Comparing Thermal Infrared Spectral Unmixing Algorithms

Applications to Bennu and other Airless Bodies

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REFERENCES

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OSIRIS-REx blind test suite used to explore **linear unmixing algorithms** for **spectra** of **fine particulate** mixtures in the **thermal IR**.

INTRO

- <u>Aim</u>: to examine different fitting algorithms to estimate modal mineralogy when using the linear unmixing model in the thermal infrared (TIR; 5-50μm or 2000-200cm^{-1}).
- Current methods [e.g., 1, 2] may not be appropriate for fine particulate materials and observations with limited prior knowledge, so alternative methods are being developed.
- Shown here is current progress for algorithm comparisons using a subset of the OSIRIS-REx TIR blind test spectra [3].

METHODS

- Most current methods use least squares techniques at their core (e.g., iterative library reduction, ILR, [1] and non-negative least squares, NNLS, [2]), which are successful for many applications [e.g., 1].
- Bayesian techniques such as Markov Chain Monte Carlo (MCMC) allow full exploration of the parameter space and quantitatively use *a priori* information.
- I begin with unmixing a selection of blind test mixtures using an ILR algorithm, ready for comparison with a Bayesian MCMC algorithm using a forward model.
- Both error in the fit and correlation between retrieved abundances are investigated in this work.

