

COMPARISON OF QUANTITATIVE ASSESSMENT OF MINERAL POWDER COMPONENTS USING SISUROCK HYPERSPECTRAL SCANNER AND FIELDSPEC PORTABLE SPECTROMETER

Viljo Kuosmanen^a, Jukka Laitinen^a and Rainer Bärts^b

^a Geological Survey of Finland, Espoo, Finland - (viljo.kuosmanen, jukka.laitinen)@gtk.fi

^b Specim Oy, Oulu, Finland - rainer.bars@specim.fi

KEY WORDS: Mineral, reflectance, quantitative, unmixing, camouflage, powder, subpixel

ABSTRACT:

Remote sensing and quantitative assessment of components of a mineral mixture is an important issue in geology and especially in mining sector. Numerous studies have shown that remote detection of mineral species using reflected VSWIR (350-2500 nm) wavelengths is difficult, because the accuracy of a quantitative assessment is intolerably low. It was noticed in this work that there exists a systematic source for bias in determining abundances of mineral components from reflectance data of mixtures. If the prime mineral components are known, as is usually the case within a mineral mine, removal of this bias makes the use of VSWIR reflectance based quantity estimation very accurate.

The preparation, experiment and analysis comprise eight parts: 1) Grinding the prime mineral components, the end-members. The prime mineral species here are apatite, calcite, phlogopite, talc, magnesite and chlorite. 2) Mixing these powders in predetermined proportions. 3) Measurement of the mixtures for reflectance by ASD's FieldSpecFR portable spectrometer. The size of the Instantaneous Field of View (IFOV) target was about 35 mm in diameter. 4) Scanning the mixtures for per-pixel reflectance by Specim's SisuROCK hyperspectral scanner. The IFOV target area was 1.2 x 1.2 mm² and the averaged area for comparison 24 mm in diameter. 5) Preprocessing the raw data into reflectance. The preparation was followed by 6) unmixing the reflectances, 7) correcting the systematic bias and analyzing the accuracy of the quantitative estimates and 8) accuracy assessment and comparison of the results from FieldSpecFR and SisuROCK.

These two reflectance data sets, one derived from SisuROCK and another from FieldSpecFR measurements, were unmixed for abundances of the end-member minerals. However, the estimated abundances appeared to be systematically and similarly biased in both cases. A frequent bias, which is not due to these instruments, statistics or computing, was 0 – 54 %. The bias is explained to be caused by mutual physico-chemical interrelations of the mineral particles and complicated paths of photons between the particles. The abundances of flaky and dust-forming minerals were highly exaggerated in this case. This suggests that the bias is related to camouflage-like phenomenon which is dependent on grain-size distribution, flatness, surface activity, etc. features of minerals.. Because the bias behaves mathematically smoothly, it was corrected using a nonlinear polynomial function. The mean absolute residual error - after the camouflage correction – became ≤ 2 %. Both the FieldSpecFR and SisuROCK data recording and interpretations can be carried out in a few minutes.

1. INTRODUCTION

1.1 Motivation

Mineral powders are everywhere. Most sediments, like sands and clays, are mineral powders. Soils are composed mainly of mineral powders. Even rocks are "solid powders". Many industries, e.g. construction engineering and mineral mining handle masses of mineral powders. Main motivation for this case study came from mining people, who study drilling powders and do enrichment of huge amounts or grinded mineral material. For the industrial processes, such as ore enrichment after mining, it is of extreme value to estimate the proportions of different mineral components quickly and reliably. Classically this is done by consequential sampling and chemical/mineralogical analysis of the samples.

In the analytical approach, sampling frequency cannot be high, therefore representativeness of the sample may remain poor. On the contrary, hyperspectral scanner can make thousands of measurements per one second without touching the target and it therefore will be a suitable method for mapping large quantities of powder materials. In chemistry, according to Beer-Lambert law, the concentration of an absorbing species in material is proportional to absorption. However, the law is not obeyed at high concentrations nor in the case of non-transparent solids which are highly scattering. Unmixing a reflectance of a mineral mixture is complicated. The reported investigations suggest 5-15 % mean absolute error, which is intolerable in mineral industry. In practice, the error is still much bigger, but people do not likely report such "failures". Detection of mineral composition is generally – with classical methods - a "slow" job, which practically takes hours per sample. Reflectance based mineral assessment is very quick (seconds or minutes), provided that a systematic bias can be eliminated. This work suggests an explanation for a mineral related bias and its elimination and a method for making accurate mineral estimations.

