

TRACE GASES INVENTORY AND CHARACTERIZATION: IMPROVEMENTS IN THE SPECTRAL ANALYSIS EXPECTED FOR THE NEXT MARS MISSIONS. A.C. Vandaele¹, F. Daerden¹, C. Depiesse¹, A. Mahieux¹, L. Neary¹, S. Robert¹, I. Thomas¹, S. Viscardy¹, Y. Willame¹, V. Wilquet¹, E. Gloesener², O. Karatekin², J. Vander Auwera³, L. Fissiaux⁴, M. Lepère⁴, and A. Garcia-Munoz⁵. ¹Planetary Aeronomy Div., Belgian Institute for Space Aeronomy (a-c.vandaele@aeronomie.be), ²Royal Observatory of Belgium, ³Service de Chimie Quantique et Photophysique, Université Libre de Bruxelles, ⁴Laboratoire Lasers et Spectroscopies, University of Namur, ⁵ESA/ESTEC, Noordwijk, The Netherlands.

Introduction: In preparation for future missions to Mars, and in particular for the ExoMars Trace Gas Orbiter (TGO), improvements in existing retrieval techniques need to be investigated. These include, for example: improvements in spectroscopy, or the use of synergies, where measurements from multiple spectral regions and/or instruments are combined. Several different avenues of development will be investigated in this study.

Most of the new techniques were applied to the detection of CO (for which vertical information is the next scientific objective) and CH₄ (to increase the probability of detection if present), but could be expanded to other atmospheric constituents, such as water (vertical information) or isotopologues (increase detection ability) in future.

Other improvements relate to the development of retrieval techniques intimately linked to global circulation modeling (GCM): one typical example would be the use of GCM fields, to take into account inhomogeneities along the Line of Sight (LOS) or across the terminator. The latter will be of direct use to the two spectrometer suites on board ExoMars, for which solar occultation will be one of the major observation modes. GCM and radiative transfer modeling will also improve the way trace gases are characterized.

In the following investigation, we will describe the different developments undertaken in our groups in preparation for the next generation of Martian data.

Spectroscopic Developments: Different improvements have been investigated, such as the use of modified line profiles including the effects of speed dependence and line mixing (very important for CO₂ and CH₄). Line lists have to be adapted and we must therefore rely on the latest laboratory studies available. We will illustrate this topic with 2 different laboratory studies performed on CO [1], HCl [2] and CH₄ [3].

Synergistic retrievals using different spectral ranges or different instruments: Most of the studies conducted to date have relied on a single spectral domain retrieval approach. Synergistic retrievals make use of absorption features present in different spectral ranges which are usually investigated independently. Typical examples include the simultaneous observation

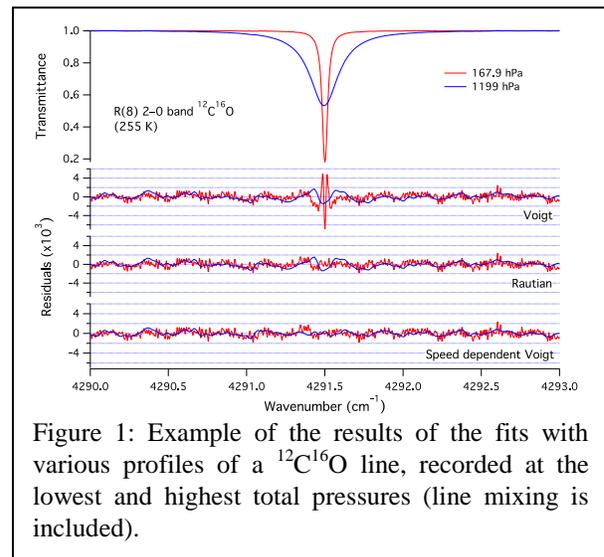


Figure 1: Example of the results of the fits with various profiles of a ¹²C¹⁶O line, recorded at the lowest and highest total pressures (line mixing is included).

of species in the thermal and short wave infrared (TIR and SWIR) showing distinct properties of absorption/emission: Sensitivity to the boundary layer is reduced in the TIR by the thermal contrast between the surface and the first atmospheric layer, and SWIR observations provide column densities with high sensitivity near the ground. TIR measurements are most sensitive in the middle atmosphere but have in most cases only little sensitivity in the lower troposphere. In contrast SWIR measurements are sensitive at any tropospheric altitude with a pronounced sensitivity to near-surface. Synergistic retrieval is expected to increase the sensitivity near the surface.

The analysis will be illustrated on CO which has two main absorption bands at 2.3 μm and 4.7 μm. Combining the information simultaneously from TIR and SWIR domains has already been demonstrated in Earth observations to improve knowledge of the lower atmosphere distribution.

