

SCOOP

Towards a synergistic study of the atmosphere of terrestrial planets

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NETWORK PROJECT

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Towards a synergistic study of the atmosphere of terrestrial planets

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FINAL REPORT

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ABSTRACT

The thermal structure of an atmosphere is a result of the radiative and convective equilibrium driven by the incidence of solar radiation, which is scattered, absorbed or emitted by the atmosphere itself and the planet surface. The energy balance is influenced by the atmospheric composition and by the presence of clouds and aerosols. In addition, the thermal structure is a driver of the global circulation, which in turn influences the atmospheric composition through vertical and horizontal transports of air masses. Therefore, understanding Mars and Venus current climate requires a multidisciplinary approach, including inter-comparison between observations and models that simulate the contributions of various processes occurring in the atmosphere of terrestrial planets.

The overarching goal of the project was the revision and exploitation of data from space missions, using a synergistic approach by combining different fields of research in aeronomy and integrating the different layers of the Mars and Venus atmospheres from the surface to the upper atmosphere. This knowledge is also invaluable for the definition of future missions.

With its scientific and public outreach success, comprising about 40 international peerreviewed publications, three chapters of the coming Venus III book, countless contributions to international conferences, to VESPA and to VIRA, but also numerous press releases, SCOOP-members interviews in the media, broad audience publications, the project contributed to consolidate the position of Belgian scientists at the international level and therefore reinforcing international collaborations as well as to the dissemination and valorisation of the scientific results towards a broader public.

1. INTRODUCTION

Being the only two planets other than the Earth within our solar system that have a stable atmosphere over a rocky core, Mars and Venus occupy a significant position in our quest for answers to some of the greatest questions, such as those regarding our origins and our place in the Universe. Terrestrial planets are a natural laboratory for the understanding of Earth-like (exo)planets, their history and their diversity.

Of particular interest to the network is the relation between the structure and the dynamics of the atmosphere that results in the transport of trace gases and how variations of greenhouse gases and aerosols in turn influence the thermal structure. Significant progress in these broad themes requires a high degree of innovation and complementarity. The SCOOP project proposed innovative science through the combined exploitation of recent measurements from MEX, VEX and other missions, together with novel retrieval tools and updated atmospheric models.

The network focused on a number of open and challenging issues in current Martian and Venusian research. For instance, the characterization of the vertical structure of their atmosphere and of the heat fluxes through the various atmospheric layers is necessary for a better understanding of the dynamics within such atmospheres, in particular the transport of trace gases, and for the comprehension of the mechanisms involved in the surface-atmosphere exchanges. In addition, a refined knowledge of the vertical and geo-temporal distribution of trace gases, which in turn, in the case of radiatively active trace gases and aerosols impact on the thermal structure of the atmosphere, can serve for the definition of future missions to Mars and Venus by pinpointing gaps in the global climatology.

For the execution of the project, the SCOOP partners had access to many data sets of planetary missions. In particular, the partners are familiar with the data of the following instruments on Venus and Mars Express since they were deeply involved in these missions: SPICAM, SPICAV/SOIR and VIRTIS. The MAVEN mission started collecting measurements in September 2014 and one of the researchers involved in this project (A. Stiepen, ULg) worked one year in the team of the IUVS/MAVEN instrument at LASP that allowed him to become familiar with the IUVS data and their processing tools and used this expertise in the framework of the SCOOP program. The international Partner 1 (Dr. R. Yelle) is moreover the Project Scientist of the MAVEN experiment. The NOMAD instrument started accumulating spectra in April 2018 when science operations of TGO (ExoMars 2016, ESA mission) were initiated. The NOMAD Science Database is managed at IASB-BIRA and it contains data for all three channels (UVIS, SO and LNO) of the instrument. All Belgian partners involved in the SCOOP, as co-Is of NOMAD, have direct and full access to this database.

2. STATE OF THE ART AND OBJECTIVES

The temperature structure of the atmosphere is an important driver of its dynamics and also reflects the vertical distribution of aerosols and clouds and of radiatively active gases present in the atmosphere. The thermal structure of the Mars thermosphere is currently surprisingly poorly known. The reason is that, so far, no space mission was specifically aimed at collecting data to build up an observational database with adequate seasonal and latitudinal coverage. For ten years, the SPICAM instrument on board Mars Express has accumulated a wide dataset of Mars day and nightglow observations. Present models such as the Mars TGCM of the University of Michigan (Bougher et al., 2009) are unable to reproduce the SPICAM observations for low to moderate solar conditions. Furthermore, results obtained from different techniques need to be reconciled (Bougher et al., 2013).

The temperature gradient between the dayside and the nightside in the Venus atmosphere creates an air flux at high altitude causing the subsolar to antisolar (SSAS) circulation at high altitudes (>120 km). The atmospheric temperature is controlled by the solar flux that reaches the atmosphere and complex greenhouse effects. Three decades ago, an international effort led to the adoption of the Venus International Reference Atmosphere (VIRA) that was published in 1985 after the significant data returned by the Pioneer Venus Orbiter and Probes and the earlier Venera missions (Kliore et al., 1985). An update to the VIRA model describing the thermal structure of the atmosphere from surface to 100 km altitude was proposed by Zasova et al. (2007) using data obtained after VIRA publication. Since April 2006, Venus Express has obtained many valuable data on the atmosphere of Venus, including more than a thousand detailed occultation profiles. Additionally, recent ground based observations supplement the spacecraft results. The determination of the thermospheric temperature is also possible using airglow observations. All these observations have shown key areas where the semi-empirical VIRA thermal structure model is deficient and can be improved using the increased coverage in latitude, longitude, local time and altitude range of recent missions.

New missions have now arrived to Mars (NASA MAVEN mission and ESA/ROSCOSMOS ExoMars TGO mission) and future missions to Venus are discussed nowadays at NASA or ISRO. The Belgian Planetary community is involved in these missions and had to be ready for the high amount of new data that are now delivered. The network had also to identify improvements that could reinforce the science return of both the current missions and the future ones.