1.2 Aims

FieldSpecFR is a portable spectroradiometer and it is effective in measuring reflectances of single targets and samples in the field. In the current study a laboratory setup of the SisuROCK hyperspectral scanner, built in 2007, was used. It is effective in scanning

quickly sample layouts or surfaces and it produces pixel array spectrometry data. These two instruments are not at all designed for the same task. However, for planning industrial operational quantity assessments it is valuable to get experience on their capacity. The aim of this study is to estimate - based on data measured by these two instruments - quantitative fractions of the end member minerals in selected mineral powders and produce some parameters for validating both estimates. From this point of view it is possible to compare the results from the two instruments.

1.3 Overview and previous work

In some case researchers have reported that it is possible to reliably estimate mineral fractions from mixtures. For example Debba et al. (2007) could estimate abundance of spectrally similar minerals using derivative spectra in simulated annealing. Unmixing reflectance from solids has been tested several times Clark (1999), Hapke et al (1981, 1984). Unmixing a reflectance of a mineral mixture is however a more complicated task than expected, it classically leads to a high error. Carvalho et al. (2001) suggest: "The abundance estimate in the intimate and macroscopic mixture can generate errors and should be corrected by mathematics adjustments with experimental data." Remote sensing methods used for this purpose are said to gain roughly 10-15% mean error of estimated quantities. Sgavetti et al (2006) state: "A quantitative analysis is however possible solely in the case of adequate particle separation, where the radiation is prevented from going through adjacent grains in its path back to the spectrometer. When the grains are close to each other, both the interference among absorption features pertaining to different minerals and the scattering effects combine to give fairly unpredictable results." Kuosmanen et al. (2008) noticed that the source of the largest error is not mathematical, statistical or computational but it is related to (physico-chemical) optical 'camouflage' of minerals, the effect of which can be computationally confined to limits that it does not prevent reliable quantity estimation.

1.4 Structure of the paper

This case study will contemplate the topic in following: Section 1 will introduce motivation, aims and some previous works. Section 2 will briefly introduce the instruments, explain the points of experiment using two and three-component powder mixtures and evidence for a camouflage effect. Section 2 also explains the mineral quantity assessment and the related errors. Section 3 will conclude the crucial results of the current case study. Section 4 lists the references and Section 4 our grateful acknowledgements.

2. INSTRUMENTS, SAMPLES AND THE EXPERIMENT

2.1 The instruments

The instruments used in the current study are as follows: SisuROCK hyperspectral scanner, 1050-2500 nm with 205 channels, manufactured by Specim, the IFOV pixel size in the current study = $1.2 \times 1.2 \text{ mm}^2$ (the most noisy channels were rejected) and the averaged area for comparison 24 mm in diameter. FieldSpecProFR portable spectrometer, 350-2500 nm with 2150 channels, manufactured by Analytical Spectral Devices, the FOV "pixel size" in the current study = 35 mm in diameter.

2.2 The experiment

The experiment and analysis of this study comprise eight parts:

1. Grinding the prime mineral components. The prime mineral species here are apatite, calcite, phlogopite, talc, magnesite and chlorite. The powders were grinded to grain size smaller than 0.33 mm. The mineral combinations were selected from the Lahnaslampi talc ore mine (talc-magnesite-chlorite) and from the Siilinjärvi apatite ore mine (apatite-calcite-phlogopite), both in Finland.
2. The mixture samples were prepared by portioning out into separate pots 0-5, 0-6 and 0-25 carefully measured volumetric quantities of each end-member mineral powder.
3. Measurement of all mixtures for reflectance by ASD's FieldSpecFR portable spectrometer. The size of the FOV target was about 35 mm in diameter, 962 mm^2 area.
4. Scanning the apatite-calcite-phlogopite mixtures for per-pixel reflectance by Specim's SisuROCK hyperspectral scanner. IFOV area was $1.2 \times 1.2 \text{ mm}^2$ and the integrated area for comparison 24 mm in diameter, 452 mm^2 area.
5. Preprocessing the raw data into reflectance.
6. Unmixing the reflectances by unconstrained linear unmixing. After optimization the wavelength area 1560-2500 nm only, was used in this work.
7. Correcting the systematic bias due to camouflage to get the final quantity estimates.
8. Accuracy assessment and comparison of the results from FieldSpecFR and SisuROCK data.

