Review Article

Hyperspectral geological remote sensing: evaluation of analytical techniques

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Abstract. Improvements in optical remote sensing spectral resolution and increased data volumes necessitates the development of improved techniques for quantitative geological analysis. Laboratory spectral studies indicate that absorption band positions, depths and widths are correlated with diagnostic physico-chemical mineral properties such as composition and abundance. Most current analytical techniques are incapable of providing comprehensive quantitative analysis of hyperspectral geological remote sensing data. Factors which must be considered for hyperspectral remote sensing campaigns include spectral resolution, analytical technique, band pass positions and spatial resolution. In many cases the volume of data required to address specific issues can be reduced through intelligent selection of band passes and analytical techniques.

1. Introduction

Technological improvements in multi-spectral remote sensing are providing opportunities for acquiring ever-increasing volumes of information as well as making more types of geological information potentially derivable. Two competing requirements must be satisfied when designing hyperspectral geological remote sensing campaigns: minimizing data volumes while maximizing information content. Consideration must also be given to the fact that data compression techniques may result in the loss of useful information and that many of the techniques developed for analysis of broad-band data (such as Landsat and SPOT imagery) may not be entirely suitable for analysis of hyperspectral data. A number of high resolution laboratory spectral studies of various classes of minerals have been undertaken to determine the quantity of information derivable from hyperspectral data and spectral resolution requirements. These studies are used to assess the applicability of various analytical techniques for deriving geological information from hyperspectral remote sensing data.

Over the years a number of analytical techniques have been developed for the analysis of remote sensing data. Most of these techniques were developed when broad-band instruments were the norm in remote sensing. With the advent of remote sensing instruments with programmable hyperspectral capabilities, such as the Compact Airborne Spectrographic Imager (Anger et al. 1994), it is necessary to examine the utility of traditional analytical techniques for hyperspectral data analysis and to determine the relative usefulness of each and potential drawbacks, if any. In order to provide a focused assessment, this analysis concentrates on the extraction

of quantitative geological information from hyperspectral data. A number of investigators have commented on the fact that new analytical techniques are required for the efficient analysis of hyperspectral remote sensing data (e.g., Mazer *et al.* 1988, Staenz 1992). Some investigators have found that hyperspectral imagery can provide greater mineralogical details than existing geological maps (Ben-Dor and Kruse 1994).

2. Spectral reflectance properties of various mineral classes

Many mineral classes, including most of the major rock-forming classes, have been the subject of systematic detailed spectral reflectance studies. The results are useful for determining the physico-chemical properties derivable from spectral analysis and spectral resolutions necessary for deriving these parameters. Some of these systematic studies are summarized below to illustrate the types of physico-chemical information that are derivable from hyperspectral data.

2.1. *Olivines*

Olivines are an important class of rock-forming minerals, whose reflectance spectra ($0.3-2.6\,\mu m$) are characterized by a broad absorption feature near $1\,\mu m$ (King and Ridley 1987). Previous spectral studies (Cloutis 1985, King and Ridley 1987) indicate that the wavelength position of the $1\,\mu m$ absorption feature varies as a function of Mg/Fe ratio with a total shift on the order of 30 nm (figure 1). The widths of the constituent bands in the $1\,\mu m$ region may also vary systematically as a function of Fe/Mg composition (Mustard and Sunshine 1992). The presence of other elements, such as Mn, Cr and Ni, can be detected by the presence of minor absorption bands shortward of $\sim 0.65\,\mu m$ (Hiroi *et al.* 1985, King and Ridley 1987, Sunshine and Pieters 1990). Overall reflectance generally increases with decreasing particle size while band depths decrease with decreasing grain size (Miyamoto *et al.* 1981, King and Ridley 1987).

These results suggest that high resolution spectra of olivines can be used to constrain the major and some minor cation abundances as well as average grain size. Given the magnitudes of the associated spectral variations, spectral resolution better than 30 nm is required in the $1\,\mu m$ region to permit the lowest level of quantitative compositional information to be derived. At increasingly finer spectral resolution, more detailed compositional information can be derived.

2.2. *Pyroxenes*

Pyroxenes are potentially important minerals for geological exploration because they are often associated with deposits of platinum group elements and chromite. Most pyroxene spectra are characterized by two major absorption bands located near $1\,\mu m$ (Band I) and $2\,\mu m$ (Band II) (figure 2). The wavelength positions of these bands can vary by up to 130 nm (Band I) and 500 nm (Band II) as a function of major element (Fe, Mg, and Ca) chemistry (Adams 1974, Cloutis and Gaffey 1991 a) (figure 3). Variations in major element composition for coexisting orthopyroxene-clinopyroxene pairs are a function of formation temperatures, enabling geothermometric data to be derived. By superimposing the spectral information with the geotherms on a compositional diagram, absorption band wavelength positions in compositional space can be used to constrain formation temperatures (Cloutis and Gaffey 1991 a).

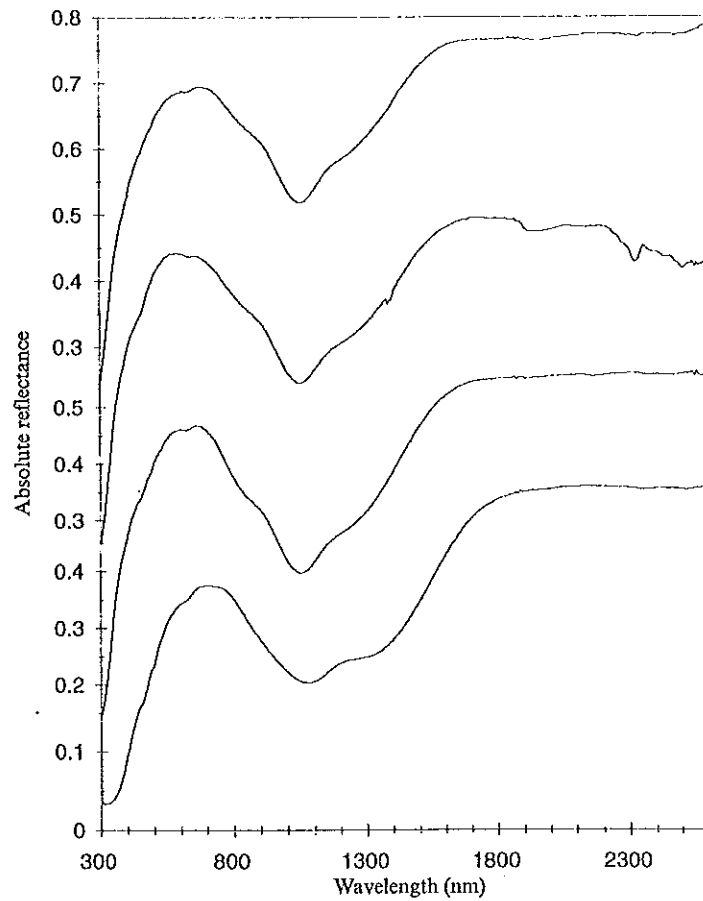Absolute reflectance values of pyroxene spectra are a function of grain size. As

Figure 1. Reflectance spectra (300–2600 nm) of <45 μm grain size olivines.

the grain size of pyroxene (and other mafic silicate minerals) decreases, overall reflectance increases; thus if grain size determination is important to the analyst, instrumental calibration becomes a critical issue. A factor of two decrease in mean particle size results in an approximately 70 per cent increase in overall reflectance (Cloutis 1985). These studies suggest that hyperspectral data can be used to derive compositional information that in turn can be applied to various geochemical issues.