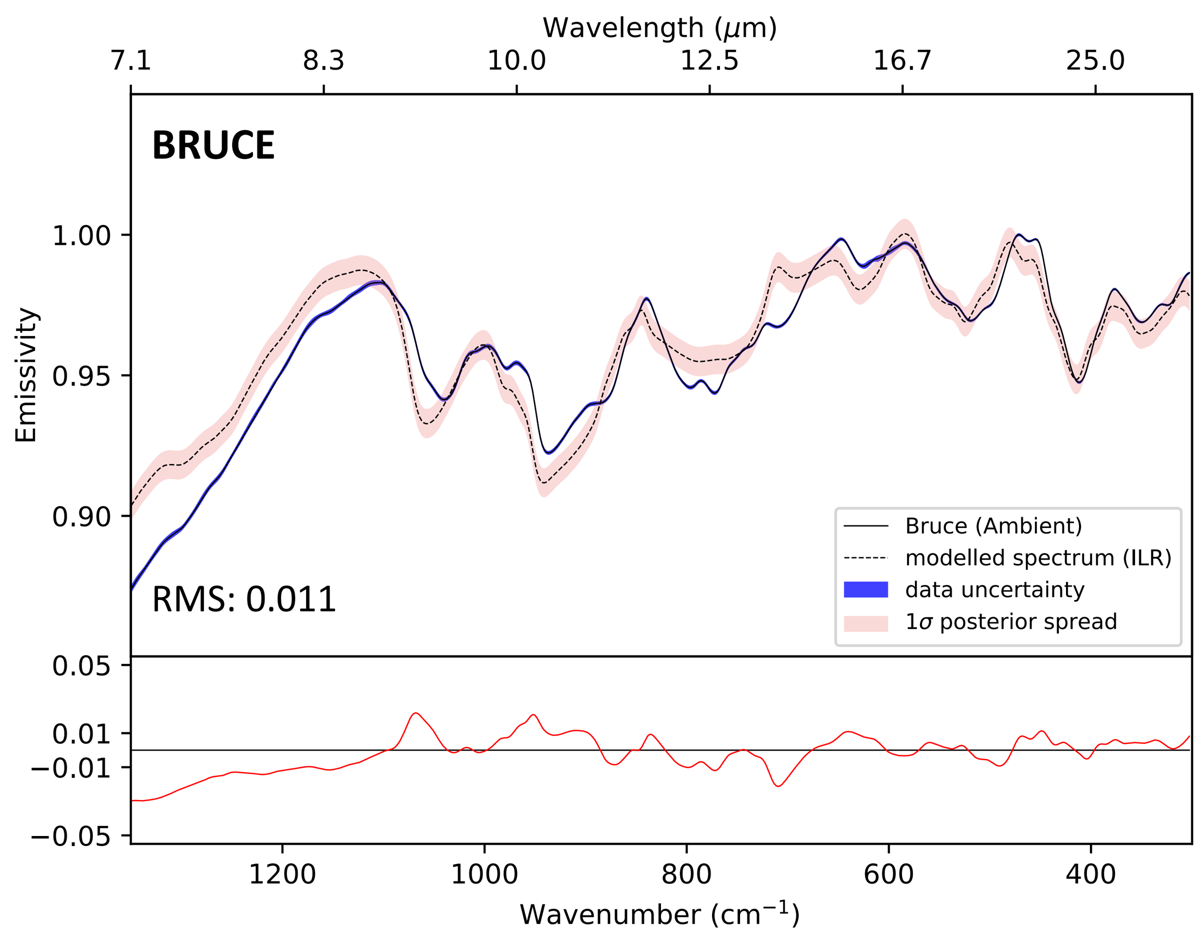
KEY RESULTS

- Preliminary derivations of the correlation coefficients from the abundance covariance matrix (calculated using ILR) indicates that most of the fitted mineral abundances are highly correlated (correlation coefficient > |0.6|).
- This could be due to an incomplete spectral library and/or evidence of additional non-linear mixing, and so requires further investigation.
- This initial work suggests that estimating modal mineral abundances of fine particulates using remote sensing data (e.g., for Bennu) may benefit from Bayesian inference techniques, in addition to current methods.