The physical conditions (illumination and its direction, powder surface area and topography, sensor distance and direction, temperature, humidity etc.) were constant throughout the experiment.

2.3 Two-component powder mixtures and evidence for a camouflage effect

If the reflectances of the mixed powders were linearly unmixed, the estimated quantities of a mineral (nearly) never coincided with the measured quantities of the same mineral. A phenomenon which we here call 'camouflage' was met in the next cases where powders of two different mineral species were mixed.

2.3.1 The talc ore minerals

The talc ore mineral mixtures were prepared from the following mineral combinations: powdered magnesite and talc (6 samples with varying proportions of the end members), talc and chlorite (25 samples), chlorite and magnesite (5 samples). These samples were measured using FieldSpecFR with a 35 mm in diameter IFOV for each sample. The reflectances were unmixing for the respective end members.

The original volumetric percentages of the end member minerals are compared (Fig. 1 and Fig. 2) to the unmixed fractions. In an ideal case the relation between the original and the unmixed proportions should follow a straight line from 0 to 1 (or from 1 to 0). However, the results show a systematic bias which contorts the unmixed fractions. The bias is dependent on the mineral species of combination and grain size. Several tests, based on mineralogical analyses, reconstruction of the mixed spectra from unmixed fractions with the endmember spectra and unmixing purely mathematical combinations of the spectra, showed that mineralogical, statistical and computational errors are very small (total average error < 1 %). But, the systematic bias is instantaneously bigger than 54 % as seen in (Figs. 1 and 2).

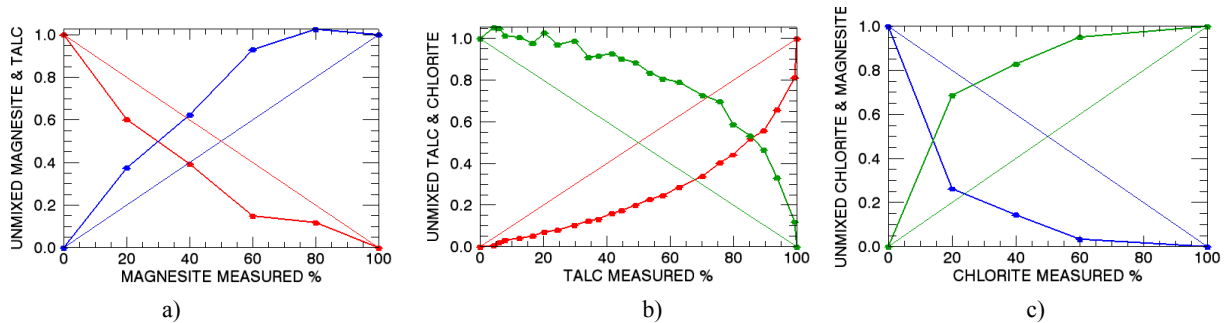


Figure 1 Two component unmixing based on FieldSpecFR data on talc ore minerals only: The curves with dots show the results from linear unconstrained unmixing and the straight diagonal lines show how the result should be. The x-axis = percentage of the first of the two components and y-axis = unmixed fractions for both components. a) Magnesite (blue) - talc (red) mixture b) Talc (red) - chlorite (green) mixture c) Chlorite (green) - magnesite (blue) mixture.

2.3.2 The apatite ore minerals

The apatite ore related mixtures were prepared using the following mineral combinations: apatite and calcite (6 samples), phlogopite and apatite (6 samples) and calcite and phlogopite (6 samples). These samples were measured using FieldSpecFR with a 35 mm in

