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Abstract

ExoMars is a two-part mission to Mars jointly led by ESA and Roscosmos. The first phase was launched in March 2016 and consisted of the Trace Gas Orbiter (TGO) and Schiaparelli lander. The TGO successfully entered orbit around Mars in October 2016 and has since begun a crucial aerobreaking campaign to circularize its orbit with a nominal 400 km altitude and 2 hr period. There are four scientific instruments on TGO: the Atmospheric Chemistry Suite (ACS), the Nadir and Occultation for Mars Discovery (NOMAD) spectrometer, 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.

ACS is a set of three spectrometers that are designed to better characterize the atmosphere of Mars with unprecedented accuracy. 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 NIR channel is combination of an echelle grating and an acousto-optical tunable filter (AOTF), and is similar to the Ultraviolet and Infrared Atmospheric Spectrometers for Mars and Venus (SPICAM/V) on Mars Express and Venus Express (Korablev et al., 2006; Bertaux et al., 2007). It has a spectral range of 0.73–1.6 μm and operates in nadir mode. It is intended to provide mapping support to solar occultation measurements. TIRVIM is a small Fourier transform spectrometer with a spectral range of 2–17 μm and resolution of 0.2 cm^{-1}. It has heritage from the Mars Express Planetary Fourier Spectrometer (PFS), operates in both nadir and solar occultation mode, and will be able to measure the physical state of the atmosphere (vertical profiles of temperature, pressure and dust opacity). NOMAD is also a multi-channel spectrometer with complimentary objectives to ACS. It consists of a pair of combination echelle-AOTF spectrometers, much like SPICAM/V and ACS NIR, that operate in both nadir and solar occultation mode. In its original configuration, TGO carried a high-resolution Fourier transform spectrometer (FTS) covering a wide spectral range to detect trace gases (Wennberg et al., 2011), supported by the nadir-viewing NOMAD instrument capable of carrying out trace gas mapping studies. The ACS MIR channel aims to reproduce the capabilities of the FTS using 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., 2017). It is capable of finer resolution than its echelle-AOTF counterparts, but is limited in its instantaneous spectral range compared to its FTS predecessor.

The ACS MIR block is thermally isolated from TIRVIM and coupled to NIR, but shares a common electronics block. It consists of an entry telescope and collimator, a large echelle grating (107×240 mm, 3.03 grooves per mm), a steerable pair of secondary grating mirrors, and a Sofradir MCT array detector The low-density echelle grating at a high blaze angle (63.43°) provides overlapping spectra at high orders. The secondary grating separates the orders and the resulting spectra are recorded by the detector with 640 pixels in the x direction corresponding to wavelength, and 512 pixels in the y direction corresponding to order. Several spectra are recorded for each order on sequential pixel rows. The secondary grating has two reflective gratings mounted side-by-side that can rotated. We

will use ten secondary grating positions, each with an instantaneous spectral width of around 16 cm^{-1} between 2380 and 4350 cm^{-1}. The spectral orders and range covered by each position are given in Table . During the acquisition of a set of solar occultation spectra, the grating position can be changed between each measurement, allowing for the retrieval of vertical profiles for several trace gases and major species at the same time.

Table 1: Spectral ranges and orders of secondary grating positions.

Grating angle	Diffraction orders	Minimum wavelength	Maximum wavelength
7.5°	205–213	2.790 µm	2.899 µm
5.7°	214–223	2.665 µm	2.790 µm
3.9°	224–235	2.529 µm	2.665 µm
2.1°	236–248	2.397 µm	2.529 µm
0.3°	249–258	2.304 µm	2.397 µm
-3.3°	142–149	3.984 µm	4.209 µm
-5.1°	150–161	3.688 µm	3.984 µm
-6.9°	162–174	3.414 µm	3.688 µm
-8.7°	175–190	3.127 µm	3.413 µm
-10.5°	191–208	2.857 µm	3.127 µm

Raw spectral images will be processed by ESA at the European Space Operations Centre (ESOC), calibrated spectra will be produced by Roscosmos at the Space Research Institute (IKI), and there are two parallel trace gas retrieval operations: at IKI, based on SPICAV retrievals, and at LATMOS, presented here. All three channels of the ACS instrument, and the other TGO instruments have been switched on and checked out on several occasions between launch and orbit capture.

