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Retrieval of the Martian surface reflectance by means of Principal Component analysis and Target Transformation using OMEGA/Mex data

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Abstract. The aim of this work is to extract the surface contribution in the Martian visible/near-infrared spectra removing the atmospheric components by means of Principal Component Analysis (PCA) and target transformation (TT). The developed technique is suitable for separating spectral components in a data set large enough to enable an effective usage of statistical methods, in support to the more common approaches to remove the gaseous component. Data collected by imaging spectrometers, such as the OMEGA (Observatoire pour la Minéralogie, l'Eau, les Glaces et l'Activité) instrument on board the ESA mission Mars Express (MEx), are particularly suitable for this purpose since it includes in the same session of observation a large number of spectra with different content of aerosols, gases and mineralogy. The methodology presented in this work has been applied to the analysis of OMEGA sessions over Nili Fossae and Mawrth Vallis regions, which have been already widely studied because of the presence of hydrated minerals. Once the surface reflectance, free from atmospheric contributions, has been obtained, the Modified Gaussian Model (MGM) has been applied to spectra showing the hydrated phase. Silicates and iron-bearing hydrated minerals have been identified by means of the electronic transitions of Fe^{2+} between 0.8-1.2 μm, while at longer wavelengths the hydrated mineralogy is identified by overtones of the OH group.

Key words. Mars, atmosphere, surface reflectance, OMEGA, mineralogy

1. Introduction

The main purpose of this work is to apply the PCA and the target transformation (TT) method to data acquired by imaging spectrometers on board space missions orbiting Mars, in order to remove the atmospheric contribution. This will allow for the isolation of the surface spectra in order to investigate hydrated mineral features. Imaging spectrometers measure a signal in the near-infrared spectral range that contains information about the atmosphere as well as about the surface. The measured spectra result in a combination of these different spectral contributions and a methodology is necessary to separate the atmospheric component from the surface reflectance. The high resolution spectral data provided between 0.4 and 2.5 μm by the OMEGA (Observatoire pour la Minéralogie, l′Eau, les Glaces et l′Activité) imaging spectrometer, on board the ESA/Mars Express, allow for the identification and mapping of different minerals (Bibring et al. 2004). However, while the electronic absorption features diagnostic of transitional elements bearing minerals (e.g., ferro-magnesian silicates) occur at wavelengths not affected by Mars atmospheric composition, the vibrational overtone absorptions bands due to water, OH^-, and $(CO_3)^{2-}$ in minerals overlap the absorption of water and CO_2 in the atmosphere. Therefore, an accurate removal of the atmospheric components (aerosols and gaseous species) is necessary to extract the actual surface contribution in the spectra.

Bandfield et al. (2000) and D'Amore et al. (2013) have already applied the multivariate analyses techniques to the Thermal Emission Spectrometer (TES) on board the NASA Mars Global Surveyor satellite and to the Planetary Fourier Spectrometer (PFS) instrument on board the ESA Mars Express (MEx) spacecraft, respectively. The authors were able to properly recover the atmospheric contribution (dust and water ice clouds) to the observed radiation in the thermal/far-infrared spectral range. Glotch & Bandfield (2006) found the surface spectral components and atmospheric spectral shapes at Meridiani Planum applying the PCA and TT to the Miniature Thermal Emission Spectrometer (Mini-TES). Glotch & Rogers (2013) used factor analysis and TT to search for carbonate decompositions products on the surface of Mars. Smith et al. (2000) successfully separated the contribution of atmospheric and surface components in TES data assuming that each spectrum is a linear combination of its components. Thomas & Bandfield (2013) used the TT on CRISM data to confirm the presence of Mg-rich carbonates near Nili Fossae region on Mars, while Thomas et al. (2014) used the TT to identify diagnostic serpentine spectral features in the CRISM near-infrared data on the same Martian region. Klassen (2009) found a set of spectral end-members applying the PCA and TT to near infrared cube images of Mars acquired by the NASA Infrared Telescope Facility. In our work, we apply the same technique, hereafter called Surface Atmosphere Separation (SAS) method, to the OMEGA data in the near-infrared spectral range. In particular, we focused on surface reflectance spectra that show the hydrated absorption bands, which occur in the spectral range between 1.8 and 2.2 μm that is strongly influenced by the atmospheric absorption of H_2O and CO_2.