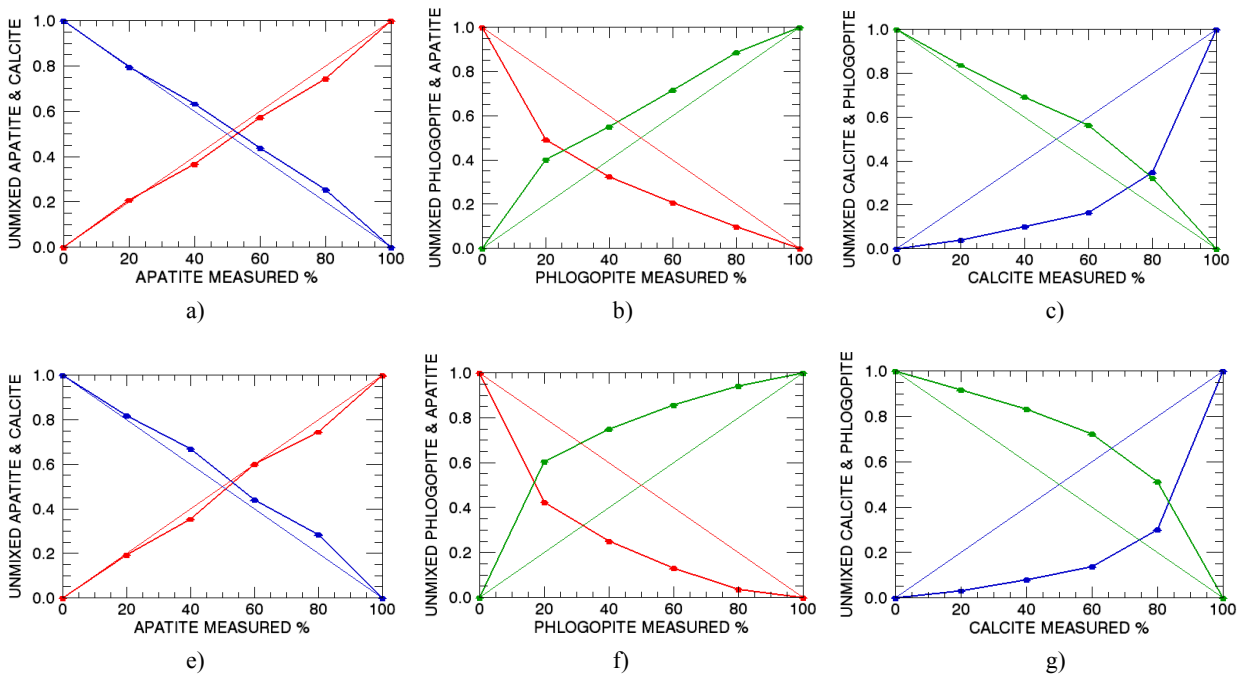


Figure 2 Two component unmixing based on FieldSpecFR and SisuROCK data: The curves with dots show the results from linear unconstrained unmixing and the diagonal lines show how the result should be. The x-axis = percentage of the first of the two mixture components and y-axis = unmixed fractions for both components. a) FieldSpecFR data, apatite (red) - calcite (blue) mixture b) FieldSpecFR data, phlogopite (green) - apatite (red) mixture. c) FieldSpecFR data, calcite (blue) - phlogopite (green) mixture. e) SisuROCK data, apatite (red) - calcite (blue) mixture f) SisuROCK data, phlogopite (green) - apatite (red) mixture. g) SisuROCK data, calcite (blue) - phlogopite (green) mixture.

SisuROCK data, apatite (red) – calcite (blue) mixture. b) SisuROCK data, phlogopite (green) – apatite (red) mixture. c) SisuROCK data, calcite (blue) – phlogopite (green) mixture.

diameter IFOV for each sample and SisuROCK hyperspectral scanner using 1.2x1.2 mm² pixel size and the integrated area for comparison 24 mm in diameter.

