VOLCANISM AND/OR AQUEOUS ALTERATION ON MARS: CONSTRAINTS ON DISTINGUISHING GLASS AND PHYLLOSILICATE IN THE THERMAL INFRARED. W. C. Koeppen and V. E. Hamilton, Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, 1680 East-West Rd, POST 602, Honolulu, HI 96822 (koeppen@higp.hawaii.edu).

Introduction: Interpretation of Thermal Emission Spectrometer (TES) data requires a detailed investigation of different minerals that show apparently similar spectral properties. For example, the TES experiment has identified surface materials (Surface Type 2) interpreted as andesitic based on the detection of a glassy component in the spectra [1,2]. Following work [3], however, has suggested that phyllosilicate minerals may be an alternative to the glassy component of [1].

Visual inspection shows the apparent spectral similarities between glasses and phyllosilicates at all resolutions, however, there are differences as well (Figure 1). Precise band minima in the 1300-900 cm\(^{-1}\) region are 20-45 cm\(^{-1}\) less in phyllosilicate phases than in glass phases. Phyllosilicates also show a deeper 465 cm\(^{-1}\) feature than 1300-900 cm\(^{-1}\) feature whereas glasses show the opposite. Unlike glass spectra, all of the phyllosilicates have an emissivity low at 500-600 cm\(^{-1}\), a region typically excluded during deconvolution due to the proximity of CO\(_2\) absorption bands.

This study aims to determine (1) if the two mineral groups are, in fact, difficult to distinguish in thermal infrared spectra of mixtures, (2) under what conditions and chemistries this problem is exacerbated, and (3) constraints on deconvolution estimates of glass and phyllosilicate abundance.

Technical Approach: Two glasses and seven granular phyllosilicate spectra were selected for analyses (Figure 1). These spectra were first individually deconvolved using an end member suite composed of the other glasses and phyllosilicates. Two-component numerical mixture sets were then generated over multiple spectral resolutions and ranges (Table 1) using one phyllosilicate and one glass spectrum. Each set was comprised of nine spectra with differing proportions of glass to phyllosilicate: 90:10, 80:20, 70:30, 60:40, 50:50, 40:60, 30:70, 20:80, and 10:90.

Table 1 – Spectral sampling and deconvolution ranges over which numerical mixtures were analyzed.

<table>
<thead>
<tr>
<th>Spectral Sampling</th>
<th>Deconvolution Range</th>
<th>Acronym</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laboratory 2 cm(^{-1})</td>
<td>1300 - 230 cm(^{-1})</td>
<td>LSS</td>
</tr>
<tr>
<td>TES 10 cm(^{-1})</td>
<td>1300-825, 508-232 cm(^{-1})</td>
<td>TSS</td>
</tr>
<tr>
<td>TES 10 cm(^{-1})</td>
<td>1300-780, 560-232 cm(^{-1})</td>
<td>NTSS</td>
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Spectra were analyzed using a linear deconvolution algorithm for emission spectra [5] which utilized a suite of user-supplied end members to model a mixed spectrum. Outputs of the algorithm include a best-fit model spectrum, the percentages of each end member used, and the RMS value for the fit.

The following end member scenarios were explored in deconvolving the numerical mixture sets: Case 1 - all glasses and phyllosilicates were included in the end member suite including those used to make the mixture; this was a control case expected to give perfect results. Case 2 - the specific glass and phyllosilicate used to make the mixture were excluded from the end member suite, forcing imperfect substitutions from other phases. Case 3 - only the phyllosilicate used to make the mixture was excluded from the end member suite.

Deconvolution Results: Individual phyllosilicate spectra deconvolved with glasses and other phyllosilicates showed less than 11% misestimation of total glass abundance. All phyllosilicate spectra could be reasonably modeled (RMS ≤ 0.01) with three or less
other phyllosilicate spectra. Deconvolution of glass spectra showed three trends: (1) silica glass was always modeled best by granitic glass (Na- and K-rich) (2) granitic glass was modeled by a combination of silica glass and phyllosilicates (dominated by saponite, and kaolinite), and (3) if only phyllosilicates were included in the end member suites, both glasses were deconvolved as almost entirely illite but were visibly poor fits.

Two-component mixture sets required a more technical approach to determine trends. For instance, high RMS values associated with a model fit by the deconvolution algorithm indicated that a major component of the mixture was missing from the end member suite. Additionally, the mean absolute value (across all mixture proportions for a set) of the modeled fraction of glass minus the known fraction of glass was a measure of model accuracy (Figure 2).

Case 1 deconvolution models perfectly simulated the known mixture and showed arbitrarily small RMS values, as expected. Case 2 models of silica glass mixtures showed high RMS values (~ 0.023-0.027) and a wide range in mean absolute difference (15-36% absolute fraction). Substitution between glass and phyllosilicates was occurring, but not producing a good model-fit. Case 2 models of granitic glass mixtures showed moderate RMS values and a narrow range of mean absolute differences coupled with poor accuracy modeling total glass abundance (~30-40% absolute fraction). Substitution between glass and phyllosilicates was occurring and producing only a moderately bad fit. Case 3 models showed low mean RMS values and most estimated the total amount of glass to within 10% (absolute fraction).

End Member Tracking. Linear deconvolution of the numerical mixture sets (with changing proportions of glass and phyllosilicate) allows us to track specifically which phases substitute for those in the mixture and how much substitution between glasses and phyllosilicates takes place. In nearly all instances, specific phyllosilicate phases dominant in Case 2 models of a mixture are also dominant in Case 3 models of that mixture. Case 2 deconvolutions of silica glass mixtures utilized the granitic glass end member, but always overestimated the amount of glass present whereas granitic glass mixtures, which utilize the silica glass end member, always underestimated the amount of glass. Case 3 mixtures overestimated glass content in five of seven cases.

Spectral Sampling and Deconvolution Range Effects. The effects of different spectral sampling and deconvolution ranges on the modeling of numerical mixtures were also examined (Table 1). LSS models provided the best overall accuracy for most silica glass mixtures, however, NTSS models were best for granitic glass mixtures and some silica glass mixtures. Both LSS and NTSS deconvolution ranges fully or partly include emissivity lows in phyllosilicates between 500 - 600 cm⁻¹. The narrowed CO₂ exclusion region of NTSS provided a typical improvement of 2-5% (absolute fraction) in model accuracy over the standard, more conservative, TSS exclusion region in nearly all instances. The specific end members used in the best-fit models did not vary significantly with spectral sampling (LSS, TSS, and NTSS), however, the percentages of those end members do vary up to 15%.

Conclusions: This study shows quantitatively that granitic glass, individually and in mixtures, is the most likely phase to be confused with phyllosilicates in the thermal infrared. Case 3 models suggest that if both glasses and phyllosilicates are present at TES-measurable quantities on the Martian surface and their spectra are nearly identical to the laboratory-measured spectra in the end member suite, substitution between glasses and phyllosilicates should not occur above ~15% (absolute fraction). Case 2 models represent a scenario in which phases present at the surface of Mars are somewhat dissimilar to those in the end member suite. In this case, substitution of glasses for phyllosilicates and vice versa may occur up to 40% (absolute fraction). A less conservative deconvolution range (NTSS) could be used to gain slightly better accuracy (2-5%) in determining total glass abundance.