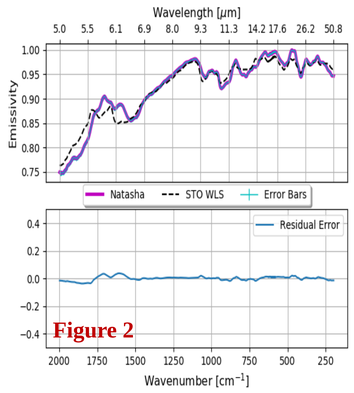

Figure 2. Ambient Anhydrous Mixture Natasha unmixed using the STO algorithm in the **Full Spectral Range**

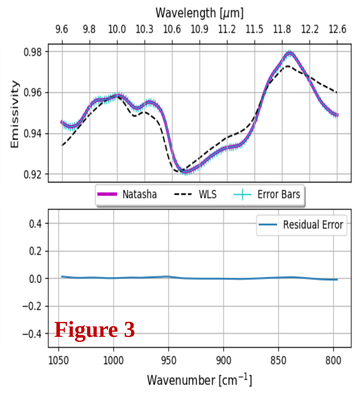

Figure 3. Ambient Anhydrous Mixture Natasha unmixed using the WLS algorithm in the **Limited Spectral Range**

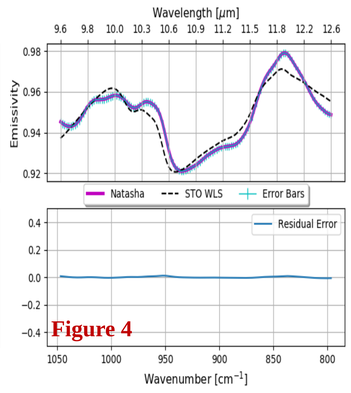

Figure 4. Ambient Anhydrous Mixture Natasha unmixed using the STO algorithm in the **Limited Spectral Range**

Table 1	WLS		STO	
	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)
Olivine	34.0	66.5	50.0	66.5
Albite		9.50		9.50
Enstatite		8.08		8.08
Troilite	42.0	4.75	15.0	4.75
Augite	25.0	1.43	35.0	1.43

Table 1. Actual and model abundances of Natasha - **Full Spectral Range** corresponding to Fig. 1 and 2

Table 2	WLS		STO	
	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)
Olivine	46.0	66.5	45.0	66.5
Albite		9.50		9.50
Enstatite		8.08		8.08
Troilite		4.75		4.75
Augite		1.43		1.43
Pyrrhotite	54.0		55.0	

Table 2. Actual and model abundances of Natasha - **Limited Spectral Range** corresponding to Fig. 3 and 4

Meteorites

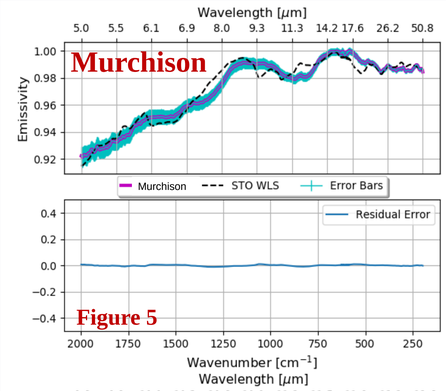

Figure 5. Murchison meteorite unmixed using the STO algorithm in the **Full Spectral Range**

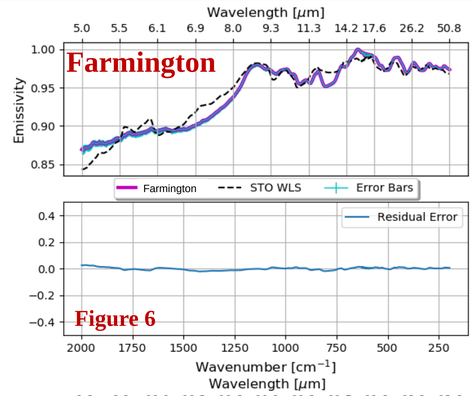

Figure 6. Farmington meteorite unmixed using the STO algorithm in the **Full Spectral Range**

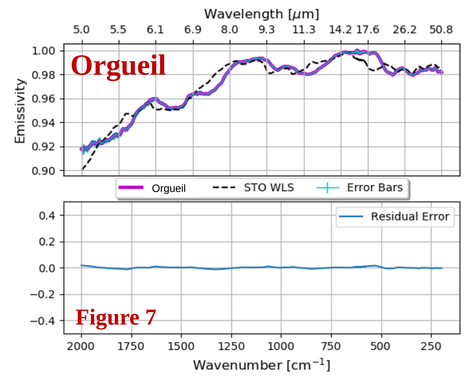

Figure 7. Orgueil meteorite unmixed using the STO algorithm in the **Full Spectral Range**

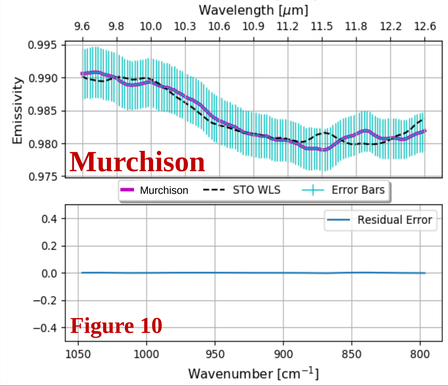

Figure 10. Murchison meteorite unmixed using the STO algorithm in the **Limited Spectral Range**