2. Instrument and dataset

In each resolved pixel (1.2x1.2 mrad instantaneous field of view, IFOV) OMEGA acquires a spectrum in 352 contiguous spectral elements (spectels) from 0.35 to 5.1 μm, with a spectral sampling ranging from 7 nm (in the visible and near infrared channel, between 0.38 and 1.05 μm) to 14 nm (short wavelength range between 0.93 and 2.73 μm) and 20 nm (long wavelength range which covers the interval 2.55−5.1 μm). The signal-to-noise ratio (SNR) is $>$ 100 over the whole spectral range (Bibring et al. 2004) for observations obtained in nadir mode and considering low solar zenith angles. The data products are organized in three-dimensional arrays (or cubes), with one spectral and two spatial dimensions (x, y, λ). Due to the MEx spacecraft elliptic orbit, the scan widths in each orbit are changed (16, 32, 64, 128 pixels) accordingly to the variation of the observing distance, e.g., 16 pixels are used for the low-elevation (<350 km, orbit pericenter) and consequently for high-resolution (300 m/pixels) observations, whereas the 128 pixels mode is adopted for elevations above 1500 km to provide wide images with spatial sampling greater than 2 km/pixel. In order to investigate regions where hydrated minerals have been already found and to include a variety of mineralogical units, in this work we focus on the two MEx orbits: 0422_4 and 0353_3.

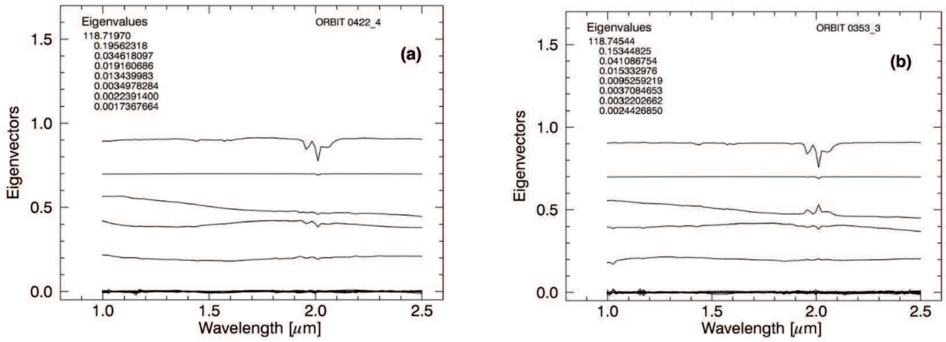

Fig. 1. Eigenvectors (shifted for clarity) retrieved using PCA for the two considered orbits. Only the first eight eigenvalues are listed.

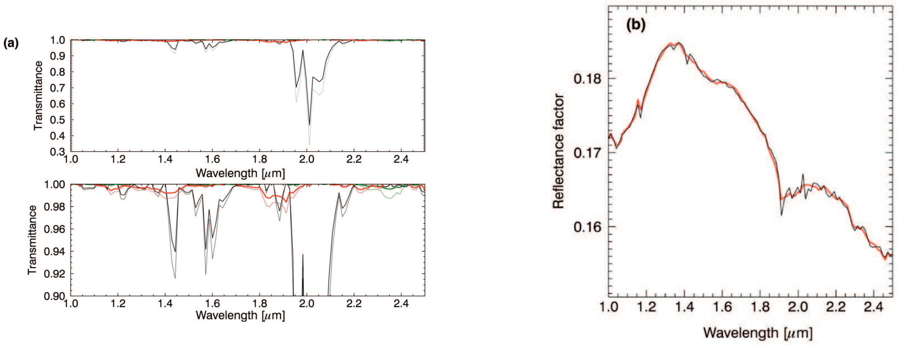

Fig. 2. (a) Retrieved transmittances corresponding to the maximum (thick line) and minimum (thin line) weights. The CO_2 transmittances are the black lines, the H_2O transmittances are the red lines and the CO transmittances are the green lines. The lower panel is a widening of the upper panel to have a better viewing of the CO and H_2O transmittances. (b) Surface trial (black line) and retrieved surface end-member (red line) for a case where the hydrated band is present.