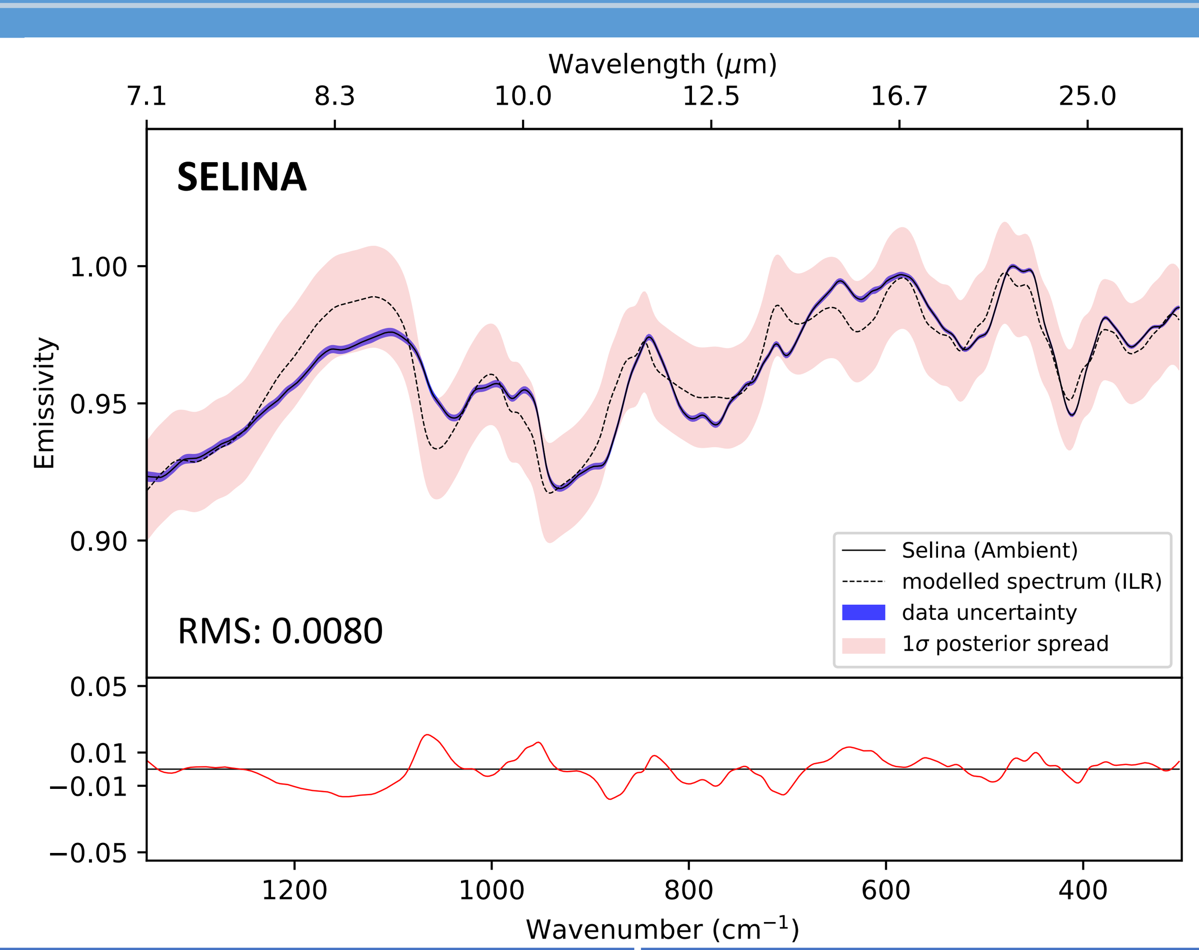
SPECTRAL LIBRARY USED

- San Carlos olivine (< 90 μm)
- Johnstown enstatite (< 90 μm)
- Kakanui augite (< 90 μm)
- Mundrabilla troilite (< 90 μm)
- Mono Lake saponite (< 90 μm)
- Minas Gerais magnetite (< 90 μm)
- New Mexico calcite (< 90 μm)
- Cronstedtite (< 90 μm)
- Pyrrhotite (< 90 μm)
- Blackbody
- Amelia albite (coarse; from ASU library)

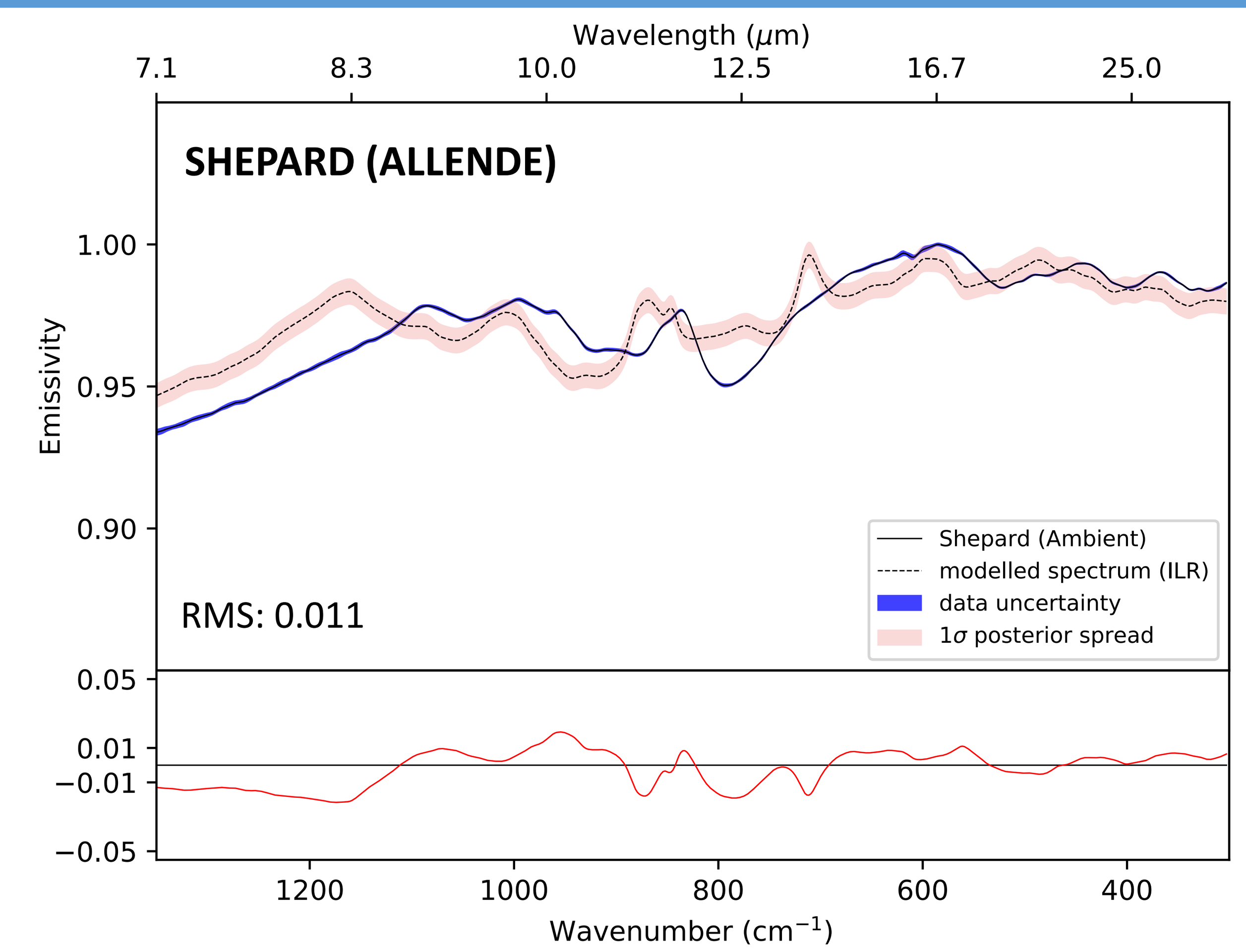
Ambient ⟹ Measured under 'Earth-like' conditions