Cross-Terminator improvements: The terminator, a very peculiar region of the atmosphere that solar occultations probe, is the limit between the day and night sides of the planet. It therefore delimits two regions in which the solar illumination and the photochemistry are quite different. Most of the solar occultation retrieval algorithms implemented nowadays [4, 5] rely on a series of assumptions, the most important one

being that the atmosphere is spherically symmetric, i.e. that identical temperature, concentration and density conditions are found at a given altitude independent of the latitude or longitude. However, it is known that densities are lower and temperatures are higher on the dayside than on the night side, particularly at the high altitudes where solar occultations sound the atmosphere. This, combined with the fact that the footprint

of the processes taking place at the terminator will be obtained by the coupling of a GCM [6] and a chemistry box model [7] with much shorter timescale, which is applied along a Lagrangian trajectory. It then will become feasible to supply the retrieval codes with best guesses of the gradients existing across the terminator and the non-homogeneities of composition along the LOS. This requires a very close interaction between retrieval codes and atmospheric models at an unprecedented level. This development will be tested on SOIR (Solar Occultation in the IR on board Venus Express ESA mission) and SPICAM (on board Mars Express) spectra obtained under solar occultation geometry.

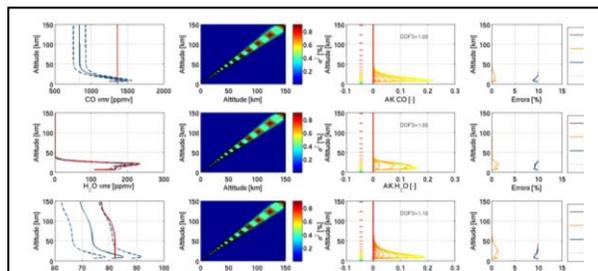


Figure 2: Retrieval profiles obtained with ASIMUT in the case of $L_s=30-60^\circ$, high concentration and no aerosols. The mode of the retrieval was set on "profile". First column of plots are the vertical profiles of vmr for each fitted species (from top to bottom: CO, H₂O and CO₂). Second column represents the variability matrix which has been set to 10%. Then the Averaging Kernels together with the degree of freedom value. And last represents the error matrices.

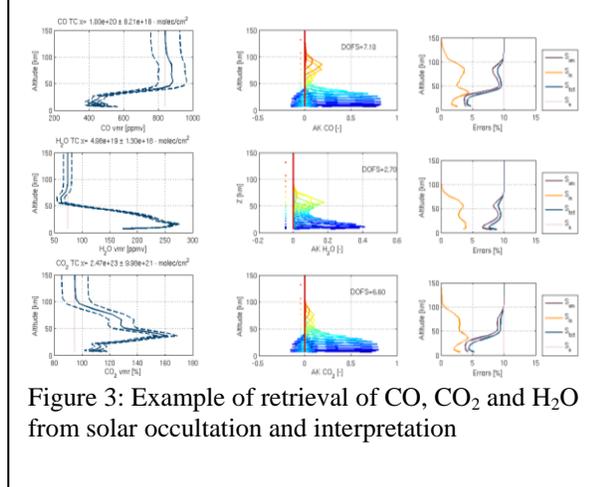


Figure 3: Example of retrieval of CO, CO₂ and H₂O from solar occultation and interpretation

of an occultation on the surface of the planet usually varies by 100 to 400 km, casts doubts on the validity of the hypothesis related to the symmetry of the atmosphere along the line of sight. We are developing a new approach to suppress these limiting assumptions: the precise modelling of trace species distributions at the terminator will be intimately coupled with the improved retrieval schemes. This is made difficult by the rapid timescales of photochemistry at sunrise and sunset, which produce acute variations in the trace gas concentrations at the terminator. Improved knowledge

GCM & modeling developments: General circulation models (GCM) describe how the 3-dimensional atmospheric structure and dynamics evolve with the time of day. GCMs are a crucial tool in the interpretation of measurements, filling in the observational gaps of time and space. Detailed model (3D and 1D) studies of Mars atmospheric chemistry in twilight conditions will help understand the diurnal cycles for a series of species. In particular, ozone (O₃) shows a complex photochemistry driven by the solar illumination. We apply the GEM-Mars GCM with interactive chemistry [6] and will combine this with a 1D model which allows for shorter integration time steps[7].

The extension of the thermal soil model in the GCM, with a model for water vapor exchange and subsurface ice and clathrate stability, will allow to study the impact of surface gas releases on the atmospheric composition.

References: [1] Tudorie, M. et al. (2012) *11th ASA conference and The 12th International HITRAN Conference*. [2] Tudorie, M. et al. (2012) *J Quant Spectrosc Radiat Transfer*, 113, 1092-1101. [3] Fissiaux, L. et al. (2014) *J Mol Spectrosc*, 297, 35-40. [4] Vandaele, A.C. et al. (2008) *JGR*, 113, doi:10.1029/2008JE003140. [5] Vandaele, A.C. et al. (2006) *ESA Atmospheric Science Conference*. [6] Neary, L. et al. (in prep.). [7] Garcia Munoz, A. et al. (2005) *Icarus*, 176, 75-95.

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