Orbit 0422_4 includes the north of Syrtis Major Planum, passing through Nili Fossae and highlands of Nili Fossae. This OMEGA observation contains 44,640 spectra and, besides the considerable mineralogical diversity, it shows significant variability in gas absorption due to an altimetry variation of 4.7 km. Orbit 0353_3, which includes 99,820 spectra, passes through Mawrth Vallis, a region located at mid-low latitude in the west part of Arabia Terra, with an elevation spanning from a minimum of −5 km to a maximum of −700 m.

3. Method description and its applications

3.1. Principal component analysis and target transformation

This Section follows closely the methodology given in Bandfield et al. (2000). In statistical methods the covariance matrix is used, with different approaches, to derive the eigenvectors, a set of N_e orthogonal spectral functions summarizing the variability of the sample. They can be organized in a $m \times N_e$ matrix R

(m being the number of spectral points), whose rows can be linearly combined to reproduce every spectrum in the dataset. More specifically, being D the full set of measured spectra (n x m matrix, gathering n sampled spectra in m spectral bands), it holds

$$D = RC \quad (1)$$

where C is a N_e x n matrix whose columns give the contribution (weights) of each endmember to the different spectra in the population. The main purpose of the PCA is to reduce the number of variables and found the minimum set of eigenvectors whose linear combinations are able to reconstruct the original measured spectra. Once all eigenvalues and eigenvectors (their initial number is equal to the original dimension of data) have been found, the dimensionality can be reduced by retaining the minimum N_e number of components that actually influence the dataset. Since the eigenvectors do not necessarily have a physical meaning, target transformation (Hopke 1989) is used to assign a physical significance to this abstract matrix by rotating the space defined by the meaningful eigenvectors to be geometrically realigned to a set of predefined axes, called test vectors, representing the possible physical contributions to the measured data. For this purpose, a set of trial (or test) spectra have been computed by means of a radiative transfer (RT) code (Ignatiev et al. 2005), each one representing the gaseous spectral end-members: carbon dioxide, carbon monoxide and water vapour transmittances. The trial spectra describing the surface components can be laboratory spectra or retrieved surface components obtained with existing methods, e.g., the so called Mons Olympus' method (Langevin et al. 2005), hereafter MO method, which is also often referred as "volcano scan" (McGuire et al. 2009). The spectral components (R matrix in Formula 1) are then retrieved fitting the trial spectra with a linear combination of N_e eigenvectors. Finally, the projection of the initial spectral population into the space defined by the retrieved spectral components allows finding the weight matrix (Hopke 1989). Considering the retrieved end-members of the surface only, the gaseous components are removed from the spectra. The validation of the method can be found in Geminale et al. (2015), where the SAS methodology has been applied to a population of synthetic spectra.

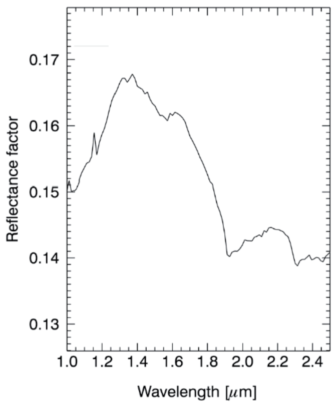

Fig. 3. Surface reflectance from orbit 0422_4 showing the absorption at 1.9 μm associated to 2.3 μm band indicating Fe/Mgrich clays.

The assumption of linear combination of spectral end-members can be done only when the dust content in the atmosphere is very low, otherwise their contribution is far from being linear. Moreover, in the visible and near-infrared range of the spectrum it is difficult to disentangle the effect of dust on the bright, dusty terrains from that in the atmosphere. For this reason we will adopt a further step to remove the effect of atmospheric dust scattering, as described in Section 4. Therefore, in our first analysis the aerosol component is not included, and the assumed contribution to the spectra is only given by the gases transmittance and surface reflectance.

