Spectral Mixture Analysis of Simulated Thermal Infrared Spectrometry Data: An Initial Temperature Estimate Bounded TESSMA Search Approach

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Abstract—At-sensor thermal infrared (TIR) radiation varies depending on the temperature and emissivity of surface materials and the modifying impact of atmospheric absorption and emission. TIR imaging spectrometry often involves extracting temperature, emissivity, and/or surface composition, which are useful in diverse studies ranging from climatology to land use analyses. A two-stage application of temperature emissivity separation (TES) using spectral mixture analysis (SMA) or TESSMA, was employed to characterize isothermal mixtures on a subpixel basis. This two-stage approach first uses the relationship between a virtual cold endmember fraction and surface temperature to extract initial image temperature estimates. Second, an isothermal SMA application searches the region within the maximum temperature error range of the initial estimate, selecting the best subpixel spectral mixture fit. Work presented includes characterizations of synthetically generated temperature and constituent mixture gradient test images, and a discussion of errors associated with selecting temperature search ranges 25% and 75% smaller than the initial temperature calculation error range. Results using this two-stage approach indicate improved overall temperature estimates, constituent estimates, and constituent fraction estimates using simulated TIR data.

Index Terms—Initial temperature estimate bounded search, spectral mixture analysis, temperature emissivity separation, thermal infrared spectrometry, unmixing.

I. INTRODUCTION

This paper presents a two-stage temperature emissivity separation (TES) algorithm using spectral mixture analysis (SMA) or TESSMA, to extract temperature and pixel fractional constituent estimates using simulated thermal infrared (TIR) radiance data. In the first step, an initial temperature estimate (TINIT) with a well-characterized error range is generated. This TINIT is used along with the assumed maximum expected error to constrain SMA searches within the projected temperature error range. This constrained SMA approach considerably reduces the number of computations required.

TIR imaging spectrometry can be used to retrieve the temperature and emissivity of objects, and has applications in geology [1], climatology [2], radiation budget analysis [3], biological process analysis [4], geophysical process analysis [5], and atmospheric plume study [6]. Other applications include surface constituent identification for land use mapping [7], disaster assessment [8], pollution detection [9], and change detection [5]. When applying TIR imagery to such tasks, it is often important to extract estimates of temperature and emissivity, which combine to contribute to thermal radiance spectra.

TES [10] and spectral mixture analysis (SMA) [1] are two classes of procedures used in TIR spectrometry to separate temperature and emissivity contributions to radiance images. TES involves separating temperature and emissivity effects using constraining assumptions about the temperature and emissivity contributions to the spectral signatures. Land surface temperature (LST) estimation is more difficult than temperature estimation over water due to the variable emissivity of land surfaces [11]. Several variations of temperature and emissivity estimation methods have been studied by various authors, including

1) split window applied to land surfaces [11], [12];
2) gray body emissivity [13];
3) normalized differential vegetation index (NDVI) correlations [4];
4) thermal independent spectral index [14], [15];
5) reference channel [16];
6) emissivity normalization [16];
7) alpha emissivity [16];
8) bidirectional reflectance distribution function [17], [18];
9) virtual cold method [1], [19];
10) automatic atmospheric correction [20].

For sensors with large footprints (e.g., advanced spaceborne thermal emission and reflection radiometer [ASTER] and moderate resolution imaging spectroradiometer [MODIS]) with nonhomogeneous subpixel surfaces, a subpixel estimate of constituents is often required. It has been suggested by Gillespie [1] that surface temperatures and subpixel constituent estimates can be extracted using SMA, which uses the concept that subpixel mixtures may be estimated as fractions of previously measured pure (or unmixed) constituents, which are referred to as spectral endmembers. One constraining difficulty is the time involved in extracting the requisite estimates from which the best endmember estimate is chosen. This is particularly difficult because the temperature contribution to radiance greatly increases the number of searches required. For simple isothermal SMA (in which all surface endmembers are at the same temperature), endmembers calculated for each emissivity sample must be searched at the temperature resolution interval desired for the entire temperature range.
Rather than take such an exhaustive approach, it is possible to constrain an isothermal search strategy using an initial surface temperature estimate, and search within the projected error range of this estimate. Optimally, one would use an estimation method or combination of estimation methods that produces the lowest temperature error to limit the temperature search range for each sample. Among the available methods, SMA was chosen for this TINIT to evaluate the method, quantify some of its limitations, and to clarify aspects of SMA in the TIR spectral region.