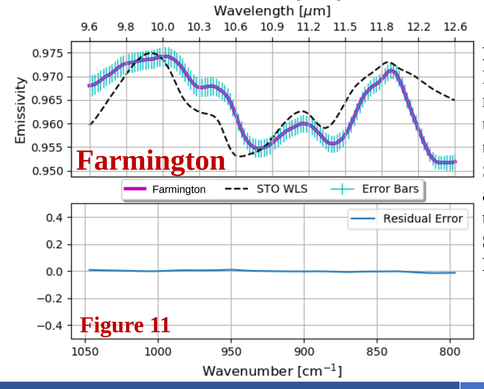

Figure 11. Farmington meteorite unmixed using the STO algorithm in the **Limited Spectral Range**

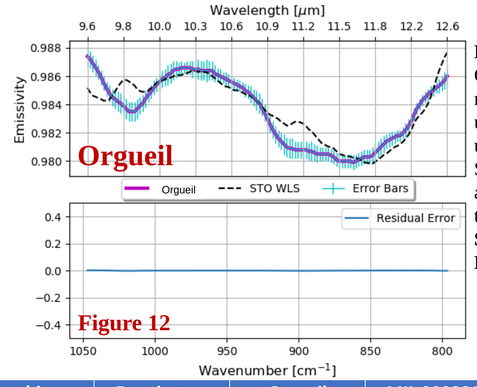

Figure 12. Orgueil meteorite unmixed using the STO algorithm in the **Limited Spectral Range**

Meteorites

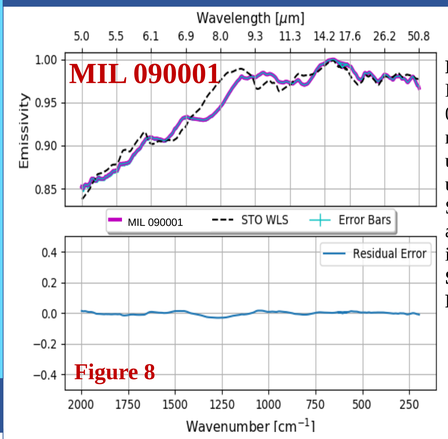

Figure 8. MIL 090001 meteorite unmixed using the STO algorithm in the **Full Spectral Range**

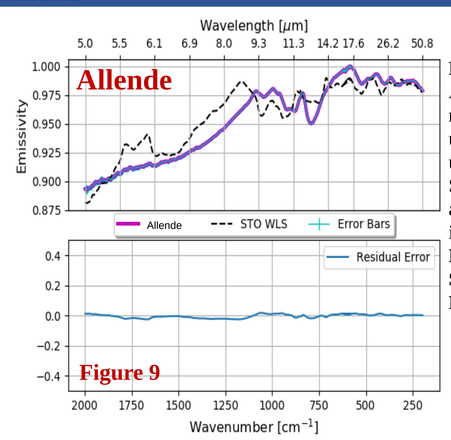

Figure 9. Allende meteorite unmixed using the STO algorithm in the **Full Spectral Range**

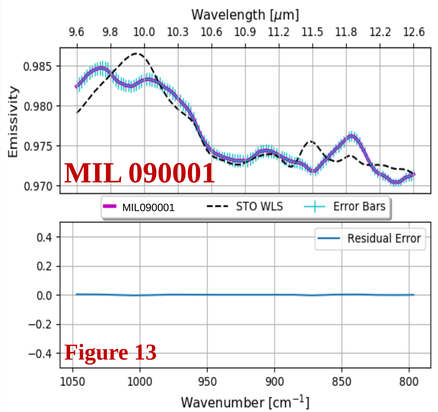

Figure 13. MIL 090001 meteorite unmixed using the STO algorithm in the **Limited Spectral Range**

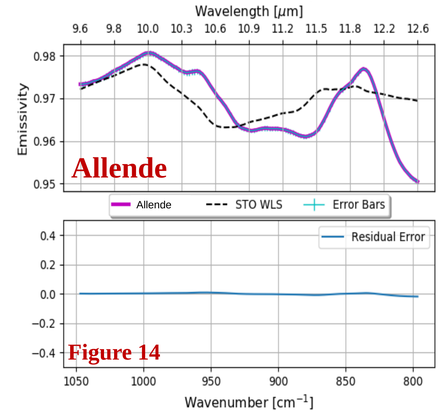

Figure 14. Allende meteorite unmixed using the STO algorithm in the **Limited Spectral Range**

Table 3	Murchison		Farmington		Orgueil		MIL 090001		Allende	
	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)
Saponite	17.0	76.2			61.0	79.1	49.0	25.9		
Olivine	17.0	11.3	38.0	39.3	16.0	4.10	26.0	23.0	52.0	80.5
Enstatite		4.00		18.9				12.4		4.20
Augite	18.0	4.00	33.0	18.9			25.0	12.4	34.0	4.20
Magnetite		1.50			23.0	6.90		2.10		
Calcite		0.80				1.00		2.90	14.0	
Cronstedtite	37.0									
Spinel	11.0									
Pyrrhotite			29.0	3.25						
Albite				11.9						
Troilite				3.25						

Table 3. Actual and model abundances of Meteorites - **Full Spectral Range** corresponding to Fig. 5 to 9

Table 4	Murchison		Farmington		Orgueil		MIL 090001		Allende	
	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)	Model (vol. %)	Actual (vol. %)
Saponite		76.2			57.0	79.1	6.00	25.9		
Olivine		11.3	16.0	39.3		4.10	6.00	23.0	25.0	80.5
Enstatite		4.00	19.0	18.9			7.00	12.4		4.20
Augite		4.00		18.9				12.4		4.20
Magnetite	48.0	1.50			43.0	6.90		2.10	75.0	
Calcite		0.80				1.00		2.90		
Cronstedtite	18.0						7.00			
Spinel	21.0						29.0			
Pyrrhotite	35.0		66.0	3.25			45.0			
Albite				11.9						
Troilite				3.25						

Table 4. Actual and model abundances of Meteorites - **Limited Spectral Range** corresponding to Fig. 10 to 14