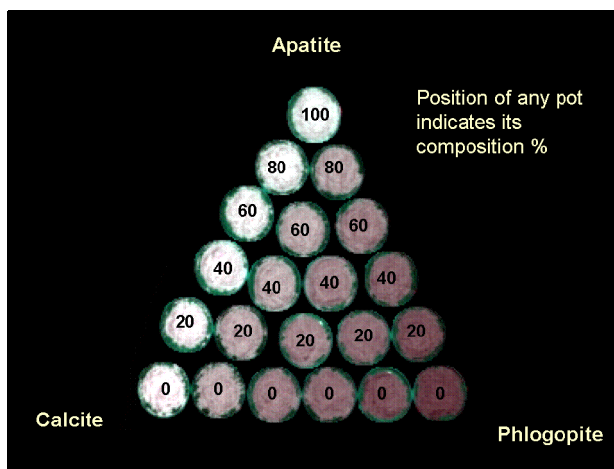
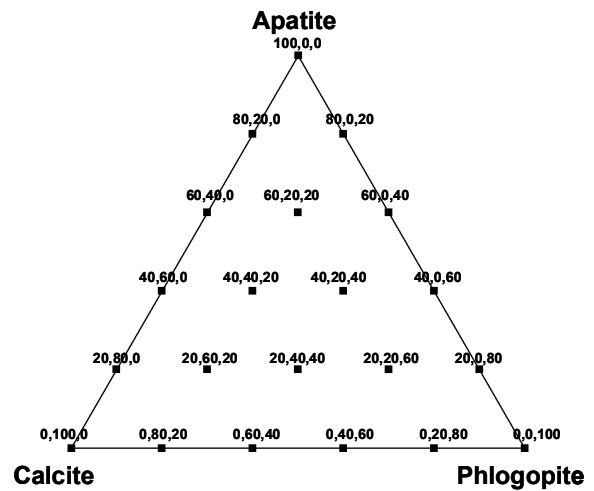
The original volumetric percentages of the end member minerals are compared to the unmixed fractions (based on FieldSpecFR data Fig. 2, a,b,c; SisuROCK data Fig. 2, d,e,f). The results again show the systematic bias which contorts the unmixed fractions. The bias is different from the previous ones and naturally dependent on the mineral combination. The mineralogical, statistical and computational errors are still very small (total average error < 1 %) as compared to the systematic bias which is instantaneously bigger than 50 % (Figs.1 and 2).

We conclude from these two-component studies that a same type of bias is present in the results derived from FieldSpecFR and SisuROCK measurements with six different mineral combinations (Figs. 1 and 2). For this reason the camouflage may be a common phenomenon and must be taken into account when two or more powder components are estimated using the reflectance method in remote sensing.

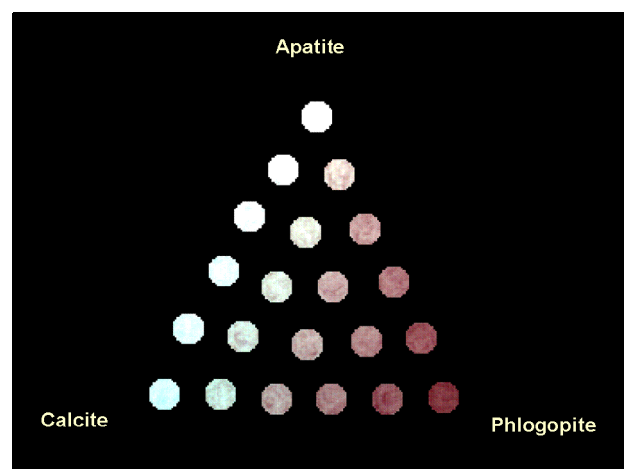
2.4 Three-component powder mixtures

The 3-component mineral powder mixtures were prepared from apatite, calcite and phlogopite using systematic 20 vol% steps in such a way that all multiples of 20 % quantity variations were covered. The mixed powders were placed into 21 plastic pots. The triangular diagram in Fig. 3 illustrates the pattern used for the measured proportional quantities of minerals and placing of the powder pots to be imaged by SisuROCK (see Fig. 4a).

Figure 3 Diagram showing the proportions of the end-member minerals in the 3-component mixtures. The numbers above the dots indicate the respective mineral percentages (V%) of apatite, calcite, phlogopite.



a)



b)

Figure 4 a) SisuROCK false-color RGB-image of the 21 mineral mixtures in pots. The mineral end-members are in the corners and the mixtures in between. Apatite contents (V%) are shown by the numbers and calcite and phlogopite concentrations also comply the

array shown in Fig 3. b) SisuROCK image after the images of the pots were trimmed in order to avoid the plastic edges. In the trimmed picture the diameter of a pot is 24 mm and each pot contains 305 pixels.