The overarching goal of the project was the revision and exploitation of data from space missions, using a synergistic approach by combining different fields of research in aeronomy and integrating the different layers of the Mars and Venus atmospheres from the surface to the upper atmosphere. This knowledge is also invaluable for the definition of future missions. To achieve this goal, the network had three main objectives,

(1) A self-consistent compilation of the three dimensional thermal structure of the Mars and Venus atmospheres for a better understanding of the related dynamics. In addition, the understanding of the mechanisms leading to the vertical structure of the Mars and Venus atmospheres obtained from compiled observations still needed clarification.

- (2) To acquire a better knowledge of the vertical distribution of radiatively active trace gases and aerosols in the atmosphere of Venus and Mars, which influences the vertical distribution of energy in the atmosphere. Indeed, infrared properties of aerosols and trace gases play a large role in trapping or emitting heat.
- (3) To improve our understanding of the spatial and temporal variability of trace gases in the Martian atmosphere. For example, the detection of methane and its variability still escapes present photochemical and atmospheric transport models. Mapping of constituents is another aspect of the climate that potentially can serve for the identification of sources of key trace gases, the quantification of the global circulation and of the atmospheric chemistry.

3. METHODOLOGY

This research programme combined analysis of data recently collected by missions to Mars and Venus, models for comparison, understanding and forecasting of evolution of various atmospheric quantities and preparation for future space missions exploring the terrestrial planets. More specifically, the methods used are:

- (1) The remote sensing of the atmospheres to detect and quantify atmospheric constituents in terms of local or integrated densities based on spectroscopic techniques. In particular the analysis of absorption and emission spectra, in the infrared (IR) and the ultraviolet (UV), to determine various atmospheric chemical species and aerosols, and indirectly derive the temperature.
- (2) Modelling of radiative transfer as it is an important and unavoidable step in the interpretation of planetary atmospheric observations. The ASIMUT and ASIMAT radiative transfer code (Vandaele et al., 2006, Mahieux et al., 2012) were used along with the associated retrieval algorithm to determine geophysical quantities and were adapted for the planet Mars, and for observations in the UV.
- (3) The elaboration of atmospheric models for the planets Mars and Venus combining data obtained with different instruments and/or using different technologies. These atmospheric models are repository of geophysical data accessible in terms of species, time, solar local time, longitude and latitude, etc...
- (4) To apply an optical model, based on the Mie theory, to derive microphysical properties of aerosols in the Venus upper haze
- (5) To develop elementary 1D-models for the interpretation of the retrievals results in terms of atmospheric processes such as: the temperature and concentration gradient across the terminator, the processes leading to atmospheric airglow, the radiative transfer on Venus to explain the discrepancy in the thermal structure between GCM and VEX observations, the clathrates outgassing from the Martian subsurface into the atmosphere

Whenever possible, the results obtained within the frame of the project were interpreted and analysed in terms of their possible use for future missions towards Mars or Venus. This is particularly true for the new or improved tools that were developed: their usability for NOMAD was investigated and the science return improvement was evaluated.

4. SCIENTIFIC RESULTS AND RECOMMENDATIONS

4.1. Venus

4.1.1 Synthesis of Venus Express measurements

Thermal structure of the Venus atmosphere

ESA's Venus Express mission has considerably increased the knowledge of the Venus atmospheric structure above ~40 km and provided enough new information above 100 km to trigger new ideas for the interpretation of the observations. In addition, we have participated in an important synthesis of current knowledge on the Venus thermal structure and dynamics. This task consisted in tabular compilations of the vertical and latitudinal structure of the temperature in the Venus atmosphere as a function of altitude as feasible from the available observations and guidance from the atmospheric models. Temperature and density measurements from different VEX instruments have been collected, critically reviewed and compared, with the purpose to build a reference atmosphere encompassing most of the Venus atmosphere. This activity has been carried out within the ISSI International Team dedicated to the Temperature and Structure of the Venus atmosphere, in which both IASB-BIRA and ULiège have been involved. An extensive manuscript has been published in Limaye et al. (2017). Figure 1a illustrates the compilation of nightside temperature measurements based on different techniques, including airglow determinations.

Figure 1b is another example resulting from this work comprising the temperature profiles based on SOIR data, among others. In this example, the compilation concerns the terminator in the Polar Regions. It illustrates the significant contributions of Venus Express, particularly at higher altitudes as it provides new information about the atmospheric structure above 100 km. The combined profiles show a complicated thermal structure in the 90 km–150 km altitude range with alternating warm and cool layers. A high variability of temperatures as well as of CO_2 densities is observed by SPICAV and SOIR in the terminator zones and seems to be caused by short-term temporal variability (all kinds of atmospheric waves) at altitudes above 100 km. This wasn't expected before the VEX mission and it is not yet very well understood. In situ measurements of the total atmospheric density at very high altitudes obtained from drag or aerobraking experiments (Müller-Wodarg et al., 2006, 2016, Rosenblatt et al., 2012) do however corroborate these results.

The role of the solar activity cycle on the distribution and dynamics of the O_2 1.27 µm nightglow has been studies based on several years of VIRTIS nadir observations. A potential source of variability is the solar EUV flux that dissociates CO_2 on the dayside and is therefore expected to control the total amount of O atoms carried to the nightside. The EUV solar flux between 0.1 and 50 nm measured by the SEM index only varied by 14% during the period of VIRTIS observations. However, Soret and Gérard (2015) did not observe any correlation between the O_2 nightglow intensity and the solar EUV flux during solar minimum conditions. We concluded that internal factors such as wave activity mask out the solar control of the oxygen night airglow variability during quiet solar activity periods.



Figure 1: Temperature profiles of the Venus atmosphere: (a) equatorial latitudes on the nightside and (b) polar latitudes at the terminator. These profiles are combined from the VEX instruments, ground-based measurements and models (Limaye et al., 2017)

Trace gases and aerosol characterization

Beside the structure of the Venus atmosphere derived from the CO_2 density, considerable progress has been made in the retrievals of trace gases (CO, SO₂, hydrogen halides, H₂O and HDO) and aerosols. The whole data set has been analysed and all SOIR results on the composition will be ingested in the updated VIRA, in combination with recent measurements from other instruments (Vandaele et al., 2016).