3.2. Trials and first guess discussion

We have applied the procedure described in Section 3.1 to OMEGA cubes 0422_4 and 0353_3, covering Nili Fossae and Mawrth Vallis, respectively. The application of the PCA to both datasets reveals that five eigenvectors (Figure 1a and 1b, for cube 0422_4 and 0353_3, respectively) have a spectral shape above the noise, meaning that at least five components mostly influence the dataset. We chose as trial spectra for the surface the reflectance obtained using the MO method, while for the gas components we consider synthetic spectra computed by means of the RT algorithm and convolved with a Gaussian kernel at the OMEGA spectral resolution. By using the already existing spectral shape for the surface end-member as a first guess in the SAS analysis we can reach meaningful solution for every spectrum in the analyzed dataset. In fact, the MO method provides a surface reflectance that at first order well represent the mineralogical diversity as reported in the OMEGA and CRISM data analysis literature and in the derived spectral indexes used to map on a global scale the different class of minerals found on Mars (Carrozzo et al. 2012).

3.3. Nili Fossae, orbit 0422_4

The eigenvectors obtained after the PCA has been applied to the spectral population of orbit 0422_4 clearly indicate that the principal components that influence this dataset are characterized by gaseous spectral features and surface spectral shape (Figure 1a). We consider a number of eigenvectors that gives the best reconstruction of the spectra when compared (by means of the chi-square test) with the original spectra measured by OMEGA. This ensures that we are observing the best combination of the retrieved end-members. Figure 2a shows the retrieved gas spectral components and their amplitude in the dataset. This is possible using the retrieved weights (*C* matrix in Formula 1) obtained by projecting the spectral population in the space defined by the retrieved end-members. Target transformation projection of surface trials in the space defined by the eigenvectors and the resulting best fit of the linear combination of the selected eigenvectors with the trial component is plotted in Figure 2b for a spectrum where the hydrated band is present. The surface reflectances obtained using SAS procedure are similar to the ones retrieved with MO method, but a reduced noise and a better evaluation of the spectral shape of the surface are obtained in the spectral region where the gaseous component is stronger, in particular around 2 μm.

In Nili Fossae region the 2.3 μm band has been detected (Poulet et al. 2005) in association with the hydration band at 1.9 μm. This combination of absorptions was attributed to Fe/Mg-rich clays. Figure 3 shows one of these peculiar spectra as an example of the result obtained by the application of the SAS procedure to a surface spectrum characterized by phyllosilicates features.

3.4. Mawrth Vallis, orbit 0353_3

In this session we present and discuss the results of the SAS procedure to the OMEGA spectra from orbit 0353_3. Figure 1b shows that the principal components obtained with the PCA have the typical features of the gas and surface shape. The absorption at 1.9 μm is present in many regions of the area as shown in the map of Figure 4a, where the violet colour indicates spatial regions where the spectral index values of 1.9 μm band (Loizeau et al. 2007) derived from the retrieved surface, are higher than 2.5%. We consider an average of nine surface spectra (the average should remove random noise), from both the MO and SAS methods, located in the region of the map indicated with a red box. These spectra are all characterized by hydrated mineral features and their average is shown in Figure 4b with cyan and red colours for MO and SAS method, respectively. To remove residuals due to atmospheric gases, the ratio with a featureless surface reflectance measured in a region (yellow box in Figure 4a) very near to the selected area has been considered and shown as green and black coloured spectra in Figure 4b for MO and SAS method, respectively. The spectrum retrieved with our statistical analysis shows clearly the main hydrated features if compared with the spectrum of nontronite (violet line) taken from the USGS mineral spectral library (Clark et al. 1993) and does not differ substantially from the normalized spectra.