A. Spectral Mixture Modeling

Spectral mixture modeling [21], also called SMA [22], is an established tool for estimating the subpixel constituent contributions to a scene using a linear or nonlinear mixing model. SMA is recognized as a method for separating constituents, such as land cover types [23], and as a method of extracting elemental and mineralogical information [22]. The basic formula describing SMA is shown in (1)

\[ L_{\text{sensor}}(\lambda) = \sum_{i=1}^{N} (f_i L_i(\lambda)) + L_{\text{err}}(\lambda) \]  

(1)

where

- \( L_{\text{sensor}}(\lambda) \) sensor spectral radiance;
- \( f_i \) spectral endmember;
- \( N \) number of spectral endmembers;
- \( f_i \) endmember fractional contribution\(^1\);
- \( L_i(\lambda) \) sensor endmember radiance;
- \( L_{\text{err}}(\lambda) \) model error: remaining spectral radiance.

SMA is an application that uses several key assumptions regarding spectral mixtures. First, it assumes that spectral mixtures are linear or nonlinear combinations of unique and separable spectral endmembers, a set of spectral constituents that are assumed to be found in an image. Each measured constituent, or endmember, must be sufficiently unique in its spectral signature from other endmembers as to be separable, or recognizably different as a spectral signature from all others. This criterion is more easily met using hyperspectral sensors, which increase the probability that a prospective endmember is separable (differentiable from all others). Most SMA applications use linear mixing models, in which mixtures of endmembers are assumed to equal the sum of the products of their fractions and their radiiances \( \sum f_i L_i(\lambda) \). Second, each spectral endmember is ideally a radiance estimate for a pure sample of a surface constituent. Usually, the model is not perfect, and some model error remains. This remaining spectral radiance is often used in a goodness of fit criterion, and the spectral mixture with the lowest model error would be selected.

This work applies the commonly used root mean squared error (RMSE) (2) as the goodness of fit criterion. Endmember fractions \( f_i \) may be partially constrained, which may provide a better model fit, or fully constrained, which makes more physical sense if mixing is linear. With partially constrained models, it is possible to arrive at solutions with negative fractions which, while not physically possible, provide an indication of a poor model fit and/or a missing model endmember approximating an image constituent. Both types of constraint are used in this temperature constrained TESSMA approach, and are shown in (1).

\[ \text{RMSE} = \left[ \frac{\sum_{\lambda} \left( L_{\text{sensor}}(\lambda) - L_{\text{model}}(\lambda) \right)^2}{N} \right]^{1/2} \]  

(2)

where

- RMSE root mean squared error;
- \( \lambda \) wavelength;
- \( L_{\text{sensor}}(\lambda) \) sensor endmember radiance;
- \( L_{\text{model}}(\lambda) \) model spectral radiance estimate;
- \( N \) number of wavelengths.

B. Virtual Cold Spectral Mixture Analysis (VC SMA)

A virtual cold (VC) endmember approach [1], treated in detail in previous work [19], is an extension of the shade concept used in visible/near infrared SMA studies to the TIR. Both original and more recent work in visible/near infrared SMA have taken multiple scattering into account by using a virtual shade endmember, which incorporates multiple scattering by solving for a unique shade endmember such as either radiative [21] or canopy shade [23]. This technique may be applied in SMA to reduce nonlinearity effects. Likewise, in the TIR spectral region, application of an analogous method uses VC to assist in the estimation of the temperature variation within a TIR image [19].

A fundamental difficulty in using this approach, however, is that the temperature-radiance relationship is nonlinear (3)

\[ L_s(\lambda, T) = \varepsilon(\lambda) \frac{2hc}{\lambda^5 (e^{hc/k\lambda T} - 1)} \]  

(3)

where

- \( L_s(\lambda, T) \) sensor spectral radiance;
- \( \varepsilon(\lambda) \) spectral emissivity;
- \( h \) Planck’s constant;
- \( c \) speed of light;
- \( k \) Boltzmann’s constant;
- \( T \) surface skin temperature;
- \( \lambda \) wavelength.

