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Spectroscopy and trace gas retrievals for the ExoMars Trace Gas Orbiter (TGO) Atmospheric Chemistry Suite mid-infrared (ACS MIR) solar occultation spectrometer using the JPL Gas Fitting software (GFIT)

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Abstract

The ExoMars Trace Gas Orbiter (TGO) intends to study the composition of the Martian atmosphere. It was jointly developed by ESA and Roscosmos and successfully entered orbit around Mars in October 2016. After a lengthy, but crucial, aerobreaking campaign, its orbit was nominally reduced to a near-circular 400 km altitude, with a 2 hour period, in January 2018. There are four scientific instruments on TGO: the Atmospheric Chemistry Suite (ACS), the Nadir and Occultation for Mars Discovery (NOMAD), the Colour and Stereo Surface Imaging System (CaSSIS), and the Fine-Resolution Epithermal Neutron Detector (FREND). This presentation will focus on trace gas retrievals for the mid-infrared (MIR) channel of the ACS instrument operating in solar occultation mode. The first solar occultation observations were made on April 21, 2018, with nominal science operations to follow. We will present the retrieval scheme, our evaluation of spectroscopic parameters, sensitivity to a priori data, results from retrievals for simulations of the Mars atmosphere, and spectral fitting results for the first set of solar occultation observations made by ACS MIR.

ACS is a set of three spectrometers that are designed to better characterize the atmosphere of Mars with unprecedented accuracy (Korablev et al., 2018). It aims to detect and quantify unknown trace gases diagnostic of active geological or biological processes, to map their distribution and attempt to identify sources, and to refine our knowledge of the vertical distribution of major and minor atmospheric gases. It has three channels: near-infrared (NIR), thermal-infrared (TIRVIM) and MIR. The ACS MIR channel uses a novel concept for atmospheric studies: a cross-dispersion spectrometer combining an echelle grating with a wide blaze angle and secondary, steerable diffraction grating (Korablev et al., 2018). It covers the wavenumber range of 2375–4340 cm^{-1}.

ACS MIR data is being processed by several groups. This presentation will focus on the data product generated at LATMOS using the Gas Fitting software (GFIT) maintained by NASA's Jet Propulsion Laboratory. GFIT if a part of the GGG software suite and is designed to be a multipurpose and robust spectral fitting suite (e.g., Sen et al., 1996; Irion et al., 2002). It was derived from early versions of the Occultation Display Spectra (ODS) software developed or the ATMOS spectrometer flown on the space shuttles (Norton and Rinsland, 1991). It is currently used for the MkIV balloon missions (Toon, 1991) and the Total Carbon Column Observing Network (TCCON) of ground-based FTSs (Wunch et al., 2011).

GFIT computes volume absorption coefficients for each gas in a chosen spectral range, computes a spectrum line-by-line, and fits the computed spectrum to the measured spectrum using a non-linear Levenberg-Marqhardt minimization. The state vector contains the continuum level and tilt, and volume mixing ratio (VMR) scaling factors (VSFs) for each target gas. GFIT is capable of fitting multiple gases at the same time. The VSF is a multiplicative scaling factor applied to the *a priori* VMR vertical profile. In principle, GFIT only modifies the magnitude, and not the shape of, the *a priori* VMR vertical profile. However, in solar occultation mode, the *a priori* can be scaled for each observed spectrum at each tangent altitude. To retrieve a VMR vertical profiles for a target gas from a set of solar occultation spectra, the set of retrieved slant columns abundances from each observation are inverted with calculated slant column paths traced through the atmosphere using a linear equation solver.

Two major spectroscopic line lists, HITRAN and GEISA, have been recently updated. Both the 2015 edition of the GEISA spectroscopic database (Jacquinet-Husson et al., 2016) and the 2016 edition of the HITRAN spectroscopic database (Gordon et al., 2017) feature significant changes to the spectroscopic parameters for CO_2. These changes were developed to support greenhouse gas measurements at Earth by TCCON, the Greenhouse Gases Observing Satellite (GOSAT) and the Orbiting Carbon Observatory (OCO-2). On Mars, while the average surface pressure is roughly 200 times less than Earth's, the VMR of CO_2 is over 2000 times that of Earth. Therefore, CO_2 absorption lines in solar occultation spectra are can be larger for Mars than for Earth, and minor changes to the spectroscopic parameters can lead to large differences in the calculated spectra. To determine whether these changes lead to improved spectral fits, we have applied both databases, as well as HITRAN 2012 (Rothman et al., 2013) to spectral fitting of Earth-observing solar occultation spectra recorded by the Atmospheric Chemistry Experiment FTS (ACE-FTS) Bernath et al. (2005). We have also investigated the effects of spectroscopic parameters recently made available for air-broadening parameters in a CO2-rich atmosphere. Parameters for some gases have been compiled by HITRAN (CO, SO_2, NH_3, HF, HCl, OCS, and C_2H_2) (Li et al., 2015; Wilzewski et al., 2016), while parameters for water vapour have been made available by Gamache et al. (2016) and Devi et al. (2017). We will present the results of our validation of HITRAN 2016 and GEISA 2015, and also show the effects that CO_2 broadening parameters have on synthetic Mars spectra.

A first attempt at spectral fitting will be done using climatological models from the Mars Climate Database (Forget et al., 1999; Millour et al., 2015). New observations of temperature and pressure made by the Mars Reconnaissance Orbiter's Mars Climate Sounder and the TIRVIM channel will be assimilated into the LMD General Circulation Model. When a more accurate assimilation is ready, the retrievals will be reprocessed using the updated *a priori* vertical profiles of temperature, pressure, CO_2 VMR, and H_2O VMR. Vertical profiles of temperature and pressure will also be retrieved by simultaneous observation made with ACS NIR and TIRVIM. These will be used to produce a third version of our MIR data product. As the mission progresses, we will quantify the differences among sources of a priori data, and study their effects on retrievals.

Much work has been done to investigate the limits of the retrieval algorithm by generating synthetic spectra for different atmospheric conditions (temperature, pressure, dust loading, and trace gas abundances). Noise is added to the spectra, they are resampled to a uniform fitting grid, and spectral fitting is performed using generic *a priori* to see how well the trace gas VMR vertical profiles used to create the synthetic spectra are reproduced. We found that given accurate temperature and pressure a priori, and a CH_4 abundance between 2–6 ppbv, we can accurately reconstruct the vertical profiles of CH_4 in the presence of noise. However, at low altitudes, due to signal attenuation from dust and interference from strong CO_2 absorption features, our retrieval becomes less accurate when the dust is high. Similarly, at high altitudes, where absorption line depths approach the magnitude of the noise, our retrieved profiles diverge from the true state of the atmosphere.

Since the end of April 2018, ACS MIR has been recording sets of solar occultation spectra. We will present our initial investigations into processing and fitting the data, focusing on the spectra and the goodness of fit for target gases in selected micro-windows. We will also present the latest state of our data processing and current best estimates of the composition and vertical structure of the atmosphere as estimated using GGG and ACS MIR.

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