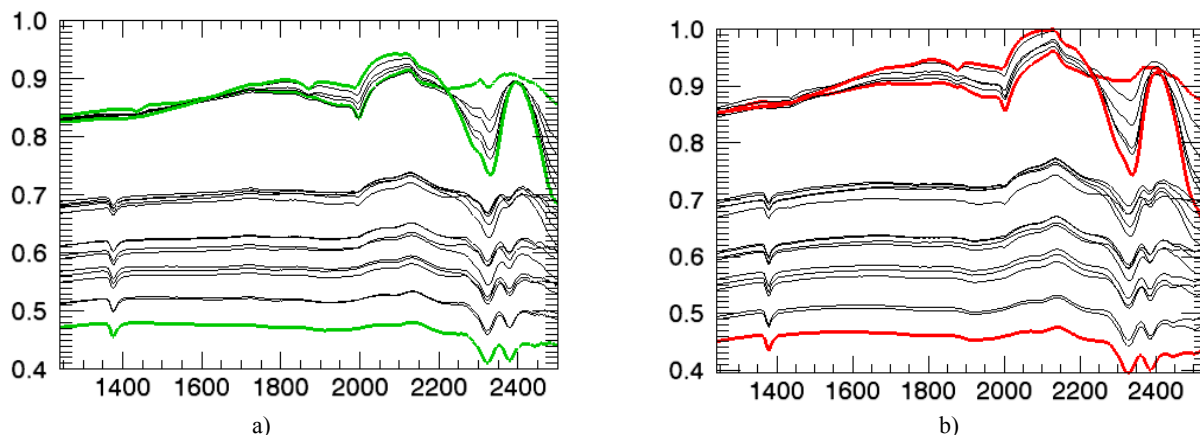


Figure 5 a) FieldSpecFR SWIR reflectance spectra of the same mineral mixtures as in Fig. 4a, measured without the pots. The green curves represent the end members. b) SisuROCK SWIR averages of the 305 pixels from each trimmed pot in Fig. 4b. The red curves represent the end members.

There is no reason to suppose that the camouflage induced bias is not present with the 3-component mixtures. The following analysis suggests that - in spite of camouflage - it is possible to make good estimates of quantities of the end member minerals in mixtures from the spectra of the mixtures.

Linear unconstrained unmixing was applied to solve the end member quantities (Figs. 6a and 7a) both from the FieldSpecFR spectra and SisuROCK average spectra (Fig. 5). The camouflage induced bias is strongly present in the results, as expected. Some negative fractions, which resulted from unmixing were not rejected. The negative fractions are indicated by the arrows outside the triangle in Figs 6 and 7.

The bias was corrected by the method defined by Kuosmanen et al. (2008). This is actually a method - not only to give training data on the classes or end members - but also to give training on the interaction of the classes or end members. The interaction is here defined by the Camouflage Function which is a smooth inverse function describing the relation between the original %-portions of the end-member minerals and the estimated unmixing fractions of the same portions. Once the Camouflage Function has been determined for a certain mineral assemblage, grain size distribution, wavelength range and instrument, the CF thereafter keeps the same and can be further used for any other samples of the same type with any proportions of end members in the mixtures. In the current project one set of measurements were used to determine the CF-correction and a new or a split set of measurements were used to evaluate the total mean absolute errors. The CF-corrected estimates are shown for FieldSpec data in Fig. 6b and for SisuROCK data in Fig. 7b.

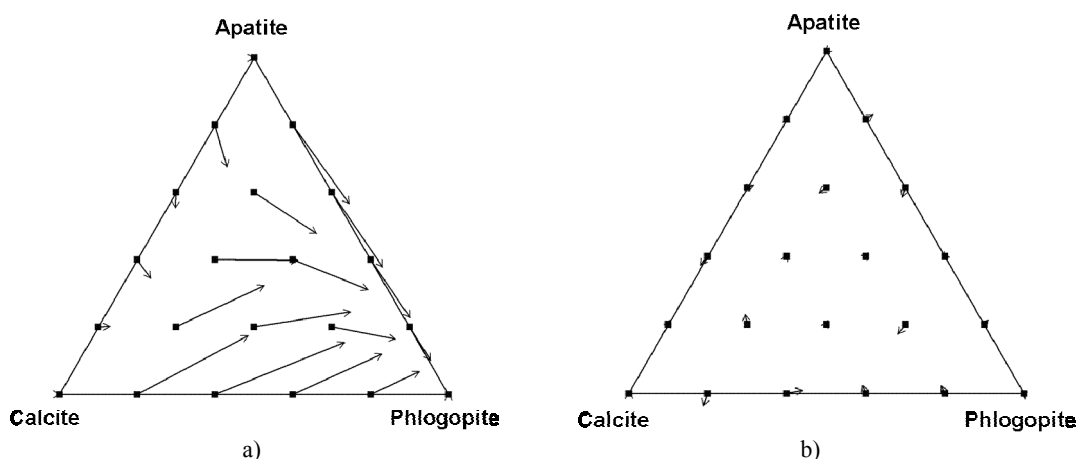


Figure 6. Estimates of the end member quantities from FieldSpecFR data in Fig 5a. The dots show the measured composition and the arrows show the estimated composition. a) Biased and estimates b) CF-corrected nonbiased estimates.