In the TIR spectral region, emitted radiance is related to the product of Planck’s radiation equation and the emissivity of the radiating object (3). Emitted surface radiance is decidedly nonlinear with respect to temperature \( T \), as seen in part of the denominator \( (e^{hc/(k\lambda T)} - 1) \). Nor is it uniform across wavelengths \( \lambda \), as also seen in the denominator \( (e^{hc/(k\lambda T)} + 1) \). These nonuniformities contribute in addition to multiple emissive effects associated with more complex scene geometries, atmosphere inhomogeneity, (e.g., partial clouds), and adjacent surfaces (e.g., trees and shrubs).

Nonlinearity in Planck’s radiation equation predicts a nonlinear surface radiancereponse (e.g., in the TIR, \( L_{13b} (300 \text{ K}) < [L_{13h} (290 \text{ K}) + (L_{13h} (310 \text{ K}) )]/2 \)). One method that addresses this nonlinearity is the application of an exhaustive analysis using all SMA endmember-temperature combinations. For large radiance datasets or large endmember sets, such an approach is computationally impractical.

As a first approximation, virtual cold spectral mixture analysis (VC SMA) assumes a linear relationship between spectral
endmembers, including surfaces composed of constituents at different temperatures. Temperature induced nonlinearity in the emitted radiance causes an estimate at an intermediate temperature to have errors in both constituent fraction estimates and in the temperature estimate [19]. As discussed in previous work [19], although the resulting endmember estimate fractions are not always representative of actual constituent fractions, there is a consistent relationship between the VC endmember fraction and the temperature of isothermal mixtures. This consistent relationship may be used to develop a lookup table, which provides an TINIT using the VC fraction. Using this TINIT, and knowledge about the error range associated with that temperature estimate, a constrained isothermal SMA search of adjacent temperatures may be used to gain more accurate results. In this application, one TES and SMA (TESSMA) method using the VC-temperature relationships is used as an initial estimate, and the temperature range around this estimate is explored for the best isothermal SMA fit to the radiance image.

II. INITIAL TEMPERATURE ESTIMATE BOUNDED TESSMA METHOD

Synthetic images were generated using a simulation of the (at-sensor) radiance of subpixel spectral mixtures. These mixed pixel images were then processed using a virtual cold SMA approach. A relationship between pixel temperature and VC endmember fractions was used to generate initial temperature estimates (TINIT = TVC SMA). These temperature estimates were then used to constrain an isothermal SMA search of the nearest 4 K around each initial pixel temperature estimate in the images. This ±4 K range is the range of possible temperatures for the selected surface given a fixed fraction. The method employed in the study of this technique is discussed in detail in the following paragraphs. A flowchart of the method is also provided in Fig. 1. Subheadings in the material that follows in this section are included in Fig. 1 to assist the reader.

A. At-Sensor Radiance Model

Synthetic radiance estimates were generated using MODTRAN 3.5 [24] simulations. The basic concept (shown as a one layer atmospheric model) is seen in (4). In this model, at-sensor radiance is described as the sum of upwelling atmospheric radiance, transmitted surface emission, and transmitted reflected downwelling atmospheric radiance

\[ L_{\text{sensor}}(\lambda) = L_{\text{up}}(\lambda) + \varepsilon_{\text{surf}}(\lambda)L_{\text{bb}}(\lambda)t_{\text{atm}}(\lambda) + L_{\text{down}}(\lambda)(1 - \varepsilon_{\text{surf}}(\lambda))t_{\text{atm}}(\lambda) \]  

where

- \( L_{\text{sensor}}(\lambda) \): sensor spectral radiance;
- \( L_{\text{up}}(\lambda) \): upwelling spectral atmospheric radiance;
- \( L_{\text{down}}(\lambda) \): downwelling spectral atmospheric radiance;
- \( L_{\text{bb}}(\lambda) \): block body surface radiance;
- \( t_{\text{atm}}(\lambda) \): spectral atmospheric transmittance;
- \( \varepsilon_{\text{surf}}(\lambda) \): spectral surface emissivity.