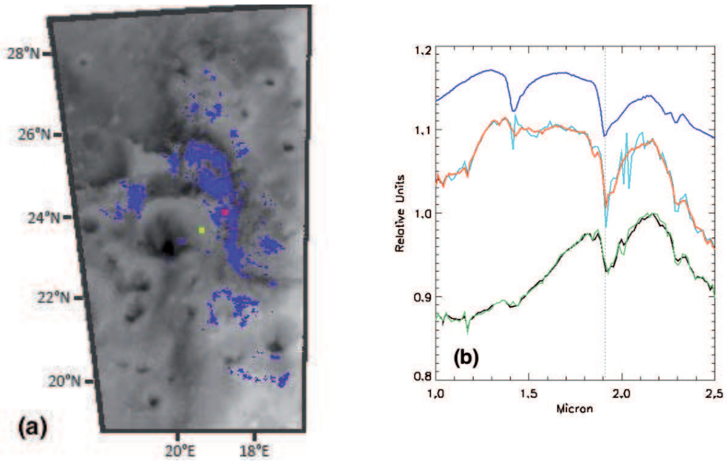

Fig. 4. (a) The violet area is characterized by a band depth at 1.9 μm higher than 2.5% (as derived from the retrieved surface) overlying the albedo map at 1 μm of orbit 0353_3. (b) The violet spectrum is a laboratory spectrum of nontronite, red and cyan spectra are surface reflectance (normalized at 1.4 μm and shifted for clarity) obtained with the SAS and MO analysis respectively and corresponding to the region indicated with a red box in the map. Green and black lines are surface reflectances measured around the pixel indicated with the red box and rationed with a featureless spectrum measured in the region indicated with a yellow box in the map, considering the MO and SAS method respectively.

4. Correction for the effect of atmospheric dust

Dust is always and everywhere present in the Martian atmosphere showing opacity variation with season and location as described in Smith (2004). Mars experiences global dust storms as well as local dust storms and small-scale dust devils. During the observational session of orbit 0442_4 the dust optical depth τ (at 1070 cm^{-1}) ranges from 0.1 to 0.2, as reported in MCD. The dust optical depth is slightly higher for orbit 0353_3, especially in the atmospheric column above craters south of 16° of latitude, where τ can be greater than 0.25. We extract the value of dust optical depth from MCD to have the value of τ influencing each spectrum. We apply the same approach reported in Vincendon et al. (2007) from visible to near-infrared spectral range (from 0.4 μm to 2.5 μm) considering that the observed reflectance factor at a given wavelength is a function of surface reflectance and τ. Taking advantage of this relationship and knowing τ a priori, we use a multiple-scattering radiative transfer code to simulate reflectance factor, assuming the most recent properties for the atmospheric dust (Wolff et al. 2009) and using the observing geometries for each observation. The grain size distribution of dust is described with a log-normal function where the grain effective radius is 1.6 μm and the effective variance of distribution is 0.35 μm. The surface reflectance factor is determined as the value that corresponds to the best fit between the observed reflectance factor and the simulated one for each wavelength.

The effect of the dust on the spectra depends on the surface reflectance. For dark surfaces the effect of dust is to increase the reflectance while, on contrary, for bright surfaces is to decrease the reflectance. For intermediate values of surface reflectance the effect of atmospheric dust is not distinguishable from that of surface dust. These effects are shown in Figure 5 where two spectra from orbit 0422_4 and two from orbit 0353_3 corrected for the effect of dust are plotted.

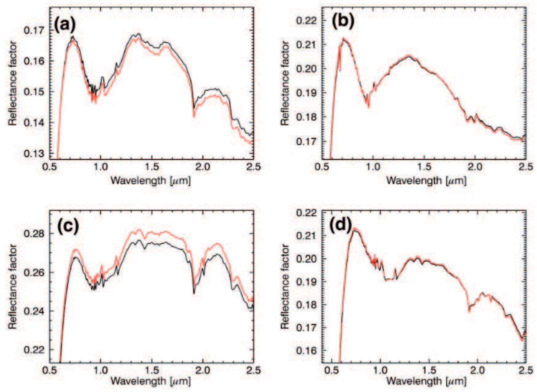

Fig. 5. (a) Orbit 0422_4: pixel 75, scan 152. (b) Orbit 0422_4: pixel 77, scan 111. (c) Orbit 0353_3: pixel 41, scan 582. (d) Orbit 0353_3: pixel 38, scan 538. The black line is the surface reflectance and the red line is the surface reflectance corrected for the effect of dust in the atmosphere. The dust optical depths are 0.137 and 0.138 and 0.217 and 0.172 for the shown spectra of orbit 0422_4 and 0353_3, respectively.