1. ACS MIR Retrievals

The LATMOS ACS MIR retrievals will be based on software prepared for the high-resolution solar occultation FTS from the original TGO configuration. We will use the GGG software suite maintained at NASA's Jet Propulsion Laboratory. GGG is 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 designed to be a multipurpose and robust spectral fitting suite and is currently used for the MkIV balloon FTS missions (Toon, 1991) and the Total Carbon Column Observing Network (TCCON) of ground-based FTSs (Wunch et al., 2011).

The main component of GGG is GFIT, which computes volume absorption coefficients for each gas in the fitting 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.

The computed spectrum is calculated using the HITRAN 2012 spectral line list (Rothman et al., 2013), with modifications provided by JPL for the TCCON collaboration. Line broadening coefficients for CO_2 need to be modified to reflect the lower pressure and colder temperatures of the Martian atmosphere, and collisional-induced broadening in 95% CO_2 atmosphere. We are implementing new broadening parameters from Brown et al. (2007) and Lavrentieva et al. (2014). In theory, the retrievals done with GGG are independent of the VMR *a priori*. For consistency, a single set of *a priori* VMR vertical profiles will be used. These will be refined as our knowledge of the Mars atmosphere increases. The VMRs of major interfering species, CO_2 and H_2O, may be updated for each occultation.

Temperature and pressure are vital parameters for accurately computing absorption line depths. A first attempt at spectral fitting will be done using climatological models from the Mars Climate Database. New observations of temperature and pressure made by the Mars Reconaissance 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 retreivals will be reprocessed using the updated *a priori* vertical profiles of temperature, pressure, CO_2 VMR, and H_2O VMR.

Much work is being 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). To test our ability to resample the spectra, very high resolution spectra are computed first, then resampled to the realistic, non-uniform spacing of an MIR order. 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 will introduce the ExoMars TGO mission, the ACS instrument and summarize the results of pre-science-operations instrument check-outs. The GGG software suite will be introduced, as will be the work done to adapt it for use at Mars with ACS MIR, such as modelling the ACS MIR instrument line shape. We will show our simulations of solar occultation transmission spectra, and present results of our effort to fit these spectra and retrieve vertical profiles of trace gas VMRs.

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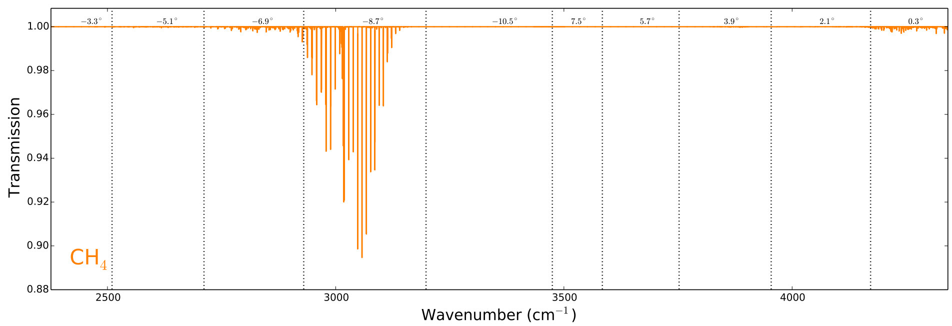

Figure 1: An excerpt from the ACS MIR spectral atlas showing the contribution from methane to the solar occultation transmission spectra. This spectrum shows all secondary grating positions, but the ACS MIR instrument can only record a spectrum for one position instantaneously. The dashed vertical lines show the range of each position. To search for methane, the $-8.7°$ secondary grating position will be used. This spectrum represents a tangent altitude of 20 km and a peak methane abundance of 6 ppmv.