The MODTRAN program requires several inputs that describe the atmospheric and surface boundaries, including atmospheric profile, surface conditions, and surface emissivity. In this study, a flight at a 3-km altitude over a 1-km elevation site was used in the simulation. The standard midlatitude continental summer atmospheric model combined with a winter water vapor profile was chosen as a first approximation of an inland desert scene.

B. Endmember At-Sensor Radiance Estimates

Five emissivity spectra from the ASTER spectral library [25] and two surface soil sample emissivities [26] were employed to provide a controlled method to simulate sensor data and for testing the TESSMA retrieval. In order to develop at-sensor spectral radiance estimates, seven spectral signatures (water, green vegetation [GV], nonphotosynthetic vegetation [NPV] such as tree bark, senesced grass, and plant litter, quartz, sandstone, and two soils) were selected Fig. 2. The original emissivity values were combined with the MODTRAN runs at a frequency interval of 3 cm\(^{-1}\) and convolved to 128 bands from 7.8 to 13.5 micrometers to represent at-sensor spectral radiance estimates for a temperature range of 260 to 350 K.

These emissivities, when employed in conjunction with MODTRAN atmospheric modeling, were used to produce sensor radiance estimates at 1 K increments in surface temperature. Using (4), the at-sensor radiances were computed. Fig. 3 shows selected radiance estimates from 260 to 350 K in 10\(^{\circ}\) increments and illustrates the nonlinearity of the at-sensor radiance with temperature. Differences in radiance are smaller at lower temperatures than at higher temperatures. This will have an effect on initial temperature estimation accuracy, as
Fig. 2. ASTER library [25] emissivity spectra for five endmembers and two measured spectra (soil1 and soil2) [26] used with MODTRAN to develop test images and endmember models.

Fig. 3. NPV sensor radiance estimates at 10°/14° temperature intervals for a 128-channel spectrometer. Estimates range from 260 to 350 K at 10°/14° intervals.

discussed later. Note that these modeled radiance estimates were used to generate both the spectral endmember model and synthetic spectral mixture image. In a practical case, data from a sensor would replace the synthetic mixture image.

C. Spectral Endmember Model

For purposes of this research, a spectral endmember is assumed to represent an at-sensor radiance of a pure (homogeneous) surface at a specified uniform surface temperature. Endmember at-sensor radiance was reformatted to develop endmember models for the virtual cold SMA (VC-SMA) (2.3, Fig. 1). The spectral endmember models were generated using the at-sensor radiance estimates for each spectral endmember. Each class, such as the one shown in Fig. 3, has one radiance spectrum, or endmember, for each temperature, ranging from 260–350 K. Endmembers for each of the seven surfaces at three different temperatures (Fig. 4) further illustrate the contributions of emissivity and temperature to at-sensor radiance.

D. Synthetic Images

Radiance estimates of isothermal (uniform surface temperature) two endmember mixtures of the seven endmembers were combined to produce two-endmember fractional mixture gradient images, one of which is seen in the image in the center of Fig. 5. These temperature and endmember fraction gradient images allow characterization of best case expectations for various unmixing algorithms. For this purpose, composite synthetic images were generated for all two isothermal endmember combinations of these seven spectral emissivities.

The lookup table generation, initial temperature estimation, and final search were conducted using the original radiance endmembers (Fig. 4) and these images. The majority of the variability in these endmembers is due to the temperature range of the endmember model. However, a recognizable and separable portion of the effect is due to spectral emissivity variations (see Figs. 4 and 5).

E. Virtual Cold Spectral Mixture Analysis Estimates

An average VC endmember $\varepsilon_{vc}$ was generated by averaging the seven spectral emissivities ($\varepsilon_{vc} = \sum \varepsilon_i / N$) and calculating their radiance at 260 K. This endmember was combined with all paired combinations of two endmembers at 330 K, using the model shown in Fig. 6. SMA endmember fractions were partially constrained (1). This produced virtual cold and hot endmember fraction estimates, which were generated by selecting the model match with the lowest RMSE.

