



Removal of atmospheric features in near infrared spectra by means of principal component analysis and target transformation on Mars: I. Method



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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. In this context, a key role is played by the estimation, from the spectral population, of the covariance matrix that describes the statistical correlation of the signal among different points in the spectrum. As a general rule, the covariance matrix becomes more and more meaningful increasing the size of initial population, justifying therefore the importance of sizable datasets. 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 first validated using a simulated dataset of spectra to evaluate its accuracy. Then, it 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. These minerals are key components of the surface to investigate the presence of liquid water flowing on the martian surface in the Noachian period. Moreover, since a correction for the atmospheric aerosols (dust) component is also applied to these observations, the present work is able to completely remove the atmospheric contribution from the analysed spectra. 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 Fe²⁺ between 0.8 and 1.2 μm , while at longer wavelengths the hydrated mineralogy is identified by overtones of the OH group. Surface reflectance spectra, as derived through the method discussed in this paper, clearly show a lower level of the atmospheric residuals in the 1.9 hydration band, thus resulting in a better match with the MGM deconvolution parameters found for the laboratory spectra of martian hydrated mineral analogues and allowing a deeper investigation of this spectral range.

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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 both the OMEGA (Observatoire pour la Minéralogie, l'Eau, les Glaces et l'Activité)

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and CRISM (Compact Reconnaissance Imaging Spectrometer for Mars) imaging spectrometers, on board the ESA/Mars Express and the NASA/MRO respectively, allow for the identification and mapping of different minerals (e.g., [Bibring et al., 2004](#); [Murchie et al., 2007](#)). 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 $(\text{CO}_3)^{2-}$ 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. The standard processing approach to remove the atmospheric contribution is to divide the spectra by a scaled atmospheric spectrum measured across Olympus Mons ([Langevin et al., 2005](#); [McGuire et al., 2009](#)). Then, the residual errors are suppressed by ratioing the target spectrum by a low spectral contrast reference spectrum of the same observational session (or cube), apparently without any relevant features and characterized by a smoother continuum (e.g., [Bibring et al., 2005](#)). [Bakker et al. \(2014\)](#) introduced a new method to obtain the surface reflectance deriving atmospheric transmission models (ATM) from the OMEGA image itself. This method has the advantage to take into account the seasonal and diurnal variability of the atmospheric gases (CO_2 and H_2O), but no attempt was made to correct for aerosols effects.

[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 and 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 and 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 and 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 .

Section 2 gives a short description of the OMEGA instrument and the set of data used in the present work. Section 3.1 summarizes the theoretical background of the PCA and target transformation approach, while the application of the method to a test case is shown in Section 3.2. Section 4 is devoted to the analysis of two OMEGA orbits passing through Nili Fossae (Section 4.2) and Mawrth Vallis (Section 4.3), where different mineral assemblages and the presence of phyllosilicates where already recognized (e.g., [Poulet et al., 2005, 2008](#); [Mustard et al., 2007](#); [Mangold et al., 2007](#); [Ehlmann et al., 2008](#); [Bishop et al., 2008a,b](#); [Noe Dobrea et al., 2010](#)). The presence of these minerals on the Noachian crust of Mars implies likely the presence of liquid water during the first

billion year (e.g., [Loizeau et al., 2007](#)) and strong climate changes between the present time and the epoch in which phyllosilicates formed. The application of the multivariate analyses techniques to OMEGA spectra in order to remove the gaseous atmospheric components is completed by the removal of atmospheric dust component as described in Section 4.4. The spectral surface component classification and deconvolution are addressed in Section 5, where it is shown that the SAS method permits an improvement in the identification of the mineralogical phases by means of MGM, in particular for the investigation of hydrated mineralogy. Finally, the discussion and conclusions are in Sections 6 and 7, respectively.

2. Instrument and dataset

In each resolved pixel (1.2×1.2 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 (VNIR) channel, between 0.38 and 1.05 μm) to 14 nm (short wavelength range, SWIR-C, between 0.93 and 2.73 μm) and 20 nm (SWIR-L, 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 peri-center) 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. Data and calibration software are publicly available through ESA's Planetary Science Archive. The OMEGA VNIR and SWIR-C channels data are co-registered according to [Carrozzo et al. \(2012\)](#). Together with CRISM, OMEGA allowed for the first time the clear detection of hydrated minerals such as hydroxides, sulfates and in particular phyllosilicates (e.g., [Poulet et al., 2005](#); [Gendrin et al., 2005](#); [Arvidson et al., 2005](#); [Milliken et al., 2008](#)).

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. 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. This observational session has been acquired on May 20th, 2004 during martian year 27 (the martian years start on 1955, April 11 at solar longitude 0° , following the convention used in [Clancy et al., 2000](#)), at solar longitude 36.1° (northern spring). The ground track goes from south to north crossing a changing elevation from -2.97 km to 1.73 km. Orbit 0353_3 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. This observational session has been acquired on April 30th, 2004 during martian year 27, at solar longitude 26.8° (northern spring) and contains 99,820 spectra.

3. Method and validation

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,

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