5. Application of MGM analysis to Martian surface spectra

Removing the atmospheric contribution in the Martian VNIR-IR spectra is crucial to study and map the surface mineralogy from remote sensing data. We spectrally analyse the two OMEGA cubes, from Nili Fossae and Mawrth Vallis, focusing on the retrieving of the Martian mineralogy by using the MGM (Sunshine et al. 1990). In particular, we focus our analysis on those minerals characterized by absorption bands centered at 1.9 μm to 2.3 μm, representative of hydrated minerals, in which spectral range the atmospheric contribution is more important. The validation of the method can be found in Geminale et al. (2015) where the MGM deconvolution has been applied to a set of laboratory spectra of minerals of recognized hydrated silicates on Nili Fossae and Mawrth Vallis.

The MGM is a statistic-base method based on the assumption that different mineral absorptions can be described with a modified Gaussian distribution superimposed on to a continuum. It is widely applied on mineral phases and mixtures analysis, in particular for the electronic absorptions (Sunshine et al. 1990; Clénet et al. 2011). Different papers used also Gaussians models to determine the vibrational overtones present in hydrated silicates, carbonates and sulfates measured in laboratories (see Sgavetti et al. (2015) and references therein). Here, we apply the MGM considering: 1) the continuum as a straight line as function of the wavenumber, with two parameters, the offset and the slope; 2) each Gaussian is described by three parameters: the band depth (in logarithm of the reflectance), the band center and the band width, or FWHM (both in nanometers). We choose a continuum that model the real strength of the absorption bands (Clenet et al., 2011) thus avoiding an horizontal continuum by choosing a fixed, tangent continuum. On the other hand, Gaussians spectral parameters are free to vary. The goodness of the fit is expressed by the RMS (root mean square) value.

The MGM approach is applied on OMEGA surface spectra of the two considered orbits where hydrated phases where recognized, as derived by both the MO method and the SAS one. Results are shown in Figure 6. We find that: a) very few differences are present in the 0.5-1.4 μm spectral region, comparing spectra after application of MO or

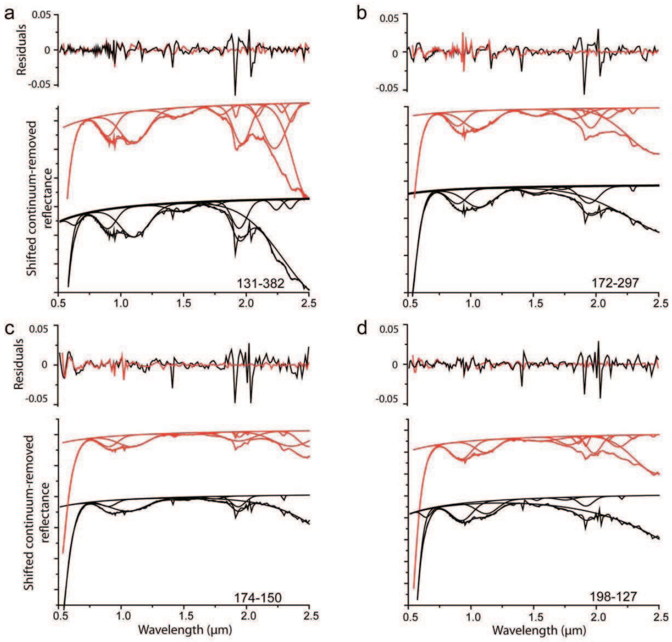

Fig. 6. Figure shows Gaussians and residuals after MGM deconvolution. Black: spectra acquired from images after MO; red: spectra acquired from images after SAS. a,b : Nili Fossae; c,d: Mawrth Vallis.