The virtual cold endmember was selected at 260 K, the low end of the image temperature range. This allowed the endmember to capture most of the temperature-related information within the spectral radiance values, while avoiding the increased nonlinearity associated with lower temperatures. The hot endmember temperature was selected at 330 K in part to allow for correct temperature estimates above and below it, and also to reduce nonlinearity effects associated with extreme temperature differences.

F. Virtual Cold—Temperature Lookup Table

The mean, maximum, and minimum virtual cold fraction estimates were computed as a function of temperature for mixtures of the seven samples. Fig. 7 shows how virtual cold fraction varies with temperature relatively independent of material type. The mean virtual cold fraction for each temperature was used to generate a lookup table relating VC fractions to temperature estimates. The generation of the VC fraction to temperature lookup table also includes calculation of the minimum and
Fig. 5. Isothermal two-endmember NPV; GV mixed pixel image and sample spectra from corners and sides of the image. The central image shows the radiance at a particular band, while the graphs around it show the spectral radiance values at several endmember fraction and temperature points in the image. A 50/50 graph represents a sample with equal fractions of NPV and GV, as seen in the second row of graphs.

Fig. 6. Nonlinearity compared to a VC SMA model. Radiances for water and green vegetation from 260 to 320 K are shown at two wavelengths, with solid circles and triangles indicating 1 K intervals. Virtual cold (VC) for these wavelengths is shown between the 260 K water and GV endmembers. The lines of hollow triangles and circles between VC and the 320 K green vegetation and water endmembers show the 100% mixture lines for three-endmember linear mixing using VC, 320 K water, and 320 K green vegetation endmembers. Mixtures containing high water fractions at intermediate temperatures are outside the triangle defined by the linear mixing lines. This illustrates the divergence of model and expected radiance as the surface temperature diverges from the temperature of the hot endmember pair. In such cases, partially constrained modeling is likely to produce negative and superpositive (> 100%) fractions and/or incorrect endmember assignments.

Fig. 7. VC fraction as a function of temperature for an isothermal SMA using seven hot endmember classes at 330 K. The temperature of isothermal endmember mixtures is consistently reflected in the VC endmember fraction. Estimates are more accurate near the 330 K endmember and degrade as the actual image temperature diverges from this hot endmember temperature. At 330 K, the virtual cold fraction is zero, and all estimates are correct. At 300 K, the mean virtual cold value is about 0.5 (50%), and the maximum absolute temperature error associated with a 50% VC fraction is 4 K.

maximum temperature for a given VC fraction. These estimates reflect an ideal case scenario, using identical models for generation and retrieval. The temperature error range is also a function of endmember variability, and additional emissivity spectra could increase this range if they fell outside the range of the original seven spectral emissivities.
Fig. 8. Ideal case unmixing of all two-endmember mixtures of six surface spectra at temperatures ranging from 280 to 320 K. The image contains 15 two-constituent mixture subimages, in which one fractional abundance grades linearly from white (100% abundance) to black (0% abundance), while the other constituent varies linearly from black to white. Adding both fractions would lead to a 100% (white) abundance image. Subimages were generated using linear mixtures of endmembers such as the mixture illustrated in Fig. 5, with temperature increasing from left to right. Columns 2–7 show the correct attribution (or unmixing) of the mixed image into its constituent classes. Absolute errors ranging from 0 (black) to 4 K (white) for the TINIT errors (input temperature errors) and temperature estimate for the search strategy (output temperature errors). Absolute temperature inaccuracies vary from 0 K (black) to 4 K (white).

G. Initial Temperature Estimates

VC fractions for these images were then used in combination with this lookup table to generate TINIT. The process may be visualized by referring to Fig. 7. For each 1 K increment, the mean VC fraction for all endmember combinations was calculated, and is shown as a solid line in the figure. In temperature estimation, the process is reversed, and the VC fraction estimates for the image are used to select the TINIT for the image (estimate T given fVC).

H. Initial Temperature Estimate Constrained Isothermal SMA Estimates

The TINIT and maximum temperature error estimates were used to limit a search strategy based on the observation that actual temperatures were within ±4 K of the initial estimates. Two endmember isothermal unmixing (SMA in which both endmembers have the same temperature) was then used to acquire more accurate temperature and endmember estimates. In this case, individual endmember fractions in the fully constrained isothermal SMA (1) were used to make more physical sense. Two additional isothermal SMA runs were carried out with search ranges of ±3 K and ±1 K to investigate unmixing errors.