The most recent results of this analysis concerns the water vapour in the Venus mesosphere (Chamberlain et al., submitted). In addition, the deuterium hydrogen isotopic ratios vertical profiles derived from water is currently being analysed. Both H_2O and HDO are targeted simultaneously in the majority of dedicated SOIR water vapour observations. H_2O is detected between 70 - 110 km and HDO is detected between 70 - 95 km of altitude: ~300 concomitant observations throughout the instruments lifetime (2006-2014).

The standard deviation of the mean water vapour profile from SOIR data on Venus (Fig.2) is significantly smaller than the variation from orbit to orbit indicating that variability is not a product of uncertainties. A common feature of note appears to be a local maximum volume mixing ratio (vmr) occurring between 95 and 105 km of altitude. It is also observed that orbit to orbit variations in water vapour abundance are much greater (up to one order of magnitude) than latitudinal and diurnal variations (Fig.3). In addition, no long-term trends or cycles appear to be obvious from the SOIR dataset, which is also consistent with previous observations, and no obvious dependence on observations obtained using the morning or evening sides of the terminator.



Figure 2: Mean SOIR water vapour volume mixing ratio (left panel) and temperature (right) panel as a function of the pressure. The shaded areas show the standard deviation of data at each pressure level. The dashed lines delineate the minimum and maximum values (Chamberlain et al., submitted).



Figure 3: On the left, VMR of water vapour at various pressure/altitude levels for successive occultations (Jan-Feb 2009): 10^{-4} mbar/~120 km (upper panel), 10^{-3} mbar/~112 km (middle panel) and 10^{-2} mbar/~103 km (lower panel). The right panel depicts the geolocation of the observations, colour displays latitude from Polar (dark red) to Equatorial (dark blue) and circles (6AM) and triangles (6PM) denote the local solar time (Chamberlain et al., submitted).



Figure 4: Mean profiles of the particle number density based on the analysis of SPICAV-IR/VEX solar occultation (Luginin et al., 2016) for mode 1 (green) and mode 2 (red).

A comprehensive review of the clouds and hazes on Venus was published following remarkable progress in the study of Venus clouds by the orbiters Venera-15, -16 in 1983, Venus Express in 2006–2014, and Akatsuki since 2016 (Titov et al. 2018). The most important contribution of SPICAV-SOIR is the vertical structure and microphysical properties of the upper haze, above the clouds layer. Indeed, a first study of the microphysical properties of the mesospheric haze suggested for the first time existence in some cases of at least two types of particles (Wilquet et al. 2009) while before that the upper haze was known to be composed of submicron sulphuric acid droplets, also present within the clouds (Venus II book, to be published). More recently, the bimodal character of the particles size distribution in the upper haze was confirmed from the analysis of solar occultations observations at 10 near-IR wavelengths with the SPICAV-IR channel (Luginin et al. 2016). Figure 4 gives the mean number density vertical profiles for the two aerosol modes identified above the clouds in the Venus mesosphere; mode 1 with $r_{\rm eff}$ = 0.12 \pm 0.03 μ m and mode 2 with $r_{\rm eff}$ = 0.84 \pm 0.16 μ m. The ratio between both number densities is about constant with the altitude.

4.1.2 Remote sensing of non-thermal emissions

We participated in a study lead by Frahm et al. (2018) (SWRI) on the highest energetic electron energy fluxes measured with ASPERA-3 on board Mars Express and ASPERA-4 on Venus Express. A total of 24 million spectra from Mars Express spanning 13 years have been examined using the electron spectrometer from all latitudes and local times. The top 10 largest differential energy fluxes at energies above the differential energy flux peak have been found. Spectral comparisons show a decade range in the peak of the electron distributions. All distributions show a similar energy maximum controlled by solar wind/planet interaction. Similarly, the largest Venus spectrum occurred near the magnetosheath bow shock and had the same shape as the most intense Mars inner magnetosheath spectrum. The Mars and Venus dayside spectra show a similar shape to the Mars nightside spectrum that included an enhanced signal attributed by Gérard et al. (2015) to discrete "auroral" precipitation. The Mars and Venus results suggest that no additional energy is needed to generate electrons forming the nightside precipitation.

A comprehensive review entitled 'Aeronomy of the Venus upper atmosphere' (Gérard et al., 2017a) has been published as a research paper in Space Science Reviews. It will also be one of the chapters of the upcoming Venus III book summarizing space (Venus Express) and ground based observational and model results about Mars upper atmosphere obtained during the recent years. This review presents aeronomical observations collected using VIRTIS and SPICAV remote sensing instruments, complemented with ground-based observations and numerical modelling. It is mostly based on measurements of airglow obtained in the nadir mode and at the limb above 90 km. These observations complement our understanding of the behaviour of Venus' upper atmosphere that was largely based on Pioneer Venus observations mostly performed over thirty years earlier. Following a summary of recent spectral data from the EUV to the infrared, we show how these observations have improved our knowledge of the composition, thermal structure, dynamics and transport of the Venus upper atmosphere. We synthetized progress in three-dimensional modelling of the upper atmosphere which is largely based on global mapping and observations of time

variations of the nitric oxide and O_2 nightglow emissions. Processes controlling the escape flux of atoms to space are described. Results based on the VeRA radio propagation experiment were also summarized and compared to ionospheric measurements collected during earlier space missions. Finally, we discussed some unsolved and open questions generated by these recent datasets and model comparisons.

Auroral optical signatures in the SPICAV and VIRTIS sets of spectra have been extensively searched on the Venus nightside but no detection could be identified.

4.1.3 Radiative transfer model

During postdoc stays at the Lunar and Planetary Laboratory (LPL, University of Arizona (UofA), Tucson, Arizona) and in close collaboration with Pr. R. V. Yelle, a *time-dependent vertical 1D non-LTE radiative transfer model* (1DRTM) was developed, in order to study the steady state of the atmospheric composition – densities and relative abundance – and thermal structure (Mahieux et al., in preparation).