SAS; b) in the NIR range, spectra processed with the SAS method allows to recognized more absorptions within the composite bands and, therefore, an higher number of Gaussians is requested with respect to the MO method, likewise for the laboratory spectra dataset. The main differences are in the 1.9-2.1 μm spectral region. In the MO surface spectra, the absorption bands are described with only two or three Gaussians despite the higher Gaussian number used for hydrated minerals, and residuals due to atmospheric contribution are high. On the contrary, in spectra corrected with SAS method, the same spectral region can be described with five/six Gaussians with a slight variation in position and depth, better fitting the overtone absorptions and revealing differences in hydrated mineralogy or in their abundance. Moreover, spectral residual is five times lower. The band centers obtained for the spectra after the SAS correction are comparable with those obtained from laboratory spectra. This indicates that hydrated mineralogy can be evidenced by applying MGM on spectra corrected by SAS, and we have seen that the selected spectra are comparable with the composition indicated in the literature (Ehlmann et al. 2008, 2009; Poulet et al. 2008). Moreover we can model the different absorption processes of these spectra. By decreasing the level of both the atmospheric residuals and random noise in the OMEGA data when retrieving the surface component, SAS method enable us to improve the investigation of hydrated mineralogy present in Nili Fossae and Mawrth Vallis by means of MGM. A higher number of Gaussians can be considered with respect to the previous technique in the 1.8-2.1 μm spectral range and a better comparison with laboratory data is reached.

6. SAS method applications and conclusions

By completely separating the atmospheric component from the surface one, the results obtained with the method described in this work have many scientific implications for the study of the Martian orbiter data in the infrared spectral range:

- Since each gas spectral end-member can be isolated and their opacities can be estimated by means the TT, it is possible to retrieve the geographical distribution of the gaseous components.
- The final surface spectra we are able to obtain are of great importance, for example, in the study of ice clouds where the knowledge of each spectral component (including the dust contribution to the spectra) is crucial to estimate the ice properties.
- The spectral index maps can be greatly improved, especially for weak mineralogical absorption bands.
- Hydrated mineralogical features in the OMEGA surface reflectance spectra retrieved by SAS (in particular in the 1.8-2.1 μm range) show a better consistency with laboratory data. The SAS surface reflectance spectra can be used to deconvolve the contribution of different minerals in the data.
- The lower level of the atmospheric and noise residuals in the retrieved surface reflectances with SAS method enables us to make a better match with the MGM deconvolution parameters found for the laboratory spectra of Martian hydrated mineral analogues, allowing a deeper investigation of this spectral range.

The removal of atmospheric contribution from reflectance spectra measured by airborne instruments is crucial to investigate the features of the surface, which are on the same spectral regions of atmospheric components. In particular, the vibrational absorption bands due to water and O-H bound in the near infrared region of the spectrum overlap with atmospheric water and CO_2, compromising the mineralogical deconvolution. The SAS method based on the principal component analysis and target transformation removes the noise and atmospheric gaseous components from the reflectance spectra, thus allowing to deeply investigate hydrated minerals on the Martian surface. Moreover, the contribution of dust in the atmosphere is also removed by modeling its effect on each spectrum. The surface reflectance obtained with the SAS method is almost free from instrumental noise and residuals due to atmospheric components (gases and aerosols) are removed. The surface reflectances obtained for two sessions of observations over Nili Fossae and Mawrth Vallis regions have been investigated by means of MGM, comparing the results obtained from spectra of the same pixel after MO and SAS treatment. In particular, surface spectra showing the hydrated phase have been selected because the diagnostic vibrational absorptions of these minerals are superimposed to the atmospheric absorptions. The information on mineralogy is obtained considering laboratory data, which allows to define the different electronic and vibrational processes to be compared with the measured spectra at Mars. Absorptions between 0.8-1.2 m can be assigned to electronic Fe^{2+} transitions, both in mafic silicates and in iron-bearing hydrated phases, while absorptions at higher wavelengths reveal the presence in the spectra of overtones of the OH group, in particular AlOH and MgOH overtones. Moreover spectra treated with SAS show a better definition of overtone processes after MGM application, showing a clear reduction of the level of the atmospheric residuals in the 1.8-2.1 μm spectral range. This residual reduction permits to better define the vibration processes indicative of the hydrate minerals present in remote sensing data and improve the comparison with laboratory data.

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