III. Results

The method produces estimates of compositional fractions and temperatures, which are portrayed in the results as images of constituent estimates and their fractions, and absolute temperature errors. For clarity, the ideal unmixing pattern is presented, followed by the fractions and temperature errors associated with the TINIT (Fig. 8). These are followed by three results of the TINIT bounded TESSMA search strategy, one in which the full temperature error range (±4 K) was searched, a second estimate using a temperature search range of ±1 K, and a third in which the search range was ±3 K.

A. Ideal Unmixing Pattern

Fig. 8 shows the ideal unmixing pattern for the two-endmember image combinations of six image spectra used in this research. In this case, seven endmembers were used, but only six are shown for clarity. The image is composed of 15 two endmember mixtures in which one fractional abundance grades linearly from white (100% abundance) to black (0% abundance), while the other endmember varies linearly from black to white. The 15 combinations shown start with a mixture of water and NPV (such as woody plant stems, dry grass, and dead vegetation), and end with a sandstone-soil subimage at
the bottom, with subimage mixture combinations shown in the left-hand column. This figure is the result of an isothermal unmixing of temperature using an exhaustive approach, which tested all two endmember combinations at all temperatures for the entire image. This is equivalent to processing the image as shown in Fig. 1 using a mean temperature of 305 K for the entire image, and a temperature search range of ±45 K, which spanned all image temperatures.

B. VC SMA Unmixing

Errors can be classified into three categories, endmember misidentification, temperature retrieval errors, and fraction errors. The VC SMA TINIT produced maximum absolute temperature errors of 4 K (Fig. 7). These errors are expressed in the fraction and constituent errors as shown in Fig. 9. This figure shows the results of calculating the best fractional estimate matches for the calculated temperatures and is equivalent to the process shown in Fig. 1, with a temperature search range of 0 K in the temperature estimate bounded search strategy.

C. Initial Temperature Estimate Constrained TESSMA

The results of the TINIT constrained TESSMA is shown in Fig. 10, which is equivalent to the process shown in Fig. 1 using a temperature search range of 4 K. As seen in this figure, the temperature-bounded search strategy produces results comparable with the exhaustive SMA results shown in Fig. 8. In this figure, the TINIT errors shown on the second column from the right have been removed because the best fit temperature was consistently in the temperature range. This results in correct endmember attributions and constituent fractions.

Figs. 11 and 12 portray the effects of underestimating the temperature error range by 1 and 3 K, respectively. When the search range is ±1 K, the maximum TINIT error is underestimated by 1 K (Fig. 11), and only a small region of fractional attribution errors exists. When the search range is ±1 K, the maximum TINIT error is underestimated by 3 K (Fig. 12), and considerable endmember attribution and fractional abundance errors exist.

IV. DISCUSSION

The discussion contains sections discussing TINIT estimates and their effects on endmember mixture estimates, followed by a discussion of the TINIT constrained isothermal TESSMA. Following these are reviews of the utility of the procedure, consequences of underestimating initial fraction estimate errors, and some limitations associated with using this method.
Fig. 10. Endmember fractions and temperature error estimates for isothermal unmixing using an TINIT bounded search strategy using a temperature search range of ±4 K. For each sample, the temperature interval around an initial estimate and bounded by the maximum expected error from this estimate is searched to find the best fit using isothermal spectral mixture analysis. The image consists of several subimages, which are two-endmember mixtures of water, green vegetation (GV), nonphotosynthetic vegetation (NPV), quartz (Qtz), sandstone (Sst), and one soil (S_1). Columns 2 to 8 contain the fractional estimates for the isothermal mixture model, with white representing 100 percent of an endmember, and black representing the absence of that endmember. Again, column 9 contains the initial temperature errors, ranging from 0 (black) to 4 K (white) absolute error. Column 10 contains the final temperature error estimates, and has the same greyscale range.