2.3. *Amphiboles*

Amphiboles are compositionally more complex than pyroxenes, consequently interpretation of their reflectance spectra is less tractable. Calcic amphibole spectra are characterized by a number of absorption features near $1\,\mu$, $1.4\,\mu$m, and $2.3–2.4\,\mu$m (Mustard *et al.* 1989). Available amphibole spectra suggest that band wavelength positions and depths are probably related to major cation abundances and may be useful for deriving compositional information. The data suggest that variations in the position of the $1\,\mu$m absorption band are on the order of 60 nm.
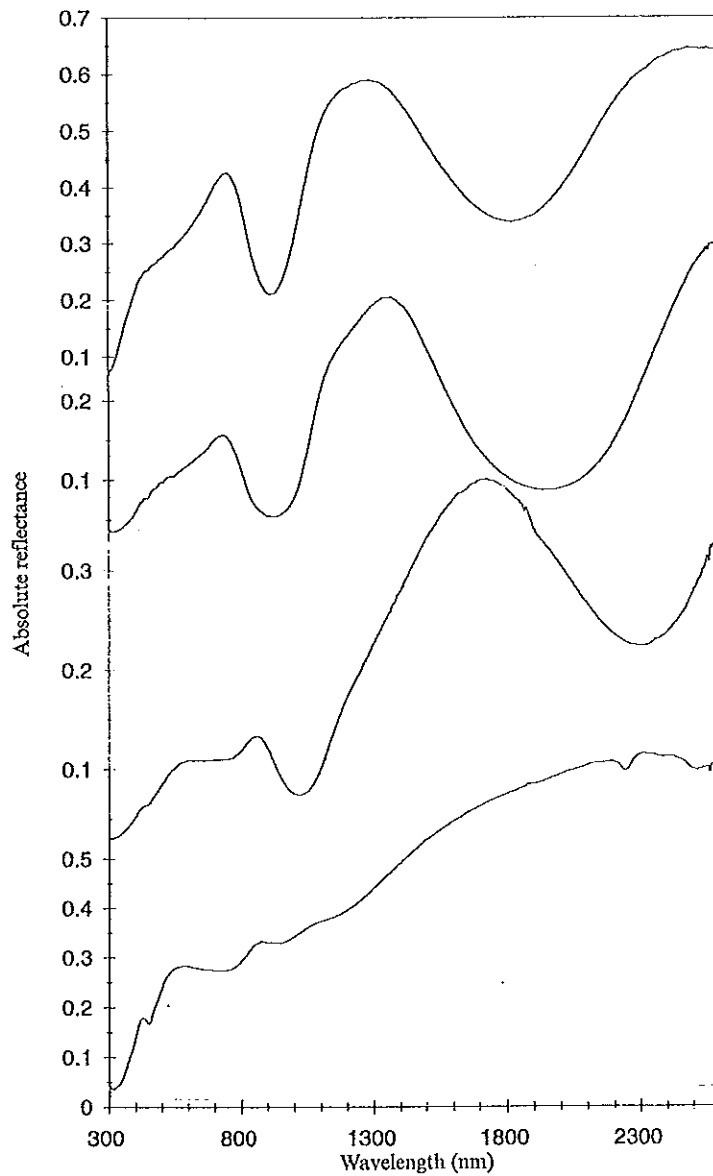
Figure 2.   Reflectance spectra (300–2600 nm) of <45 μm grain size pyroxenes.

2.4. *Feldspars*

Plagioclase feldspars are another important group of solid solution, silicate rock-forming minerals. Their reflectance spectra are generally characterized by an absorption feature in the 1·1–1·3 μm region, attributable to ferrous iron (Adams and Goullaud 1978). It was found that band wavelength position and depth are a function of iron content, and that iron content is roughly correlated with anorthite content. Decreasing grain size results in an increase in overall reflectance and decrease in band depth (Crown and Pieters 1987). It appears that high resolution spectral data
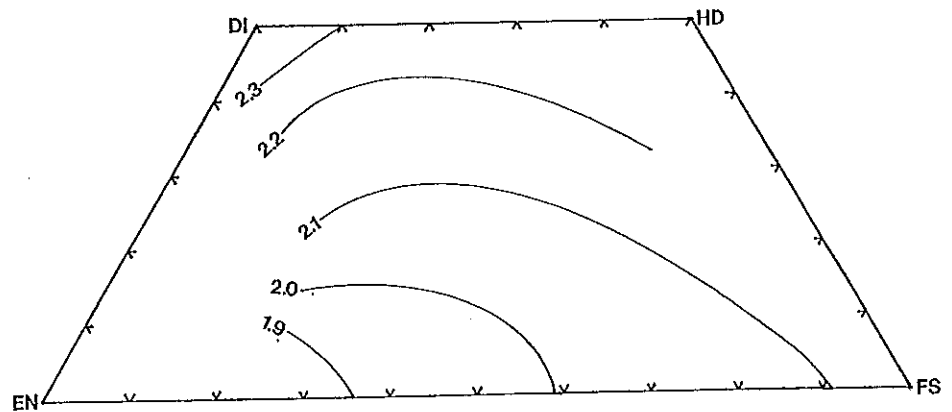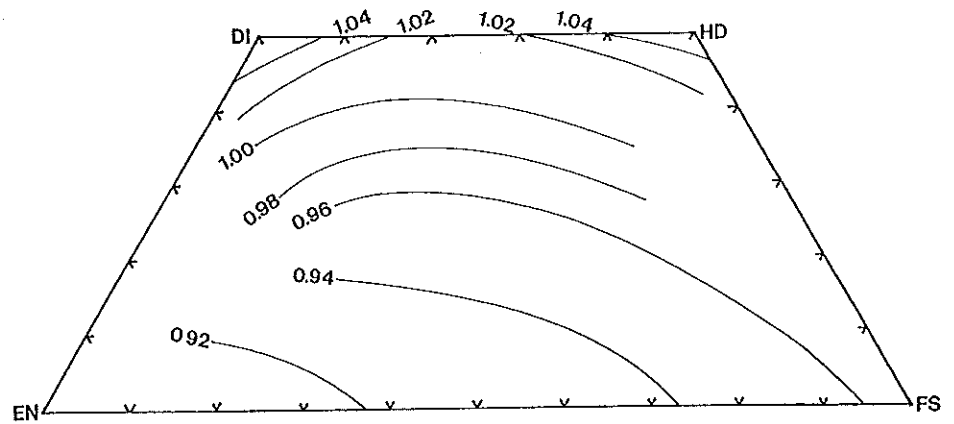
Figure 3. Pyroxene compositional tetralateral with wavelength positions of Band I (upper) and Band II (lower) superimposed (in microns).

(200 nm minimum spectral resolution) can be used to constrain major (Ca, Na) and minor (Fe) element abundances and grain sizes.

2.5. *Clay/phyllosilicate minerals*

Clay minerals are important elements for geological remote sensing because they are common products resulting from weathering of exposed rock surfaces. Clays exhibit a wide variety of spectral properties but identification of specific species often depends on small differences in the number, depth and wavelength positions of absorption bands (Hunt 1979, Hunt and Hall 1981, Crowley 1984, King and Clark 1989).