This model takes into account the radiative heating and cooling contributions of the different gaseous and aerosol species, the thermal conduction and the species diffusion within the atmosphere. It assumes hydrostatic equilibrium. It considers the density profiles of the main species present in the atmosphere. It is currently set up for Venus, and will easily be adapted for the Martian atmosphere. This model is a powerful tool to study the influence of external forcing parameters, such as the solar zenith angle, the solar input radiance, density sources and sinks originating from chemical reactions or transport, etc., and to understand where each species is radiatively active. It returns the vertical profiles of the simulated species, the temperature profile, the different heating and cooling sources, and the values of the mass and energy exchanges at its boundaries. These are located at the transition between the mesosphere to the troposphere at the bottom and between the thermosphere at the top of the domain, which will help constrain the escape to space of the lightest species. It also calculates the non-LTE vibrational populations of the species of interest, currently CO_2 , the main species of both Venus and Mars atmospheres.



Figure 5: Example of steady-state thermal balance results from 1DRTM for the Venus terminator conditions (Mahieux et al., in preparation). Left: main species heating (plain) and cooling (dashed) terms. Right: non-LTE ratio of the CO_2 vibrational states, grouped in 9 groups as a function of their energy, given in HITRAN notation.

In Figure 5, we present an example of the 1DRTM radiative heating and cooling terms calculated for the Venus terminator conditions and the CO_2 non-LTE population ratios for

different vibrational states. The calculated non-LTE populations can then be compared to measurements performed by space-borne instruments.

When using 1DRTM to simulate the mean SOIR profiles, excess heating induced by CO_2 non-LTE heating is observed from 80 to 98 km, while extra cooling is observed from 98 to 120 km. We expect the aerosols to be responsible for the extra cooling and heating in those two regions. Thus, we want to add aerosol species with a small radius in the upper region to equilibrate the heating/cooling profile with a mean radius of 0.01 µm, for which heating is larger than cooling. In the lower region, we will add larger aerosols (0.2 µm), that have a cooling radiative balance.

4.2 Mars

4.2.1 Solar wind interaction with the Martian atmosphere

The ultraviolet aurora

Three types of Martian aurora have been recently discovered based on Mars Express and MAVEN in situ and ultraviolet remote sensing measurements. Significant progress in their characterization has been accomplished in the framework of the SCOOP program.

Discrete aurora

The full SPICAM database collected on the nightside during the Mars Express mission was analysed to identify the presence of the CO Cameron and CO_2^+ doublet UV auroral emissions and characterize signatures of the UV auroral events. A total of 16 events were detected in the nadir direction and three additional ones were observed at the limb, all of them in the Southern hemisphere (Gérard et al., 2015; Soret et al., 2016). We found that auroral emissions are located near the statistical boundary between open and closed field lines measured by magnetometers at 400 km. From a total of 113 nightside orbits with SPICAM nadir pointing in the region of residual magnetic field, only 9 show confirmed auroral signatures. The mean energy of the electron energy spectra measured during concurrent ASPERA-3/ELS observations ranges from 150 to 280 eV. The peak altitude of the CO Cameron bands has been estimated to be 137±27 km. These observations have been reproduced by a Monte-Carlo model of electron transport in the Martian thermosphere for mono-energetic electrons between 60 and 200 eV. We have modelled these auroral emissions using electron energy spectra simultaneously measured with ASPERA-3/ELS. The simulated altitudes are in very good agreement with the observations. UV auroral emissions detected with SPICAM in Mars' southern hemisphere are consistent with the scenario of acceleration of electrons by transient parallel electric field along semi open magnetic field lines, but the exact mechanism remains to be explored.

Modelling of these emissions requires an accurate knowledge of the various cross sections involved in the photon and electron (auroral or photoelectrons) collisions with the atmospheric constituents. Some of these cross sections however are still poorly known. A series of new laboratory measurements of the cross sections for electron impact on CO_2 and CO has been initiated at the University of Colorado with our implication. A first article (Ajello et al., 2019) was recently published. We have measured the 30 and 100 eV far ultraviolet (FUV) emission cross sections of allowed Fourth Positive Group (4PG) band system (A¹ $\Pi \rightarrow$

 $X^{1}\Sigma^{+}$) of CO and the optically forbidden O (${}^{5}S \rightarrow {}^{3}P$) 135.6 nm atomic transition by electron impact on CO and CO₂. We derived a model FUV spectrum of the 4PG band system from dissociative excitation of CO₂, an important process observed on Mars and Venus. The determination of the total OI (${}^{5}S$) emission cross section at 135.6 nm is accomplished by measuring the cylindrical glow pattern of the metastable emission from electron impact by imaging the glow intensity about the electron beam from nominally zero to ~400 mm distance from the electron beam.

Diffuse aurora

Unexpected aurora observations were made with the IUVS instrument on board MAVEN. Starting in December 2014, many efforts were made to confirm and explain the detection of auroral UV features in the Northern hemisphere, far from the Martian remnant crustal magnetic field. These diffuse auroras were observed low in the atmosphere, suggesting that high energetic electrons are the cause of the excitation of Mars' atmosphere. This discovery was published in an article in Science (Schneider et al., 2015). The diffuse aurora reveals a new type of direct solar wind-atmosphere interaction during energetic solar events. The Monte Carlo model electron transport model has been adapted to the high electron energies of the diffuse aurora (Fig. 6).



Figure 6: Limb integrated production rate of the CO_2^+ UVD (a) and CO Cameron band (b) emissions for different electron energies. Quenching of the CO a state is not considered in panel (b). The electron energy flux at the top of the model is 1 mW m⁻² for all simulations (from Gérard et al., 2017b).

The energy dependence of several emissions has been modelled and the role of collisional deactivation of the Cameron bands has been assessed (Gérard et al., 2016). These model calculations have been compared with in situ measurements of auroral particle precipitation by the plasma instrument package on board MAVEN. We have calculated the nadir and limb production rates of several UV emissions for a unit precipitated energy flux.