The whole SisuROCK image was also unmixed per pixel, the biased abundances are coded in Fig. 8a with intensity of colors (R = apatite, B = calcite, G = phlogopite). The average based CF-correction was applied to that unmixed image and the unbiased abundances are seen as color coded in Fig. 8b. These images are in agreement with the respective diagrams demonstrating the results from the average SisuROCK spectra.

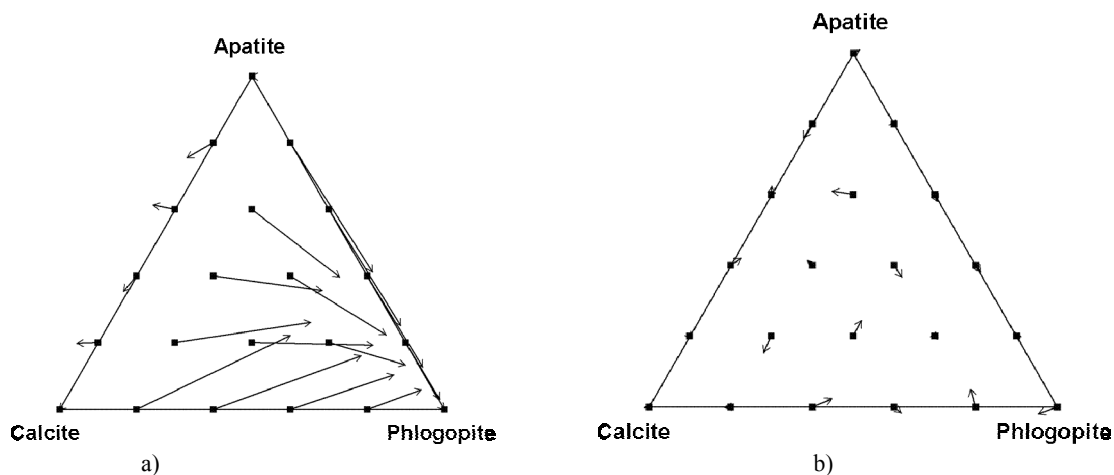


Figure 7. Estimates of the end member quantities from SisuROCK average spectra in Fig 5b. The dots show the measured composition and the arrows show the estimated composition. a) Biased and estimates b) CF-corrected nonbiased estimates.

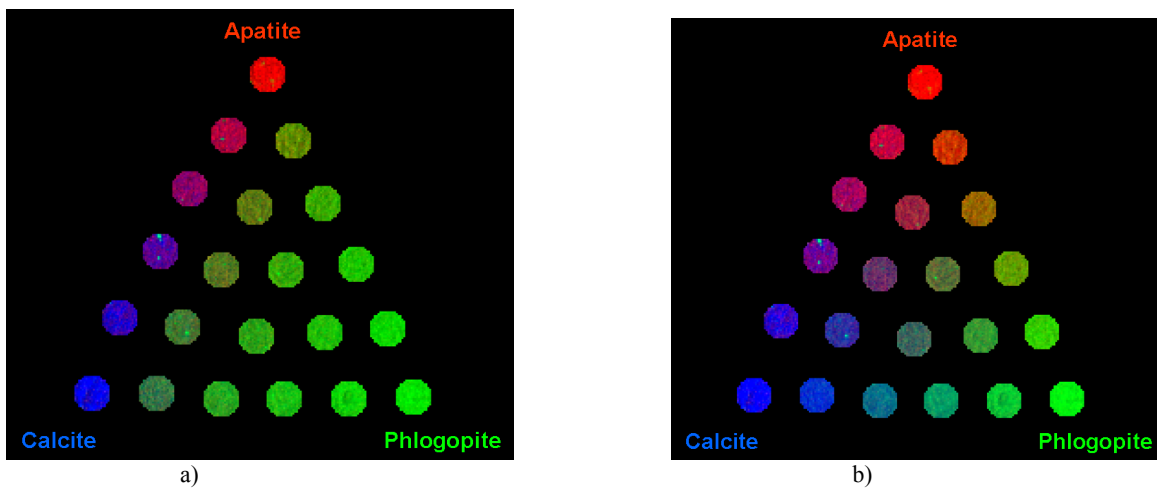


Figure 8 a) Per pixel unmixed SisuROCK image: biased pixel estimate. b) Per mean CF-corrected per pixel unmixed SisuROCK image: nonbiased pixel estimate.