For most clay minerals, it has been found that the wavelength regions most useful for species discrimination are located near 1·4 μm, 1·9 μm and between 2·2 and 2·6 μm.

Spectral resolution in these regions should generally be better than 15–20 nm to permit accurate clay species discrimination and identification (King and Clark 1989). Spectral resolution on the order of 100 nm is only useful for identifying the presence or absence of clay minerals (Hunt 1979).

2.6. *Iron oxides/hydroxides*

Iron oxides/hydroxides and clay minerals are nearly ubiquitous weathering products for a range of rock types (Cloutis 1992). Different iron oxide/hydroxide species can be discriminated on the basis of absorption band wavelength positions. Differences in band positions between different species may be as small as 10 nm (Hovis 1965, Morris *et al.* 1985, Sherman and Waite 1985). Even smaller band position shifts may be useful for discriminating small differences in composition (Morris *et al.* 1985). Consequently high resolution reflectance spectra may be necessary for quantitative analysis of iron alteration minerals (Townsend 1987). Iron oxides/hydroxides also exhibit variations in absolute reflectance and band depths as a function of grain size, although the variations are not as systematic as for other mineral groups.

2.7. *Carbonate minerals*

Carbonate minerals are important because of their abundance, and potential economic significance (Gaffey 1987). Carbonate spectra exhibit a number of diagnostic absorption bands in the 0·3–2·6 μm region. Band wavelength positions, depths and widths can be used to characterize a wide range of physico-chemical properties, including species type, minor element composition, degree of site distortion and site symmetry (Gaffey 1985, 1986, 1987).

Band position differences on the order of a few nm are often required to discriminate different carbonate minerals (Gaffey 1987). Spectral studies have also shown that drying, heating, annealing and roasting may affect the physical and chemical properties of carbonates. The results suggest that spectral data may be used to infer diagenetic conditions (Gaffey *et al.* 1991).

2.8. *Mineral mixtures*

A number of studies have examined the spectral properties of mineral mixtures. These studies have shown that the spectral properties of intimate mixtures are not simple linear combinations of the end member spectra (e.g., Cloutis *et al.* 1986, Crown and Pieters 1987). A detailed discussion of the complexities inherent in unravelling mineral mixture spectra is beyond the scope of this paper. Empirical laboratory spectral studies can be used to unravel the relative effects of the end members but the time involved in generating and analysing sufficient numbers of mixture spectra is significant. Nevertheless these types of studies are useful for providing information on the spectral parameters which are affected by the introduction of additional mineral species and which spectral properties are most useful for deriving the various physical and chemical parameters of interest (Cloutis *et al.* 1986, Cloutis and Gaffey 1991 b).

A comprehensive study of the spectral properties of olivines and pyroxenes (Cloutis *et al.* 1986) found that the most diagnostic spectral parameters for deriving the physical and compositional properties of the mixtures include absorption band positions, band depths, band areas and absolute reflectance values. These parameters

are the same as those which have been determined to be most diagnostic for monomineralic assemblages.

In general the introduction of a second mineral will affect all of the key spectral parameters such as band depths, wavelength positions, widths, areas, and absolute reflectance. These results, and the fact that in operational remote sensing a spectrally 'pure' pixel is rarely encountered (i.e., a pixel containing only a single, spectrally homogenous material), are the major impetus for the development of techniques which can be used to derive the spectral properties and abundances of various end members.

3. Hyperspectral versus broad-band remote sensing

The advent and continued growth of hyperspectral remote sensing imaging systems, which acquire tens to hundreds of bands of spectral information for each pixel in a scene, will necessitate the development of techniques which can efficiently and accurately analyse the tremendous volumes of resultant data. Obviously, the techniques which are developed and applied to data analysis will depend on the nature of the problem being addressed and the level of accuracy required. The high spectral resolution geological study results suggest that hyperspectral remote sensing provides the potential to conduct previously unimagined levels of geological mapping and exploration. Consequently, analytical techniques developed for analysis of broad-band spectral data, such as Landsat and SPOT imagery, may be incapable of taking advantage of the full range of information present in hyperspectral remote sensing imagery. Some of the issues of importance in hyperspectral remote sensing are discussed below.

3.1. *Spatial resolution variations*

The issue of spatial resolution is one which will be of increasing importance in future remote sensing campaigns. The advent of terrestrial remote sensing satellites with spatial resolutions on the order of a few metres (e.g., Duval *et al.* 1989, Rast and Bezy 1990, Henderson 1995), will impact geological remote sensing in a number of ways. Increased spatial resolution will provide a greater likelihood of imaging pixels which are more 'pure' in the sense that as pixel size decreases fewer components will be present in a given pixel. This will result in improvements in spectral unmixing as end member spectral signatures will be more readily obtainable (see § 4.4 below).

Increased spatial resolution will also facilitate detailed surficial mapping. If, as expected, smaller pixels result in less mixed pixels, more subtle surface composition variations will be mappable than are currently possible. This capability has already been demonstrated in a number of studies (e.g., Kneppeck and Ahern 1989, Marceau *et al.* 1994).

3.2. *Spectral resolution variations*

Spectral resolution will affect the quality and quantity of geological information derivable from optical remote sensing imagery. The results of some previous studies are briefly discussed below to illustrate how spectral resolution variations can affect geological interpretations.

Rowan *et al.* (1977), using ground-based high resolution spectra and Landsat Multi-Spectral Scanner (MSS) imagery, found that some limited lithologic discrimination was possible using Landsat MSS band ratios which minimizes the effects of topography and overall albedo. Spectral normalization was also found by Pieters

(1983) to be effective for minimizing the effects of viewing geometry. Rowan *et al.* (1977) noted that lithologic discrimination was dependent on the presence of ferric iron oxides. A similar spectral study by Townsend (1987) found that different iron-alteration minerals could be discriminated with appropriate band passes.

Hunt and Salisbury (1978), Blom *et al.* (1980), and Kruse (1989) compared hyperspectral to broad-band data for lithologic discrimination. In all cases, the higher spectral resolution data provided greater classification accuracies while broad-band instruments provided only limited lithologic mapping capabilities.

High resolution reflectance spectra of a suite of soil samples have been used to ascertain that a number of spectrally active soil constituents could be derived from statistical analysis of the spectral-compositional data (Ben-Dor and Banin 1994). The number of data points required to derive the compositional parameters ranged from 25 to 3113, suggesting that instruments with a limited number of spectral bands would be incapable of discriminating the various soil properties.

Field-based spectra were used by Rowan and Kahle (1982) to determine that Landsat Thematic Mapper (TM) imagery could provide some broad lithologic discrimination on the basis of the presence of some spectrally diagnostic minerals, but would be incapable of discriminating some types of hydrothermally altered and unaltered rocks. They concluded that high spectral resolution data in the 2·0 and 2·5 μm regions would be required for enhanced lithologic discrimination.