True abundances (Total: 1.0) [3]		Modelled abundances (Total: 1.011±0.0027)	
San Carlos olivine:	0.70	San Carlos olivine:	0.44 ± 0.00074
Johnstown orthopyroxene:	0.085	Kakanui augite:	0.054 ± 0.0014
Kakanui augite:	0.015	Mundrabilla troilite:	0.18 ± 0.0018
Amelia albite:	0.10	New Mexico calcite:	0.047 ± 0.00018
Fe-Ni metal:	0.05	Cronstedtite:	0.29 ± 0.0012
Mundrabilla troilite:	0.05		



True abundances (Total: 1.0) [3]		Modelled abundances (Total: 1.012±0.011)	
San Carlos olivine:	0.595	San Carlos olivine:	0.42 ± 0.0011
Johnstown orthopyroxene:	0.072	New Mexico calcite:	0.052 ± 0.00028
Kakanui augite:	0.013	Pyrrhotite:	0.27 ± 0.0075
Amelia albite:	0.085	Cronstedtite:	0.16 ± 0.0022
Fe-Ni metal:	0.0425	Blackbody:	0.11 + 0.0076
Mundrabilla troilite:	0.0425		
Organics (synthetic IOM):	0.050		
New Mexico calcite:	0.050		
Mono Lake saponite:	0.025		
Morris County lizardite:	0.025		



True abundances (Total: 0.999) [4]		Modelled abundances (Total: 1.012±0.0024)	
Olivine:	0.827	San Carlos olivine:	0.089 ± 0.00061
Pyroxene:	0.063	Kakanui augite:	0.15 ± 0.0012
Anorthite:	0.011	Cronstedtite:	0.30 ± 0.0011
Phyllosilicate:	0.019	New Mexico calcite:	0.063 ± 0.00014
Metal:	0.010	Blackbody:	0.41 ± 0.0016
Fe-Oxide (magnetite+rust):	0.003		
Sulfide + Sulfate:	0.066		

EXTRA INFO

BACKGROUND

- The emissivities of coarse particulate minerals in a mixture add together linearly in proportion to their abundances to create a composite spectrum [1], based on the assumption of surface only emission.
- Mineral abundances of mixtures are commonly found using linear least squares techniques [e.g., 1, 2]. These methods have known issues with fine particulates [1].
- Degree of degeneracy in retrieved abundances is often poorly constrained with these methods (i.e., multiple mineral assemblages could provide statistically good fits but only one outcome is considered).
- Bayesian inference techniques (e.g., MCMC) provide an alternative approach to modelling by exploring a parameter space which may be restricted by the quantitative inclusion of *a priori* information.

DATA USED

- The OSIRIS-REx blind test study presented spectral measurements of materials thought to be compositionally analogous to target asteroid (101955) Bennu [3].
- For preliminary testing, a subset of three olivine-rich samples from the blind test study were chosen; Bruce, Selina and Shepard (Allende), which have increasingly complex compositions.
- The mineral end-members within the mixtures were prepared to particle size fraction < 38μm (fine), and the San Carlos olivine also included a 38 – 105μm size fraction (coarse). Bruce and Selina contained an olivine mixture of 85 wt. % fine particulates and 15 wt. % coarse particulates. Shepard was composed of a mixture of three different size fractions: ~11 wt. % 105 – 150μm; 22 wt. % 38 – 105μm; 67 wt. % <38μm [3].
- These data are challenging to analyse with least squares techniques due to their complex compositions and being dominated by fine particulates, hence the interest in new techniques.

STILL TO COME

- Completion of MCMC unmixing algorithm.
- Full comparisons between Bayesian methods and least squares methods (e.g., ILR, NNLS).
- Development of Bayesian spectral unmixing toolkit and applying this to datasets such as those from OTES (on OSIRIS-REx), Spitzer, and meteorite samples.