A. Initial Temperature, Class, and Fraction Estimates

The errors in TINIT and resulting endmember calculations are a consequence of previously discussed nonlinearities inherent in this technique. One of the basic assumptions of SMA is that the resulting image is a linear combination of the fractional contributions of the image constituents. One of the previously discussed difficulties of a simple SMA approach in the TIR, rather than the visible/near infrared, spectral regime is that anisothermal endmember mixtures are nonlinear (Fig. 6). Also inherent in the use of partially constrained SMA (1) is the limitation that although the endmembers define the extreme range for mixtures of their classes, and only positive fractions adding to 1.0 are allowed (Fig. 6). The radiance nonuniformity with wavelength, visible in the curved lines in Fig. 6, contributes along with nonuniformity in temperature to confound the TINIT, contributing to endmember misidentification.

As previously discussed [19], SMA using this virtual cold technique was found to provide TINIT with a maximum ±4 K error range. Also, endmember and fraction estimates near the hot endmember temperature were good, but they became increasingly less accurate as the actual temperature departed from that of the hot endmember. Fig. 9 shows the results of the temperature and endmember estimation process. This figure has the same general format as Fig. 8, and the column on the right contains the calculated temperature error (TINIT-TISO). This synthetic image covers isothermal mixtures from 260 to 350 K, and was used to estimate the initial temperature error range (±4 K) used as the search range in the subsequent bounded search strategy.

B. Initial Temperature Estimate Constrained Isothermal Unmixing

As expected, the TINIT constrained TESSMA shown in Fig. 10 resulted in correct temperatures, endmember constituent assignments and constituent fraction estimates when the TINIT error range (±4 K) was used as the search range. This result occurs in the absence of confounding error sources. The fundamental benefit is found in the reduced time that it takes to process these images.

When the temperature search range is slightly underestimated, the search range is insufficient, and occasional fractional abundance errors are to be expected (Fig. 11). These fractional abundance errors were relatively infrequent, and constituent identification was correct for this set of endmembers.
When the temperature search range is significantly underestimated, considerable fraction errors should be expected, as well as constituent misclassification (Fig. 12). Our results indicate that it is important to properly characterize the error range of the initial estimate to search within a sufficient range of the initial estimate and achieve good final results. This effect should be exacerbated by other error sources, such as a missing library endmember match, sensor noise, or poor atmospheric modeling.

Figs. 9, 11, and 12 illustrate another aspect of the TINIT. The TINIT error range is reduced around the hot endmember temperature (Fig. 7). Underestimating the temperature error by 1 K produces correct estimates for the hot 2/3 of the image (Fig. 11). Underestimating the temperature error by 3 K produces good estimates for approximately 1/3 of the image, centered on the hot endmember temperature (Fig. 12). Using the TINIT results in correct estimates for a narrow band a few Kelvin around the hot endmember temperature. Selecting the hot endmember temperature at the expected average surface temperature should produce the best results using a narrow search range.

C. Error Sources

It is important to note that this method uses synthetic images whose endmembers match those of the spectral library. In addition, the atmosphere model used to generate the endmember library is the same as that used for the synthetic mixture image. When either of these diverge, endmember fraction accuracy, and eventually constituent attribution accuracy should degrade. It is also likely that the temperature error range of the TINIT would also increase as model and image atmospheres diverge.

Several difficulties contribute to errors in retrieved fractions and error estimates, among them

1) errors in atmospheric modeling, particularly temperature and water vapor profiles,
2) sensor models and noise degradation effects,
3) errors in the spectral library (i.e., missing endmembers),
4) scene geometry effects (e.g., buildings, bunch grass, shrubs, trees) on attributions (i.e., multiple reflection and emission).

We believe one of the most important problems to be solved before TESSMA can be applied to real data is to correctly characterize the atmosphere, which is possible using a hyperspectral sensor. The water vapor and temperature profiles together dominate the atmospheric variability, and are primary contributors to error when they are incorrectly estimated. These factors change over time and space, and may vary within the scene itself. Errors in estimating either profile are likely to generate at-sensor radiance estimates that depart from modeled radiances. Departures may result in systematic errors in temperature, which will translate to errors in endmember attribution and fraction estimates. For example, preliminary analysis of measured thermal data...
demonstrated that errors in estimating the atmospheric water vapor content resulted in SMA analyzes with unrealistic water fractions on land surfaces (results not shown). Similar results are expected if flight height and/or surface elevation varies, producing a different path length to the surface.