Proton aurora

Important work on the Martian proton aurora and its characteristics has been achieved. The most innovative aspect was the study of this new (third) type of Martian aurora resulting from the interaction between the solar wind protons, the hydrogen corona and the Martian upper atmosphere. A thorough analysis of the Mars Express hydrogen Lyman- α emission profile observed with the SPICAM instrument at the dayside limb led to the conclusion that it is occasionally enhanced between 120 and 150 km over the dayglow background (Fig. 7).

The auroral peak brightness ranges from the instrumental detection threshold up to about 3 kiloRayleighs, superimposed on the background Lyman- α dayglow emission excited by resonance scattering of solar radiation by the hydrogen corona. The observations have been described in a paper by B. Ritter et al. (2018), the postdoctoral researcher funded by the SCOOP contract. The proton aurorae are caused by charge transfer collisions between the incoming energetic solar wind protons and neutral constituents. The brightness enhancements were observed concurrently with perturbed solar wind conditions such as coronal mass ejections during active periods.



Figure 7: Limb profile of the Lyman- α dayside emission during proton auroral precipitation plotted versus the tangent point altitude for an aurora (blue) and a non-auroral case (black). The difference is shown in magenta (from Ritter et al., 2018)

Interaction of charged particle beam with the Martian atmosphere

New developments also included a study of the role of a crustal magnetic field on the electron precipitation and its effect on the backscattered component and the precipitated energy flux (Bisikalo et al., 2017). In collaboration with our partners from the Astronomical Institute of the Russian academy of Sciences (INASAN), the role of the aurora as a heat source for the upper atmosphere by the auroral precipitation has also been numerically simulated (Shematovich et al., 2017). These model studies are based on an extensive use of the Monte Carlo model developed by the Russian partners of this contract and adapted to auroral precipitation in the Martian atmosphere, dominated by CO₂ and atomic oxygen. Observations have shown the occasional presence of localized ultraviolet nightside emissions associated with enhanced energetic electron fluxes. These features generally occur in regions with significant radial crustal magnetic field. We have used the Monte-Carlo electron transport model to investigate the role of the magnetic field on the downward and upward electron fluxes, the brightness and the emitted power of auroral emissions. Simulations based on an ASPERA-3 measured auroral electron precipitation indicate that magnetic mirroring leads to an intensification of the energy flux carried by upward moving electrons - from about 20% in the absence of crustal magnetic field up to 33-78% when a magnetic field is included, depending on magnetic field topology (Fig. 8).



Figure 8: Upward (black line) and downward H^+ (red line) fluxes at 160 km for the case of proton precipitation without (a) and with induced magnetic field B=15 (b), 20 (c) and 30 (d) nT. The orange

line shows the energy spectrum of the precipitating magnetosheath proton flux (from Bisikalo et al., 2018)

Conservation of the particle flux in a flux tube implies that the presence of the B-field does not appreciably modify the emission rate profiles for an initially isotropic pitch angle distribution. However, we find that crustal magnetic field results in increase of the upward electron flux, and, consequently, in reduction of the total auroral brightness for given energy flux of precipitating electrons. We also investigated the role of the induced magnetic field on proton precipitation based on MAVEN measurements of in situ upward and downward proton energy spectra (Bisikalo et al., 2018). We demonstrated that the presence of the magnetic field significantly modifies the intensity of the backscattered proton flux relative to the precipitated component. Simulations with incident ENA H atoms yield a guite similar peak altitude but a broader line profile. We have shown that the presence of an induced magnetic field somewhat increases the line width and significantly decreases the brightness of the Lyman- α emission. The simulated limb peak altitude and intensity are compatible with those observed with SPICAM on board Mars Express (Fig. 9). This intensity increase is a signature of Doppler-broadened optically thin emission caused by the beam of fast H atoms resulting from the proton collisions with the atmosphere. Simulations with the Monte Carlo collisional model adapted to the Martian atmosphere have been performed as a support study to these new findings (Gérard et al., 2018). We have performed numerical simulations of the Lyman- α production rate and line profiles at different altitudes, partly based on in situ measurements of the energy spectrum of energetic protons in the magnetosheath region by the SWIA instrument on board the MAVEN satellite. The calculated Lyman- α line profile is significantly broader than the core of the planetary thermal H atom. Therefore, as much as 98% of the auroral emission is produced outside the optically thick hydrogen core and creates the intensity enhancement observed from MAVEN. The simulated intensity and altitude of the Lyman- α emission are consistent with the observed characteristics of the proton aurora.



Figure 9: Calculated distribution of auroral Lyman- α limb intensity for proton precipitation in the absence of an induced magnetic field. Dotted curves: without CO₂ absorption, dashed curve: including

the effect of CO_2 absorption along the line of sight for an observer at an altitude of 350 km. The model prediction is in good agreement with the characteristics of the observed Lyman- α auroral enhancements (from Gérard et al., 2018).

We also investigated the dependence on the intensity of an induced horizontal magnetic field. We have found that the presence of the induced B-field strongly controls the penetration of the H/H+ beam and the production of auroral Ly- α radiation (Fig. 8).

4.2.2 Remote sensing of upper atmospheric composition from non-thermal emissions

Composition and seasonal variations

The detailed study of the dayglow emissions observed with IUVS at the limb has provided new information on the global distribution of CO_2 and O, the two major constituents of the Martian thermosphere. Tools for these studies have been developed and a first set of results on the variability of CO_2 in the lower thermosphere and mesosphere have been obtained. The adopted methodology combining airglow observations and modelling is outlined in Fig. 10. The full set of IUVS ultraviolet limb scans collected by MAVEN near periapsis has been downloaded from the NASA/PDS archives. Limb profiles of seven different emission features from CO, CO_2^+ , and OI, and five of them have been completed so far. In a first step, we concentrate on the oxygen multiplets at 130.4, 135.6 and 297.2 nm, the CO Cameron bands and the CO_2^+ UV doublet (UVD). Limb scans of dayglow emissions complement each other and comparison to GCM simulations have also been made to investigate the oxygen redistribution by large-scale transport. A quantitative study of the dayglow emission observed during limb scans with the MAVEN IUVS spectral imager started in 2017.