High spectral resolution airborne imaging spectrometer (AIS) data were evaluated by Pieters and Mustard (1988) for mapping mineralogical variations. They found that the data could be used to identify the presence of several mineral components of the surface materials and analysed in a spatial context. The level of analytical accuracy was such that specific geological problems, such as eruption/flow patterns, could be addressed. They determined that the signal to noise ratio of the data is the ultimate limitation to the accuracy of deconvolving individual spectral components. It was also determined that spectral coverage affects the ability to derive minera-logical information.

King and Clark (1989) and Clark *et al.* (1990) measured high resolution reflectance spectra of various minerals. Wavelength positions and depths of some diagnostic absorption bands were found to be correlated with various compositional parameters. It was determined that spectral resolution greatly affected the ability to derive these compositional parameters and to discriminate different phyllosilicate species. While increased spectral resolution would enhance the ability to discriminate the different species, in a practical remote sensing campaign this would result in increased data volumes. However, it was found that with increased spectral reso-lution, less wavelength coverage was required to discriminate among various ser-pentinites. It was also found that the ability to discriminate different minerals and to derive compositional information increased with increasing spectral resolution.

Singer *et al.* (1984) examined the ability of broad-band optical remote sensing instruments (Landsat TM and SMIRR) to discriminate and identify specific rock types and mineral species. They determined that while some discrimination of iron oxide species may be possible with these instruments, they can not be used to discriminate different species of clays and carbonates and for mineralogical analysis of basalts, and are poorly suited for iron oxide species discrimination. It was suggested that band passes of 25 nm or better would be required to accomplish these tasks.

These aforementioned studies all suggest strongly that geological and mineralo-gical discrimination is greatly dependent on spectral resolution as well as indicating

that some spectral regions are more diagnostic than others for mineralogical discrimination. The spectral resolution and wavelength intervals sampled will depend on the geology of the study area, as well as the types of issues which a remote sensing study is designed to address. Further summaries of geological remote sensing campaigns can be found in a number of textbooks such as Sabins (1987).

The effects of varying spectral resolution on the spectral properties of clays are illustrated in figure 4. It can be seen that for clay spectra with narrow absorption
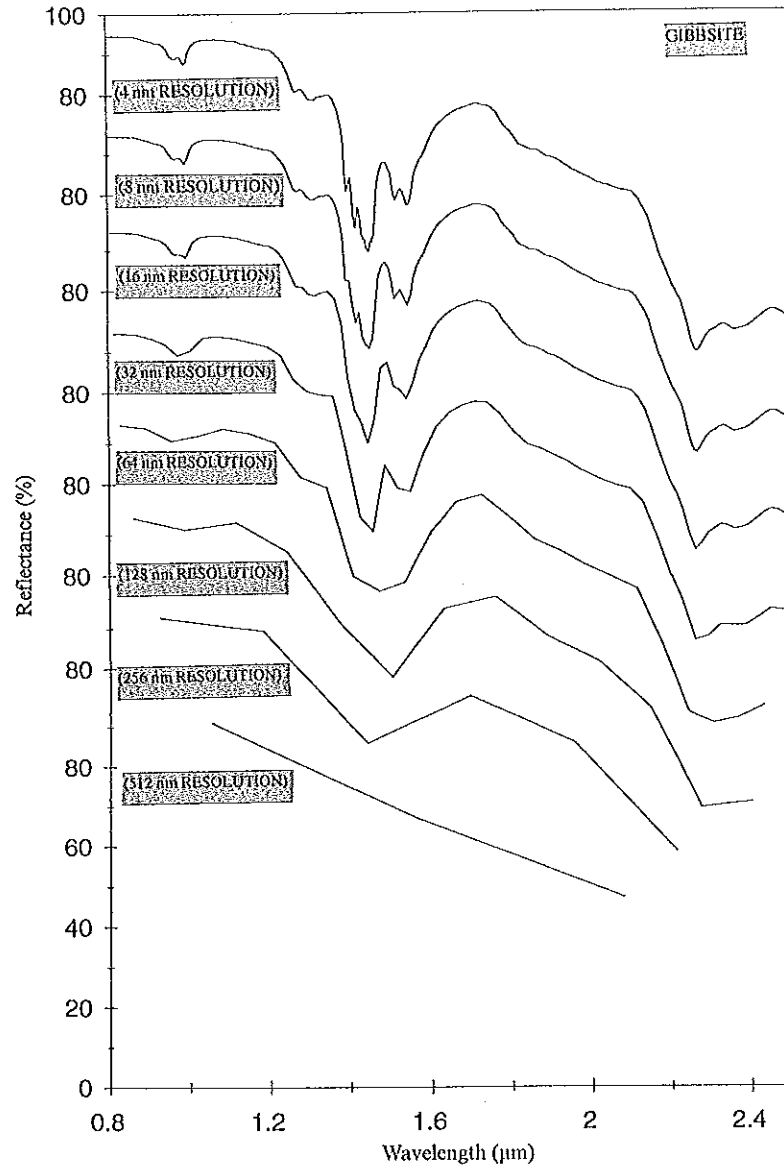

Figure 4.   Effect of successive halving of spectral resolution on the reflectance spectrum of gibbsite (Grove *et al.* 1992).

features, a doubling of spectral resolution from 8 to 16 nm can result in the apparent 'disappearance' of absorption bands in the 1·4 μm region (gibbsite in this case).

3.3. *Spectral band pass position effects*

With the advent of hyperspectral remote sensing systems which are programmable in terms of spectral resolution, the issue of band pass wavelength position may be a factor in qualitative data analysis and perhaps for quantitative analysis as well. Hyperspectral imaging systems will provide the opportunity for direct mineralogical mapping and mineral species identification. As mentioned above, mineral species discrimination in some cases relies on differences of a few nanometres in wavelength positions of absorption bands.

The effect of altering band pass wavelength positions is shown in figure 5 for two spectra of dickite, both with 16 nm resolution. The wavelength positions of the band passes differ by 8 nm. The appearance of the absorption feature near 1·4 μm is dramatically different for the two spectra, even though spectral resolution is the same in both cases (16 nm). At 32 nm resolution, the two absorption bands are not visually resolvable.

4. Techniques for analysis of hyperspectral remote sensing data

The laboratory spectral studies cited above provide some guidelines for assessing the applicability of various analytical techniques to hyperspectral data analysis. The applicability of each technique will of course depend on the particular issues being addressed. Since hyperspectral data provides the opportunity for conducting quantitative geological/mineralogical information extraction, various techniques can be evaluated for how well they address these issues.

The hyperspectral studies summarized above indicate that quantitative mineralogical information can be derived from spectral parameters such as band wavelength positions, depths, widths, areas and absolute reflectance values. Evaluation of the various 'preprocessing' techniques which may be applied to hyperspectral imagery to correct for atmospheric effects (in order to derive absolute reflectance values) and for geometric distortions are beyond the scope of this study. A number of the most common analytical techniques are summarized briefly below along with some specific applications of each. These results are useful for assessing the benefits and limitations of each as well as for assessing their potential for analysis of hyperspectral data.

4.1. *Derivative analysis*

Derivative spectroscopy involves fitting mathematical functions to reflectance spectra and determining various orders of derivatives. The benefit of derivative analysis is its ability to provide rapid determination of inflections points (which may be indicative of overlapping absorption bands) as well as reflectance maxima and minima. Derivative analysis has been applied to the analysis of extraterrestrial reflectance spectra (Huguenin and Jones 1986), water quality parameters (Dick and Miller 1991, Goodin *et al.* 1993, Farrington *et al.* 1994), and vegetation stress monitoring (Demetriades-Shah *et al.* 1990). It was found that derivation could be used to deconvolve overlapping absorption bands and to derive various target parameters. For geological remote sensing, derivative analysis can be used to derive various significant spectral parameters such as band positions, depths, and perhaps band widths (Huguenin and Jones 1986).