The FieldSpecFR nonbiased estimates (Fig. 6b) were compared to SisuROCK nonbiased estimates (Fig. 7b) in the following way: The nonbiased quantity estimates were subtracted from the original quantities to get the residual. Then the average absolute residual E was used as a parameter for the comparison. The computed average absolute residual error E for FieldSpecFR based estimates $E_{FS} = 1.23\%$ and for SisuROCK data $E_{SR} = 1.92\%$.

3. CONCLUSIONS

In this case study the areas for comparison were slightly different: target IFOV of FieldSpecFR = 962 mm² and the trimmed pot area of SisuROCK image = 452 mm². Therefore this comparison is not complete but indicative. The two instruments, as it is well known, are not designed for the same task. However, for planning industrial operational quantity assessments it is valuable to get experience on capacity of these instruments. The computed average absolute residual errors E for FieldSpecFR and SisuROCK are less than 2%. This high accuracy and high speed of the quantitative estimation speaks for that these methods can be used for example in operational control engineering and monitoring industrial conveyor belt feeding in mining and other industries.

4. REFERENCES

References from Journals:

R. N. Clark, "Chapter 1: Spectroscopy of Rocks and Minerals, and Principles of Spectroscopy," in Manual of Remote Sensing, Volume 3, Remote Sensing for the Earth Sciences, A.N. Rencz, editor. John Wiley and Sons, New York, pp. 3 – 58, 1999.

B. Hapke, "Bidirectional Reflectance Spectroscopy: 1. Theory", JGR, Vol 86, pp. 3039-3054, 1981.

- B. Hapke and W. Eddie, "Bidirectional Reflectance Spectroscopy: 2. Experiments and Observations", JGR, 86, pp. 3055-3060, 1981.
- B. Hapke, "Bidirectional reflectance spectroscopy. 3. Correction for macroscopic roughness," Icarus 59: pp. 41-59, 1984.
- P. Debba, E.J.M.Carranza, F.D. van der Meer and A. Stein, 2006, "Abundance estimation of spectrally similar minerals using derivative spectra in simulated annealing," IEEE Trans. Geosci. Remote Sens., vol.44, no. 12, pp. 3649-3658.
- V. Kuosmanen and J. Laitinen, 2008, "Quantitative Mineral Assessment of Apatite, Calcite/dolomite and Phlogopite Powder Mixtures, Using VSWIR-reflectance." IEEE Transactions on Geosciences and Remote Sensing. TGRS-2007-00306, 11 p.
- M. Sgavetti, I. Longhi, S. Meli and L. Pompilio, 2006, Accuracy in mineral identification: image spectral and spatial resolutions and mineral spectral properties. Annals of Geophysics, Vol. 49, N. 1.

References from websites:

O.A. de Carvalho, A.P.F. de Carvalho, R.F.Guimarães, P.R. Meneses, 2001, Intimate and Macroscopic Mixture Analysis by Linear and Nonlinear Regression. Study Case: Garnierite x Goethite and Garnierite x Asbolan
ftp://popo.jpl.nasa.gov/pub/docs/workshops/01_docs/2001Carvalho_intimate_web.pdf

5. ACKNOWLEDGEMENTS

We are highly indebted to Specim Oy for giving the possibility to hyperspectrally scan our mineral samples. The authors are also grateful to Mr. Jouko Kallioinen and Mr. Jukka Karhunen Mr. Nils Gustavsson, (from the Geological Survey of Finland) for their support during this work. We also like to thank Mr. Olli Härmälä and Mr. Jarmo Aaltonen (from Kemira Oy) and Mr. Ilkka Tuokko and Erkki Kuronen (from Mondo Minerals Oy) for giving access to their mineral materials.