Figure 10: Block diagram of workflow for dayglow studies and the interactions between IUVS observations and models.

The 130.4 nm oxygen emission that is mainly produced by resonance scattering and photoelectron impact on O atoms. The 135.6 nm OI emission results from electron impact on O and is therefore a direct proxy of the O density distribution. Both emissions peak near 130 km. The 297.2 nm multiplet shows two emission peaks. The lower one (near 85 km) is solely excited by photodissociation of CO_2 by solar Lyman- α and is therefore directly proportional to the total CO_2 density. Its study has provided a new method to determine the CO_2 density in the lower thermosphere, a region currently not accessible to *in situ* measurements. The CO_2^+ UV doublet and the CO Cameron bands are essentially produced by dissociation of CO_2 by photons and photoelectrons. Consequently, their peak altitudes (120-130 km) are also excellent proxies of the column density (pressure level) overlying the emission peak.

So far, we have analysed two Martian years of dayglow measurements of the CO Cameron bands and the CO2⁺ UVD at 298-299 nm with the IUVS instrument on board the MAVEN orbiter. We show that the altitude and the brightness of the two emissions peaks are strongly correlated, although data were collected over a wide range of latitudes and seasons. We obtained averaged limb profiles and compared them with numerical simulations based on updated calculations of the production of the CO and the CO2⁺ emissions. All model simulations use the solar flux directly measured on board MAVEN with the Extreme Ultraviolet Monitor (EUVM) and the neutral densities provided by the Mars Climate Database (MCD) version 5.3, adapted to the conditions of the observations. We have shown that the altitude and the shape of the sample limb profiles are generally well reproduced using the MCD neutral atmosphere. The simulated peak intensities of the CO_2^+ UVD and Cameron bands are in good agreement considering the uncertainties on the excitation cross sections and the calibration of the IUVS and EUVM instruments. Seasonal-latitudinal maps of the Cameron and UVD peak altitude observed during two Martian years show variations as large as 23 km. Model simulations of the amplitude of these changes are in fair agreement with the observations except during the southern summer dust period (Ls = $270^{\circ}-320^{\circ}$) when the calculated rise of the dayglow layer was underestimated.

The O(¹S) metastable atoms radiatively relax by emitting photons at 557.7 nm and 297.2 nm. Limb profiles of the 297.2-nm dayglow have been collected near MAVEN periapsis with a spatial resolution of 5 km or less. The production of both 297.2 nm layers is dominated by photodissociation of CO_2 . Their altitude and brightness is variable with season and latitude, reflecting changes in the total amount of CO_2 present in the lower thermosphere. The lower emission peak near 85 km is solely produced by photodissociation, so that its peak altitude is an indicator of the changing altitude of the unit optical depth pressure level and the overlying CO_2 column density (Gkouvelis et al., 2018). Its intensity is directly controlled by the Lyman- α solar flux reaching the Martian upper atmosphere. To calculate the expected limb intensity, we combine photodissociation sources with chemical processes and photoelectron impact excitation. To determine the relative importance of the excitation processes, we apply the model to the atmosphere. We find very good agreement with the lower peak structure and intensity if the CO_2 density provided by the Mars Climate Database is scaled down by a factor between 0.50 and 0.66. We also determine that the previously uncertain quantum yield for

production of O(1S) atoms by photodissociation of CO₂ at Lyman- α wavelength is about 10%. In a second study, we used the specificities of the O(¹S) source to investigate.

A summary plot of the seasonal variation of the altitude (and pressure level) of the CO_2^+ UVD and O(¹S) emissions is shown in Fig. 11. It shows that emissions at both levels exhibit similar seasonal variations. In particular, the combined effects of the higher surface pressure during the summer season in the southern hemisphere, combined with the increased atmospheric dust load during dust storms, moves up the pressure levels and the peak altitude of the airglow. The CO_2 density provided by the Mars Climate Database (MCD) requires some adjustment by as much as a factor of two as shown in the top panel (percentage change required for best altitude fit). These data will be useful to correct models of the Martian upper atmospheric density.



Figure 11: Seasonal variation of the observed (large dots) and modelled (red small dots) altitude of the CO_2^+ UVD and OI 297.2 nm dayglow emissions observed during two Martian years. The altitude changes correspond to variation in the CO_2 column density overlying the emission peaks. The small red dots indicate the modelled altitudes. The upper plot shows the CO_2 scaling factor needed to match the observed peak altitude of the $O(^1S)$ (black) and CO_2^+ UVD (red) emission peaks. We note the general increase of the altitude after Ls=180°, during the dust season.

A third study concentrated on an overview of two Martian years of oxygen dayglow limb observations of the UV emissions at 130.4 nm and 135.6 nm. We showed that the observed 130.4 nm airglow brightness is dominated by resonance scattering of the solar multiplet with a smaller contribution (15-20%) by electron impact on oxygen. Over 95% of the 135.6 nm

line excitation arises from electron impact on oxygen. We have used in situ solar flux measurements of the EUV solar flux monitor on board MAVEN to remove the solar-induced variations. We have analysed the variations of the maximum limb intensity and altitude with season, solar zenith angle and latitude. The 130.4 nm and 135.6 nm peak brightness and altitudes are strongly correlated and behave similarly. Both emissions have been modelled for selected data using Monte Carlo codes to calculate emissions arising from electron impact on oxygen and CO₂ and to test the sensitivity to the atmospheric content in CO₂ and O. Additional radiative transfer calculations have been made to model the optically thick 130.4 nm multiplet. Model densities and temperature from the Mars Climate Database served as inputs. Both simulated limb profiles have been found in good agreement with the observations despite some deviations (Fig. 12). Simulations indicate that the observed limb brightness is dependent on the oxygen and CO₂ contents, while the peak emission altitude is mainly driven by the CO₂ content due to absorption processes. We deduce [O]/[CO₂] mixing ratios between 1.8% and 2.9% at 130 km for datasets collected at L_S = 350° in Martian years 32 and 33.