The signal to noise ratio can affect the accuracy of derivative analysis. In most
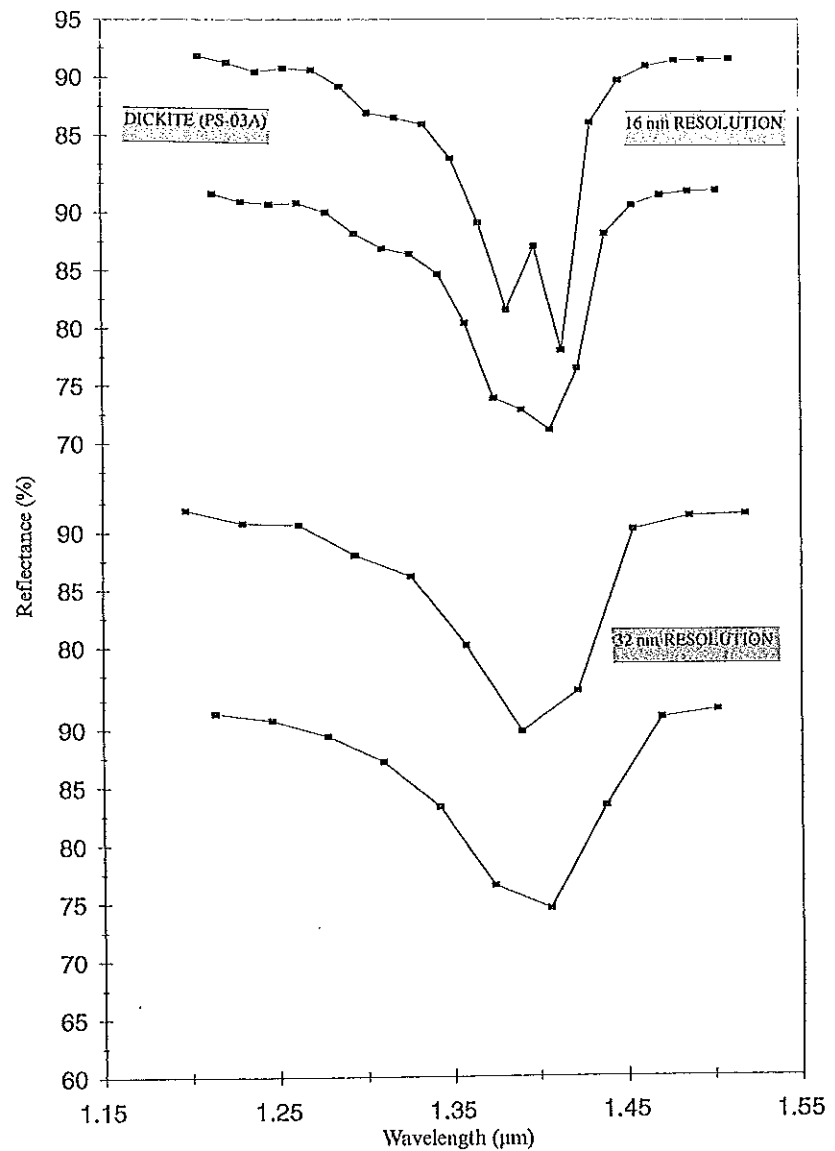
Figure 5. Effect of varying band pass positions on the reflectance spectra of dickite (Grove *et al.* 1992).

cases it has been found that some level of spectral preprocessing (generally involving some form of noise suppression) is required prior to derivative analysis. It has long been known that the accuracy of derivative analysis is sensitive to the signal to noise ratio of the data; progressive differentiation will increasingly accentuate this noise.

A review of derivative spectroscopy by Singer and Geissler (1988) found that the noise and other small random variations in reflectance spectra will have a pronounced effect on the derivative results. It was determined that lower order derivatives are less sensitive to noise and hence more useful in operational remote sensing.

4.2. Vegetation 'red edge' derivative analysis

A variation of derivative spectral analysis involves analysis of the so-called vegetation 'red edge'. Reflectance spectra of vegetation commonly exhibit a steep rise in reflectance near 750 nm, termed the vegetation red edge. A number of investigators have attempted to use the wavelength position and shape of this reflectance rise to characterize various vegetation parameters (e.g., Horler et al. 1983, Filella and Peñuelas 1994). More detailed analyses involve modelling this wavelength region using inflection ratios (Campbell and Esaias 1983) and derivative spectra. These models suggest that various plant parameters can be derived from various characteristics of the red edge (e.g., Miller et al. 1990, Feng and Miller 1991, Miller et al. 1991). It has been found that the vegetation red edge is a function of a number of environmental and plant parameters and given the complex interplay of the various parameters, may in fact not be useful for many of its anticipated uses (Banninger 1989, Boochs et al. 1990, Railyan and Korobov 1993). 'Red edge' derivative analysis is essentially a specialized application of derivative spectroscopy discussed above, with many of the same advantages and disadvantages of derivative spectroscopy.

4.3. Spectral matching

One approach to the analysis of remote sensing data for surface characterization or change detection is spectral matching. This approach involves matching scene spectra to reference spectra or comparing scene spectra to a spectral library in order to highlight differences. Spectral matching has been used to isolate spectral features of interest for detailed analysis (Goetz et al. 1990, Yasuoka et al. 1990) and for direct comparison of scene to reference spectra (Goetz and Srivastava 1985, Ben-Dor and Kruse 1994). It has also been used for geological analysis of hyperspectral remote sensing data using neural networks (Segl et al. 1994). The effort required in spectral library searching has necessitated the development of new search criteria whereby robust analyses are possible while minimizing searching times (Kawata et al. 1987). Lyon and Zhu (1989) argue that in addition to absorption band wavelength position and depth, spectral shape is an important criterion that should be included in spectral analysis as it can greatly simplify spectral matching using pattern recognition.

4.4. End member mixing models

In order to improve the quantity and quality of information derivable from remote sensing imagery, a number of techniques have been developed which can be broadly classified as spectral mixing models. These models generally involve analysis of spectral data in order to determine target parameters such as the fractional abundances of various end members within a pixel, or the identification of additional components not used in the end member analysis. These techniques have been applied to a number of geological mapping studies (Adams et al. 1986, Mustard and Pieters 1987 a, Boardman 1990, Sabol et al. 1992, Ben-Dor and Kruse 1994, Farrand and Harsanyi 1995) as well as other land cover mapping applications (Foody and Cox 1994, Gong et al. 1994).

