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Vertical distributions of CO, H₂O, HDO, and temperature in the atmosphere of Mars after a year of observations with the ExoMars Trace Gas Orbiter (TGO) Atmospheric Chemistry Suite mid-infrared (ACS MIR) solar occultation spectrometer

K. S. Olsen (1), J. Alday (2), L. Baggio (1), D. Belyaev (3), A. Fedorova (3), A. Grigoriev (3), F. Lefèvre (1), O. Korablev (3), F. Montmessin (1), A. Patrakeev (3), L. Rossi (1), A. Shakun (3), and A. Trokhimovskiy (3)

(1) Laboratoire Atmosphères, Milieux, Observations Spatiales (LATMOS/CNRS), Paris, France, (2) Department of Physics, University of Oxford, Oxford, UK, (3) Space Research Institute (IKI), Moscow, Russia (kevin.olsen@latmos.ipsl.fr)

Abstract

The ExoMars Trace Gas Orbiter (TGO) began its nominal science phase in April 2018 after arriving at the red planet in October 2016 and undergoing a lengthy aerobraking campaign. It carries a stereo camera (CaSSIS), a neutron detector (FREND), and two spectrometer suites aimed at investigating the atmosphere: the Atmospheric Chemistry Suite (ACS), and the Nadir and Occultation for Mars Discovery (NOMAD). This presentation focuses on data analysis for the mid-infrared (MIR) channel of ACS, operating exclusively in solar occultation mode. We will describe work done to produce a Level 2B data product of calibrated transmission spectra and then show results from performing trace gas retrievals on target gas species, such as H₂O, HDO, CO, and CH₄.

ACS MIR is a cross dispersion spectrometer consisting of an echelle grating with a wide blaze angle and a secondary, steerable diffraction grating (Korablev et al., 2018). The secondary grating is used to separate high diffraction orders and access a spectral range of 2300–4400 cm⁻¹. The simultaneous spectral range observed during an occultation is around 200 cm⁻¹ wide, and the spectral resolution is around 0.04 cm⁻¹.

1 Level 2B data processing

Raw detector images (Level 0B) are processed at IKI and LATMOS. These undergo several corrections to produce Level 1A data, including: correcting hot pixels and accumulation errors, removing the dark background and flat field, vertical and horizontal sub-pixel registration, and performing an orthorectification transformation. After these steps, transmission spectra

(Level 2A) are computed using a reference observation of the sun, and observations made during atmospheric occultation. Level 2A data consists of an image of transmittances for each altitude in an occultation. The x -axis corresponds to wavenumber, and the y -axis corresponds to diffraction order. Each observed diffraction order covers 15–20 rows, and this extent corresponds to the vertical field of view of the instrument (~ 3 km). The first step in processing Level 2A data is to select rows for analysis. We are currently working near the edge of the optical entry slit, which is identified by the inflection point of an incident light intensity curve for a given order.

The second step is wavenumber calibration for the selected rows. A first-guess wavenumber vector is created for each order. The corresponding row of the solar reference observation (made outside the atmosphere) is then used to perform wavenumber calibration by fitting peak positions of solar lines to a reference solar atlas measured by the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) (Hase et al., 2010). If strong absorption lines of CO₂, H₂O, or CO are present in an order's spectral range, the wavenumber calibration is refined by comparing measured absorption line centres to modelled spectra.

Finally, *a priori* temperature (T) and pressure (P) are determined. Initial T and P , and the abundances of major gas species, are taken from the Mars Climate Database (Forget et al., 1999; Millour et al., 2015). Where available, CO₂ lines across an absorption-rotation band are fit by the retrieval code. This set of fitting results is evaluated to estimate corrected vertical profiles of T and P (Olsen et al., 2015). This method is not always available, and other sources of more accurate T and P data include: ACS MIR retrievals performed at the University of Oxford, ACS near infrared (NIR) retrievals performed at IKI, and nadir ACS ther-

mal infrared (TIRVIM) data assimilation performed at the Laboratoire de Météorologie Dynamique.

2 Retrievals

Retrievals are performed using the Gas Fitting software (GFIT) maintained by NASA's Jet Propulsion Laboratory. GFIT is 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 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-Marquardt minimization. To retrieve volume mixing ratio (VMR) vertical profiles for a target gas from a set of solar occultation spectra, the set of retrieved slant column abundances from each observation are inverted with the slant column paths through the atmosphere using a linear equation solver.

Absorption features of CH₄ have not yet been observed in the Martian atmosphere by ACS or NOMAD (Korablev et al., 2019). We are continuing to search for it and other trace gases, such as HCl, C₂H_n, HCN, OCS, and HF.

With ACS MIR, we have been able to produce the first vertical profiles of CO abundance. These are characterized by being well mixed up to 70 km, and then increasing in abundance above, where CO₂ is photolyzed. Our initial observations are of very similar profiles at both high and low latitudes. These will be presented alongside model output from the LMD GCM (Forget et al., 1999).

We will also present vertical profiles of water vapour and HDO. H₂O is very dynamic in the atmosphere of Mars and we have observed very large seasonal changes related to increased dust content from local and global dust storms. Of key interest is the vertical distribution of HDO, and the D/H ratio. HDO in the Mars atmosphere is enriched relative to Earth, indicating that there are mechanisms for hydrogen escape from the atmosphere, preferential towards the lighter isotope (Clarke et al., 2017). The D/H ratio may also be impacted by ice cloud formation and seasonal sublimation cycles of the ice caps. We are also interested in the behaviour of water vapour above 50 km which is enhanced in the presence of dust and can accelerate

H escape.

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