### D. Linear Mixing Constraints

One fundamental problem in the use of SMA in any wavelength range or region is the identification of representative endmembers. In the event that an endmember is present at the surface, but absent from the library, SMA will produce errors [26]. In the TIR, because spectral differences between endmembers (i.e., emissivity) are often low, these types of errors are likely to lead to larger errors in fractional abundance than is typical in the VNIR where spectral contrast is greater. In contrast, temperature errors are likely to remain modest K, except in the event that an unknown material has an emissivity that departs significantly from any member of the library. In the event this is true, the missing endmember may be identifiable because the error in fit will be large in the image. A good example of this is provided by Soil 2, which would have generated large errors in the models if it had been left out of the library (Fig. 2) but was present in the image. One very likely source of endmember variability is in soil endmembers, where compositional information (e.g., sands, silts, clays) and grain size effects can lead to significant variability in emissivity [27].

Complex scene geometries, intimate mixing of inhomogeneous substances, and multiple reflectance and emission effects associated with vegetation and/or structures involve unaccounted for reflectance of radiant energy emitted from another surface, and are not modeled in standard linear mixture approaches. Reflected radiative contributions from surfaces at different temperatures would further confound the process. For situations in which such factors are relevant, more computationally intensive techniques incorporating scene geometries [29] or nonlinear mixing models would be more appropriate.

### E. Processing Time

Accuracy of the TINIT affected the overall time required to run the next stage of the process. Evaluation of each temperature step requires 21 model evaluations per sample, and an exhaustive evaluation would require (models × temperatures) evaluations, or $21 \times 91 = 1911$ evaluations per sample. Using VC SMA, if the initial temperature estimation process (21 model evaluations) results in a perfect temperature estimate, the next stage will require only 21 more model evaluations, for a total of 42 evaluations per sample. This is rarely the case, and the actual number of evaluations per sample is (models × (2 + 2 × maximum absolute error/resolution)), or $(21 \times (2 + 2 \times 4 K/1 K)) = 210$ evaluations. In this case, when the error range of the TINIT is searched using the initial temperature constrained isothermal TESSMA, the resulting
estimates are correct, resulting in a factor of nine increase in speed over the exhaustive approach for processing this temperature range.

V. CONCLUSIONS

The constrained TESSMA technique produces a near-perfect unmixing of temperature, endmember attributions, and fraction estimates under perfect conditions, a result not attainable using non-SMA approaches of TES. However, reality has been and will continue to be a more challenging situation. Further research would be required in order to evaluate the relative performance of this and other approaches to TES for a given sensor over a variety of scenes.

A new approach is presented for mapping surface temperature and composition at subpixel scales using thermal imaging spectrometry. This paper presents a conceptual overview of this approach, a basic research structure for exploring this concept, and an outline of future work in support of this approach of extracting and refining temperature estimates and classifying hyperspectral TIR data on a subpixel basis. This approach utilizes a TINIT using virtual cold as a proxy for temperature, followed by a temperature constrained search algorithm to better estimate pixel constituents, their fractions and their temperature. Initial results, using simulated mixtures over a 260 to 350 K temperature range, demonstrated that this approach has the potential of estimating temperatures at accuracies less than or equal to 1 K, with near perfect identification of surface constituents and their fractional abundance. Major limiting assumptions in this test case include perfect modeling of atmospheric effects, uniform temperatures within a pixel (isothermal mixing) and the existence of a spectral library that includes all materials within the scene. When applied to real image data, errors in atmospheric modeling, atmospheric heterogeneity, anisothermal sub-pixel temperatures, and variability in the emissivity of materials will result in decreased accuracy. A fundamental goal of future research will be to determine the sensitivity of the constrained TESSMA technique to these errors.

Sensor fusion holds much promise for TESSMA, particularly with the introduction of sensors such as ASTER and MODIS. Bounding endmember and possibly fraction estimates using V/NIR data provides another means of extracting isothermal and anisothermal endmember temperatures. Combining multiple estimation methods may also yield better overall results.

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REFERENCES


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