The ability to detect different surface materials in end member analysis of broadband data is a function of spectral contrast, noise and spectral resolution (Shipman and Adams 1987, Sabol et al. 1990, Zhang et al. 1993). Some studies have concluded that for simple land cover targets, only a few end members are required to fully characterize a scene (Johnson et al. 1984, Smith et al. 1984, Huete and Escadafal

1990). Other studies have determined that full scene characterization requires the analysis of residual spectra which result after the end members used in the analysis have been modelled (Green and Craig 1985, Herrmann *et al.* 1988, Hutsinpiller 1988, Roberts *et al.* 1993), or the application of successive mixture analyses (Chabrillat *et al.* 1994). In some cases improved analysis may be possible by applying mixture models to data initially processed by other means such as principal components analysis (Hurcom *et al.* 1994). End member mixing analysis of hyperspectral data can be used to address issues which may otherwise be intractable using broad-band data (Smith *et al.* 1990).

4.5. *Maximum likelihood classification*

Maximum likelihood classification (MLC) is an analytical technique based upon assigning pixels to various classes on the basis of similar spectral properties, on the assumption that the probability for each spectral class is in the form of a multivariate normal model with dimensions equal to the number of spectral bands. This technique has been extensively applied to the analysis of broad-band remote sensing data. Computational requirements increase significantly with increasing number of spectral bands. In order to reduce computational demands, Jia and Richards (1994) found that processing time could be reduced by dividing hyperspectral data into several wavelength subgroups. However, in contrast to other techniques such as derivative analysis, MLC includes the noise in the data and hence would not result in an inadvertent loss of potentially useful spectral information. In this sense it provides solutions with the highest probability of being correct (DeNoyer and Dodd 1991). The greatest advantage of MLC is its ability to rapidly assign scene pixels to any one of several classes.

4.6. *Principal components and canonical analysis*

Principal components analysis (PCA) is an analytical technique based upon a transformation of spectral axes such that spectral variability is maximized. This technique is found to be quite useful for analysis of remote sensing data for which certain channels exhibit high degrees of dependence. PCA has been applied to various geological remote sensing projects involving both broad-band and high resolution data (Lee *et al.* 1990, Bogliolo *et al.* 1994) as well as in laboratory spectral analysis (Devaux *et al.* 1988 a, b). Loughlin (1991) found that PCA of selected Landsat TM bands could be used to highlight mineralogical variations of interest while minimizing the effects of non-desirable mineralogical variations. Rundquist and Di (1989) have developed a variation of PCA, termed band-moment analysis which accounts for variations in reflectance value distributions such as mean, standard deviation, skewness and kurtosis. These values are applied on a band-by-band basis and hence are poorly suited for deriving parameters such as band positions and band widths.

Canonical analysis is essentially a variation of principal components analysis in which the principal components are designed to maximize the separability between different land cover classes (e.g., Avery and Berlin 1985). Most of the benefits and limitations of principal components analysis apply to canonical analysis as well. Canonical analysis has been used by a number of investigators to provide lithologic discrimination (e.g., Merembeck *et al.* 1977, Podwysocki *et al.* 1977). However the limitations of broad-band data limit this technique to very generalized lithologic discrimination.

4.7. *Linear regression*

Linear regression is a technique, adapted from analytical chemistry, for determining parameters of interest from spectral data. This technique requires the availability of a statistically robust number of spectra from which spectral-compositional relationships are derived. Linear regression can be applied to either unprocessed or derivative spectra. This technique has been found to be useful for deriving various crop and water quality parameters (Dekker *et al.* 1990, 1991, Shibayama and Akiyama 1991). Linear regression can also be used to select diagnostic wavelength regions, thereby reducing the volume of data required to address particular issues (Dekker *et al.* 1990).

4.8. *Ratio analysis*

A technique related to analysis of residuals resulting from end member mixing models is ratio analysis. In this technique, target spectra are first divided by a reference spectrum. This allows features of interest to be accentuated. This technique has been applied to the analysis of water and plant spectra for pigment identification and analysis (Chappelle *et al.* 1990, 1992). This technique possesses a number of operational limitations common to some of the other analytical techniques.

4.9. *Spectral decomposition*

Under this heading are included a number of analytical techniques designed to derive quantitative spectral-compositional relationships from empirical studies. Huete and Escadafal (1991) analysed soil spectra in terms of underlying 'basis' curves. They found that linear combinations of four of these basis curves could be used to reconstruct outdoor soil spectra. Huete (1986) applied a similar technique to the analysis of soil–plant mixture spectra. Lucey *et al.* (1989 a, b) used laboratory reflectance spectra of lunar samples to generate a grid of three component mixtures which were used to match lunar surface spectra and to derive mineralogical abundances.

4.10. *Spectral deconvolution*

Optical remote sensing data rarely contain 'pure' pixels, i.e., a pixel composed entirely of a single component which is spectrally homogenous across the entire pixel. Such pixels are generally required for various analytical techniques such as end member mixing and for radiometric calibration. Normally, a pixel will contain more than one type of material and/or be spectrally heterogeneous. In order to fully decompose a remote sensing image, the various components in the scene must be identified and their abundances and other physico-chemical properties quantified. In hyperspectral remote sensing data, the presence of more than one scene component will often lead to overlapping absorption bands. In order to quantify the scene, the relative spectral contributions of each component must be determined.

Much effort has been expended on developing techniques to deconvolve composite spectra into individual components. Various curve fitting techniques have been developed based on presumed shapes of absorption bands and degrees of overlap. It has been found that the ability to resolve overlapping absorption bands is a function of the signal to noise ratio and the degree of overlap (e.g., Kaper *et al.* 1966, Maddams 1980, Nadler *et al.* 1989, Pierce *et al.* 1990). Techniques have been developed to resolve component spectral features within these limitations (e.g., Kauppinen *et al.* 1981, Harbecke 1986, Hawthorne and Waychunas 1988).

In the area of hyperspectral geological remote sensing, Kruse (1988) developed a technique to determine the position, depth and width of the strongest absorption band in each pixel in AIS imagery. He found that this parameter could be used for limited mineralogical mapping. Mineralogically significant factors, such as band position and width, would normally not be derivable from broad-band data. Green and Craig (1985) have developed techniques for removing the effect of background continuum from reflectance spectra so that individual absorption bands can be isolated and analysed. They found that this approach is useful for comparing reflectance spectra from diverse sources.

4.11. *Theoretical treatments*

Under this heading are included a variety of methodologies which attempt to model reflectance spectra on the basis of scattering and absorption properties of minerals and rocks. Hapke (1981) developed approximate analytical solutions to the radiative transfer equation describing the scattering of light from particulate surfaces. This approach allows the spectral reflectance properties of a wide range of particulate surfaces to be modelled. However, even with the simplifications, application of the model to the analysis of reflectance spectra relies on the determination of some optical properties of the materials being studied as well as some simplifying assumptions whose validity may not be widely applicable.

Johnson *et al.* (1992) have developed a number of simple algorithms for modelling the reflectance spectra of mineral particulates. The derived approach involves a number of steps and ultimately relies on deriving a synthetic spectrum that best matches a target spectrum. An alternative approach to modelling reflectance spectra is the so-called 'isograin model' (Hiroi and Takeda 1989, Hiroi and Pieters 1991, 1992). This model involves calculating the proportion of light scattered and reflected from multiple layers and requires the input of optical constants for the constituent minerals. The results of this model compare favourably with the more rigorous model of Hapke cited above (Hiroi and Pieters 1994).