Figure 12: Model-data comparison for the datasets from MY 32 (a) and MY 33 (b). The mean profiles are plotted as points with horizontal variability bars reflecting the brightness variation within each dataset. The solid lines represent the total modelled brightness, the dashed lines the major and the dashed-dotted lines the minor contributor to the modelled brightness.

Remote sensing of hemispheric transport and global wind characteristics in the upper atmosphere

The analysis of the NO nightglow emission collected at the limb with SPICAM on board Mars Express has been finalized (Stiepen et al., 2015). This study had shown that the NO emission strongly varies in morphology and intensity with the Martian season. Comparison with 3-D models showed a good agreement with the predictions, although the observed distribution appeared less systematic and more complex than the numerical simulations. An extensive study of the NO nightglow distribution at the limb has been performed used UUVS limb observation on the nightside. Large seasonal and latitudinal intensity gradients have

been discovered based on analysis of three seasons of observations. By mapping the NO emission, insight was gained on the seasonal atmospheric transport and the impact of the circulation on the distribution and chemistry in the upper atmosphere. Signatures of standing waves were discovered in the longitudinal structure of the airglow brightness. These results were compared with the 3-D model calculations from the LMD model including partial photochemistry. Similarities and differences have been identified. A paper reporting IUVS characterization of the NO nightglow distribution and 3-D LMD model predictions has been published by Stiepen et al. (2017). In particular, they showed the impact of tides in this region, as well as large discrepancies in model-to-data comparisons regarding the day-to-night hemispheric transport in the mesosphere.

Additionally a new study, still in progress, was initiated in 2016 to analyse global disk images collected during the apoapsis phase of the MAVEN orbit (Fig. 13). They gave unprecedented snapshot views of the nightglow emission and provided unexpected results. This analysis has provided the first global mapping of the NO nightglow at Mars. These disk images collected by IUVS/MAVEN showing the fine structure of the NO nightglow have been studied in detail. For example, the presence of waves and tides appear to partly control the seasonal and longitudinal transport of N and O atoms. In particular, the wave structures observed at different local times and planetary longitudes have been characterized by combining a large number of apoapsis images to determine the physical nature and sources of the waves. A manuscript reporting these findings is in preparation.



Figure 13: spherical projection of the NO nightglow brightness observed during MAVEN orbit 3102. We observe the expected enhancement in the brightness near the southern winter pole, but on this occasion, we also observe equatorial enhancements of similar magnitude near longitudes 120°E and 150°E.

4.2.3 Development of tools for NOMAD data analysis

Modelling the terminator

In order to handle concentration gradients along the line of sight when retrieving density profiles of atmospheric components from solar occultation measurements, we aim at suppressing the limiting assumption of spherically symmetric atmosphere while 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.

The GEM-Mars general circulation model (GCM) was used to provide several 3D gridded fields as a priori for the retrieval codes. To provide input profiles, the model was run at a horizontal resolution of 4x4° (approximately 237 km longitudinal spacing at the equator) and 103 unevenly spaced vertical levels from the surface up to about 150 km. The spacing of levels near the surface is of the order of meters, increasing to about 1 km in the 10-50 km altitude range. A simulation was performed for a generic Mars year with average dust loading (not year specific) resulting from the dust-lifting scheme in the model with orbital parameters set to MY 28. The dynamical and chemical integration timestep was 1/48th of a Mars sol (30 minutes). For the gradients, profiles of temperature and ozone were provided at each model timestep for the period 2 hours before until 2 hours after sunrise/sunset for each grid point the occultation traversed.

Figure 14: Examples of retrieved ozone slant densities derived using GEM-Mars gradients (red lines) compared to profiles derived at LATMOS (orange lines). ASIMUT profiles retrieved assuming a spherically symmetrical atmosphere (black lines) are also shown (Piccialli et al., submitted).

An example of the results of this analysis (Piccialli et al., submitted) is displayed in Figure 14 showing the impact that the use of a gradient has on retrieved O_3 profiles (red lines) compared to retrievals assuming a spherically symmetrical atmosphere (black lines). The impacts of gradients on O_3 retrievals is strongly related to the model results (data not shown). Sunset O_3 retrievals are about < 20% smaller than retrievals obtained assuming a spherically symmetrical atmosphere. At sunrise, the impact of gradients on the retrievals is negligible. In the subset of SPICAM-UV spectra used for this analysis, all selected sunset occultations are



located near the equator while sunrise occultations are situated at high latitudes south. Therefore, we plan to extend the analysis to the whole SPICAM database and to NOMAD/ExoMars observations.

Development of tools for the analysis of NOMAD LNO data and the mapping of trace gases

The remote sensing of a target gas from space can be performed in different spectral domains and under different geometries such as nadir or limb observation viewing. Because each of these spectral regions and geometries has its advantages and disadvantages, the possibilities to combine several types of measurements in a synergistic way have been studied in view of improving the investigation of the Martian atmosphere and increasing the science return of the ExoMars TGO mission.

For this purpose, the radiative transfer model ASIMUT was modified, sometimes in-depth, as to be able to run on different spectra measured by different instruments, it has also been improved for retrieval in the IR in the nadir geometry. Scripts were developed in Python to perform the runs on the High Performance Computing System of the Belgian Space Pole in order to decrease the computation time.

These IT solutions were thoroughly tested during the theoretical study related to ExoMars TGO (Robert et al., 2017) based on synthetic spectra of a Fourier transform spectrometer working in the middle to far infrared and of a grating spectrometer working in the middle infrared. The theoretical study was a necessary step, as it enabled us to control the runs and focus on the synergy itself. This work has been undertaken with a particular focus on the ExoMars TGO 2016 mission, accommodating two IR instruments that might operate in a complementary way. A database of synthetic spectra was created taking into account the expected characteristics of two representative instruments, based on the known specifications of the TGO instruments available at the time of this study.

