Linear deconvolution of ATR-IR spectra of mineral mixtures for planetary surface studies

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Abstract

Attenuated total reflectance (ATR) is an infrared spectroscopic method useful for compositional analysis of powdered samples. ATR-IR is frequently used for chemical phase ID, but is seldom used in geological studies. Because it is effective with small grain sizes, ATR-IR could be a powerful tool for *in situ* mineral identification on future planetary lander missions, especially for the analysis of fine-grained regoliths, atmospheric dust, and outcrop grindings. Here we test the ability of the ATR-IR technique to quantitatively determine the modal mineralogy of powdered mineral mixtures. Mixtures were prepared from four mineral endmembers - olivine (Fo_{90}), plagioclase (An_{60}), calcite and gypsum - in known volumetric proportions and in a variety of grain sizes. ATR spectra of mineral mixtures and endmembers were collected in the range 400-4000 cm^{-1}. Spectra of mixtures were modeled using the deconvolution method of Rogers et al. (2006), modified so that a measured grain-size distribution (GSD) could be included as a weighted factor in the fit. The signal-to-noise ratio increased for each mineral with decreasing grain size. This is expected because finer grain sizes have a better contact with the ATR crystal. For mixtures of a single grain size, the deconvolution-modeled proportions generally matched actual proportions within 10-20%. Occasionally, the deconvolution model produced poor matches to actual mineralogy and observed spectral shape. To assess the effect of clinging fines, fine-grained (<10 μm) calcite and gypsum were added in increments from 0 to 30% to a mixture of coarsely particulate (74- 147 μm) olivine and plagioclase. The fine-grained components of these mixtures were strongly overrepresented in the model - possibly the result of non-ideal mixing and surface area dominating over volume in linear spectral addition. Increasing the weight of the GSD in the deconvolution model mitigated the overestimation of fines, but increased the RMS error of the spectral fit. Given the present results, we conclude that deconvolution of ATR-IR spectra can quantitatively predict the mineralogy of fine-grained mixtures, but for mixed grain-size samples, it may be necessary to grind the mixture to a uniform particle size.

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