Mustard *et al.* (1986) and Mustard and Pieters (1987 b, 1989) developed a number of simplifications to the Hapke (1981) model which greatly simplify its application to reflectance spectral analysis. For accurate analysis the model requires empirical data in the form of reflectance spectra over a range of phase angles and well characterized particle size distributions. In situations where this information is lacking, relative mineral abundances can still be derived.

Kinoshita and Miyamoto (1990) developed a methodology for predicting the reflectance spectra of mineral mixtures on the basis of the reflectance and transmittance properties of the mineral components. The disadvantage of this method is its reliance on knowing both the reflectance and transmittance properties of potential end members.

4.12. *Modified Gaussian model analysis*

The last few years have witnessed the development of a new analytical technique for analysis of reflectance spectra—the modified Gaussian model (MGM). This technique was developed in order to address inconsistencies in the use of Gaussian or Lorentzian profiles in fitting of absorption bands. Comparative analysis of the MGM to other curve fitting models indicates that the algorithm is firmly rooted in crystal field theory and hence provides more valid results (Sunshine *et al.* 1990). MGM is used to model reflectance spectra as a series of modified Gaussian curves

with each curve characterized by a central wavelength position, width and depth. Using this method, the characteristic absorption bands present in reflectance spectra can be quantified.

While this technique is fairly new, it has been applied to a number of geological studies. These include characterizing mineral chemistry of tremolite–ferroactinolite solid solution series minerals (Mustard and Sunshine 1992), deriving compositional information for olivines (Sunshine and Pieters 1990), deriving compositional and abundance information for pyroxenes and pyroxene mixtures (Sunshine et al. 1988, Sunshine and Pieters 1993), deriving mineralogical and mafic silicate compositional information for the surface of Mars (Sunshine and Mustard 1994), lunar and terrestrial basalts (Sunshine and Pieters 1991) and martian meteorites (Sunshine et al. 1993). MGM analysis can be used to identify the presence of specific minerals in mixtures, to quantify compositions, and to identify the presence and perhaps types of any accessory phases (Mustard 1991). For pyroxene reflectance spectra it was found that modal abundances of pyroxene mixtures could be estimated to within 5–10 per cent without predetermined knowledge of end member spectra and that the results are largely independent of particle size.

5. Discussion

Few studies have been conducted to compare the quantity and quality of lithologic information derivable from hyperspectral data with different analytical techniques. Feldman and Taranik (1988) compared the results obtained using band ratios, principal components analysis and spectral matching for geological mapping of a study area in Nevada from AIS hyperspectral imaging data. They found that spectral matching provided the highest level of discrimination of alteration minerals followed by principal components and band ratios. Several papers in the volume edited by Vane and Goetz (1985) also compare the results of applying various analytical techniques to the analysis of airborne hyperspectral data. In general it was found that the use of spectral libraries provided the highest levels of classification accuracy. Clark and Roush (1984) have reviewed the various techniques developed for analysis of reflectance spectra. They found that while empirical studies are useful for some applications, the development of bidirectional reflectance theories are more promising because of their wider applicability.

Many analytical techniques specifically developed for analysis of hyperspectral remote sensing data are limited, largely for practical reasons, in that they fail to provide a sufficient capability for analysing the full range of compositional information inherent in parameters such as absorption band positions, depths, widths, and areas (Mazer et al. 1988, Staenz 1992). Given the relative paucity of comparative studies, the results of hyperspectral laboratory and comparative studies cited above can be used to assess the relative efficacy of various analytical approaches for the effective analysis of hyperspectral remote sensing data.

No single analytical technique can be used to fully deconvolve hyperspectral data in the absence of ancillary data. However, comparison of the various techniques suggests that some are more suited than others for hyperspectral data analysis for a variety of reasons, such as ability to isolate diagnostic absorption features, ease of application, and reduced computational demands.

The maximum likelihood and principal components techniques, which were largely developed for analysis of broad-band data could, in theory, be applied to analysis of hyperspectral data for direct lithologic discrimination. However each

possesses certain inherent limitations which would limit their usefulness for full quantitative analysis of hyperspectral data.

Maximum likelihood classification (MLC) is not particularly well suited to this task because of its inability to properly analyse mixed pixels. Meaningful quantitative information from spectral parameters such as band wavelength positions, widths, depths and shapes are also not directly derivable from MLC. Its greatest benefit is in rapidly assigning scene pixels to any one of several classes. MLC could perhaps be combined with other analytical techniques such that pixels are assigned to one of several classes on the basis of certain lithologic/spectral parameters and the pixels in each class subsequently analysed using other techniques.

One of the advantages of principal components analysis (PCA) is that spectral discrimination can be maximized in the first few principal components. However, determining the physical significance of each principal component is difficult. In addition, since mineralogically significant variations may be associated with minor spectral differences, these differences are often relegated to the higher order principal components which are normally ignored in the analysis, since the first few principal components can generally account for upwards of 95 per cent of the spectral variation. Consequently, PCA is perhaps better suited for identifying gross mineralogic and lithologic variations rather than quantitative mineralogical identification and mapping.

If full mineralogical discrimination were required, such that end member abundances and subtle variations in composition could be derived, this would require an exceedingly large number of end members for maximum likelihood classification or analysis of the full complement of principal components. In the latter case, relating the various principal components to mineralogically significant factors would be difficult at best.

Derivative spectroscopy, whereby spectra are fitted by various mathematical functions which are then differentiated may introduce artifacts due to noise amplification. Intuitively one expects that some information may be lost in derivative analysis due to noise suppression (filtering) and curve fitting. The major impediments to derivative analysis are the extensive preprocessing required (and associated sensitivity to filter type), undesirable amplification of spectral noise, and potential loss of information during filtering and curve fitting. The major benefit of derivative analysis is its ability to often resolve partially overlapping absorption bands. Derivative spectroscopy is probably less robust than analytical techniques that do not require differentiation, such as MGM, since these non-differentiation techniques are not affected by noise amplification and filtering.

Spectral matching is a promising analytical technique if probable target spectra are available in spectral libraries. However, extraneous factors such as viewing geometry effects and grain size variations, which are not central to mineralogical identification, must be accounted for if valid interpretations are to be derived. These effects can often be minimized through spectral normalization (Pieters 1983, Barnes *et al.* 1989). Spectral matching is probably more useful for scene change detection (Yasuoka *et al.* 1990) rather than the identification of unknown scene components. It appears that the full benefits of spectral matching would be realized when combined with other analytical techniques such as MGM or various modelling algorithms.

Linear regression is somewhat useful for spectral analysis because the analysis can be targeted to derive scene parameters of interest. A potential drawback is the possibility of the presence of additional spectral components in a scene which could

adversely affect the spectral-compositional correlations. Consequently, the results for one study area may not be applicable to other areas. In addition, ground-based (non-spectral) data are normally required for analysis.

The major limitations of end member mixing models are that the number of end members must be less than the number of spectral bands of data used in the analysis. This would normally not be a problem for hyperspectral imagery. In addition, the identification of 'pure' end member spectra is sometimes problematic. The presence of additional scene components not included in the analysis could lead to erroneous results and their identification and abundance could only be addressed by analysis of the 'residuals', an area of research which requires further investigation.

Ratio analysis has the advantage of resulting in no loss of information. However, it is probably of limited usefulness for many of the reasons outlined for linear regression: the results from one study area may not be applicable to other targets due to the presence of additional, unanticipated scene components. In addition, linear regression would probably yield similar statistical results without the need for the intermediate step of reference spectrum division. The main advantage of this technique appears to be providing a visual enhancement of spectral differences but does not supplant other analytical techniques; rather it represents an intermediate processing step.

Spectral decomposition may be useful for studies with very limited objectives and extent. This technique appears to be more suited for analytical laboratory work where material characterization is performed on a single type of material. The heavy reliance on empirical data and limited applicability outside of narrowly defined project objectives also limits its widespread utility.

The majority of the theoretical treatment studies cited above are designed to model the spectral reflectance properties of mineral mixtures. The major impediments to widespread applications of these models can be attributed to any one of a number of reasons: the difficulty of application, the requirements for empirical data—sometimes extensive—limited applicability in some cases, and the number and nature of simplifying assumptions. Nevertheless, this avenue of approach is perhaps the most promising because of the probability that continued development of these techniques will lessen the requirements for supporting empirical data.

Spectral deconvolution is a potentially powerful analytical technique provided proper curve shapes are used in the analysis. In order to interpret the various absorption features, it will probably be necessary to refer to reference spectra contained in some sort of spectral library.

MGM analysis possesses a number of advantages over other analytical approaches. The mathematics are more firmly rooted in the physical processes of electronic absorptions; the sensitivity can be limited by the signal to noise ratio, and can be used to reduce hyperspectral data volumes by reducing reflectance spectra to a series of modified Gaussian curves with almost no loss of information. In addition, this technique can be used to identify the minerals contributing to a reflectance spectrum, and to constrain their abundances and compositions. The MGM method has also been found to be relatively insensitive to particle size variations (Sunshine and Pieters 1991). MGM analysis could also readily be applied to the data in spectral libraries, resulting in simplified spectral searching.

Given the goal of geological remote sensing to quantify reflectance spectra in terms of the abundances and compositions of the spectrally contributing components, MGM analysis represents an important advance in this area, particularly if the

results found for the mineral species examined so far can be extended to other species. To date there are no indications that this expansion cannot be accomplished. This technique is particularly well suited for analysis of hyperspectral geological remote sensing data and with continued improvements in software its application will be further simplified, permitting increasing automation of spectral analysis.

Spectral deconvolution and MGM appear to hold the most promise for detailed spectral analysis. These approaches are potentially capable of isolating absorption features of interest which laboratory spectral studies have found are capable of providing detailed information on factors such as mineralogical compositions and end member abundances. The major drawback to these approaches is the requirement of a spectral library in a form suitable for analysis with the particular methodology employed.

It should be evident that no analytical technique can provide quantitative mineralogic/lithologic information without a knowledge of the spectral properties of potential target materials. Otherwise the analysis results in the identification of unknown components whose abundances and compositions are poorly constrained at best. Consequently spectral libraries in some form will continue to be an essential component of quantitative mineralogic/lithologic analysis.

The quantity of data which would be acquired even in the course of a modest hyperspectral remote sensing campaign can number in the millions of individual spectra. If quantitative mineralogical information is required, each of these spectra must be individually analysed. The consequence of the relative infancy of the various spectral deconvolution techniques is that they have not yet been fully adapted for automated data analysis. Once the validity of these techniques is more fully demonstrated, dramatic improvements in ease of application are expected. This has already proven to be the case for spectral matching (e.g., Segl *et al.* 1994) which, it appears, will be a central feature of spectral deconvolution in some form.

The ability to conduct increasingly detailed geological interpretation of remote sensing data is largely correlated with spectral resolution. Programmable hyperspectral scanners (Anger *et al.* 1994) allow spectral resolution to be varied for a particular application, resulting in reduced spectral resolution (and reduced data volumes) for wavelength regions of low diagnostic potential.

Using the pyroxene spectral study as an example, the resolution of the spectral data used in the analysis was on the order of 5 nm. This translates into 461 data points per spectrum ($0\cdot3$–$2\cdot6\,\mu$m). However, it was also found that much of the diagnostic compositional information was 'concentrated' in certain wavelength regions. The spectral resolution necessary for characterizing these minerals will depend on the types of information and level of accuracy required. At a minimum, three data points are required to characterize an absorption band, one on either side of the feature and one (ideally) at the band minimum. For pyroxenes with two major absorption bands this translates into six or less data points. Since the wavelength position of the band minimum is not known a priori, the full possible range of band minima should be sampled. If the level of accuracy for this parameter is set at 25 nm, then 6 bands and 20 bands are needed to sample Band I and Band II, respectively. For non-diagnostic spectral regions, the spectral resolution may be dictated by the spectral properties of additional components in the target area.

Another approach to reducing the volume of hyperspectral data, before or after data acquisition, is suggested from the results of the modified Gaussian method. With MGM each absorption band can be characterized in terms of wavelength

position, depth and width. For a two-pyroxene mixture, ~13 absorption bands are present. This translates into 39 values of position, depth and width, a better than order of magnitude decrease in data volume (from an original 461 point spectrum).

6. Summary and conclusions

A number of laboratory spectral studies have shown that spectral parameters such as band minimum position, band depths, band widths, band areas, absolute reflectance, and ratios of these various parameters can be used to extract compositional information. The spectral parameters can be used to quantify, or at least severely constrain, important physical and chemical properties such as major, and in some cases minor, element chemistry, end-member abundances, and grain sizes. This type of information along with ancillary geomorphometric information readily obtainable from spatial analysis of hyperspectral imagery may allow a detailed geological, geochemical and geothermometric history of a target region to be constructed. The spectral reflectance properties of rocks and minerals have also been found to be a function of grain size, particle packing and viewing geometry (Adams and Filice 1967). Ratioing or normalization can often reduce these effects so that spectral–compositional relationships can be better delineated (e.g., Pieters 1983).

Of the various analytical techniques examined which can potentially be applied to quantitative analysis of hyperspectral geological remote sensing data, those which were developed for analysis of broad-band data appear to be poorly suited for efficient quantitative analysis of hyperspectral data. The most promising techniques appear to be those involving various forms of curve fitting, such as MGM, which permit mineralogically diagnostic spectral features such as band depths, wavelength positions and widths to be derived.

Spectral resolution is a key factor in determining the quantity and quality of information derivable from hyperspectral data. An analysis of spectral properties of various materials by Price (1994) has revealed that high spectral resolution data, on the order of 10 nm, offer unprecedented opportunities for uniquely identifying a range of rock, soil and vegetation types.

Hyperspectral remote sensing provides both challenges and opportunities for studying the Earth's surface. The large volumes of data require that analytical techniques be developed which are efficient and capture the full range of information contained in the data. Variable spectral resolution and/or curve fitting can be used to reduce data volumes as much as possible while still sampling the most diagnostic regions of the spectrum to a desired level of accuracy. A variety of analytical techniques can then be applied to the data depending on the issues being addressed and desired levels of accuracy.

A key requirement in the development of robust analytical techniques for hyperspectral data will be additional comparative studies to augment the few which have been undertaken. For geological applications this will require the acquisition of hyperspectral remote sensing data over a well characterized study area and extensive analysis of the data using a variety of the analytical techniques cited above. Plans are underway to conduct such a study for an area in northern Canada, involving the acquisition of ground-based and airborne high spectral and spatial resolution data as well as detailed field mapping.

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