The systematic retrievals that have been performed show a positive impact of synergies in the quantification of CO, as can be seen in Figure 15. Both vibrational bands, i.e. the 1-0 around 4.7 μ m and the 2-0 around 2.3 μ m can be targeted respectively by the ACS and NOMAD instruments, provide interesting synergistic possibilities. The results presented are a good indication that our retrieval tools are mature enough and ready for an optimal scientific use on the spectra recently acquired with NOMAD and ACS. In particular, the synergy L1/L1benefits from both spectra and from the information contained in both bands of CO measured by the instruments. This is confirmed by the retrieved VMR values and their a posteriori uncertainties. The L1/L1 synergy profile is very close to the true solution and presents the smallest error bars at each season.



Figure 15: Statistical distribution of the 50 retrievals (in the column mode) of CO in the four cases (non-synergy (NOMAD ; ACS) ; L1/L1 synergy and L2/L1 synergy) in the nadir mode with low VMR (321 ppmv) on the left and a high VMR (1362 ppmv) on the right. The four different L_s periods are indicated in different colors. The first guess value was 841.5 ppmv in all cases and is not shown on the plots. All results within 2 ppmv are binned together. The black vertical line on each plot represents the GEM value expected to be retrieved. The colored vertical line indicates the mean abundance at each season with their respective error bar.

Nevertheless the results presented by Robert et al. (2017) must be considered with caution, as our study did not embrace all aspects of the Martian environment. Emissivity was considered as constant while it may vary spectrally and aerosols were not considered even though we know their importance in the Martian atmosphere. The retrievals themselves were also simplified as the vertical temperature profile was assumed to be known. Usually the atmospheric temperatures are derived from the CO_2 density and therefore have an

associated uncertainty. The assumption used in this study is excluding this additional uncertainty.

The next step was to use these tools on actual experimental data from instruments on-board Mars Express and as anticipated, the results from this test case are harder to interpret for several reasons: (1) in order to quantify the science return of the spectral synergy, co-located measurements of both instruments are necessary, (2) observations for which surface, clouds and aerosols loadings are known would facilitate the task, (3) the thermal part of the spectra, i.e. the 1-0 band complicated the retrieval of the CO VMR, as the impacts of emissivity and surface temperature are important, and (4) the 2-0 band is shallow, as it is spectroscopically expected. However, the test case enabled us to go further in the development of our tools and understanding of nadir measurements of the Martian atmosphere. This work paved the way to more collaborative studies and revealed itself enriching and future research ideas emerged along the task.

Search for nightglow or auroral detection with the of NOMAD- UVIS channel

A thorough study of possible opportunities to use the instruments on board the EXOMARS TGO orbiter to study the Martian upper atmosphere, including non-standard observing modes, has been performed and published in Space Science Reviews (López-Valverde et al., 2018).

A study was conducted to examine whether the NOMAD or the ACS sensors on board TGO will be able to provide information on the distribution of the CO₂ and CO₂⁺ dayglow emissions. The detectability of other dayside and nightside emissions has also been investigated, such as the CO₂⁺ FDB bands, the OI 297.2 nm and the green line forbidden emissions on the dayside. The NO δ and γ UV nightglow, the discrete and diffuse nightside aurora. In the infrared, the NO band at 1.22 μ m and the OH (Δ v= 1) sequence are potential candidates for detection. The conclusion was the need to perform limb scan observations with the NOMAD nadir channels during the course of the TGO mission.

Numerical inversion of limb observations

The development of an inverse Abel transform method for the analysis of occultation observations of the dusty atmosphere of Mars has been undertaken. Accounting for the extinction of several constituents leads to the resolution of severely ill-conditioned linear systems. The resolution of ill-conditioned linear systems generally requires special techniques of linear algebra such as the Tikhonov regularization, a method often used in the study of inverse problems. It was found that using a simple representation of the vertical profile of the properties of the dusts (the so-called α -parameter modelling of dust extinction) could lead to erroneous retrieval when the dust properties vary rapidly with height. We explored the possibility of accounting for a variation of the dust properties inside of the bins of the retrieval grid. We found one method to include that variation that still produces triangular elements (to be linearly combined to produce a piecewise representation of the profile) that still admit an analytical forward Abel transform, which is necessary to produce an efficient inversion method. The analytical result does, however use hypergeometric 2F1 functions, which are difficult to compute. We conceived an efficient and simple computation method of the needed 2F1 functions that can be used over the range of physical parameters

that we anticipate for the inversion of realistic profiles. Final software implementation is still under way.

In parallel, we explored the possibility of explicitly accounting for the exponential dependence of the density profile of any atmospheric constituent. We found this could be done analytically using a series development of the Jacobian of the Abel transform about its limit at infinity. We showed that this result can be used for both planetary and cometary atmosphere and produced a convincing demonstration of the use of these results in the case of the $O(^{1}S) \rightarrow O(^{3}P)$ emission at 297.2 nm in the Mars atmosphere. The reach of this new idea is however less promising than it may have seemed at first sight, especially in the case of a cometary atmosphere, because the exponential dependency produces large values of the second derivative of the fitted profiles, that complicate the use of a Tikhonov regularization, especially when the profile to be retrieved varies over many orders of magnitude. These last results were presented at the AGU fall meeting held in last December in Washington.

4.2.4 Clathrate modelling

Clathrate stability zone

At present-day, as stability conditions of methane clathrates are met in the near subsurface of Mars, the spatial variation of the top of their stability zone is strongly dependent of mean annual surface temperature. Consequently, CH₄-rich clathrate hydrates are stable closer to the surface at high latitude (few meters deep) and deeper in equatorial areas (few tens of meters deep) due to the larger surface temperature in these regions.



Figure 16: Depth (m) of the top of clathrate stability zone in present-day Martian subsurface for CH_4 -rich clathrates formed from a gas phase with 90% of methane. The first layer of the thermal model has properties that fit with the thermal inertia derived from MGS TES observations (Putzig and Mellon, 2007), while the second layer has properties representative of dry basalt or ice-cemented soil depending on the latitude. Local detections of methane are reported in black: Gale crater (Webster et

al., 2015, 2018) is represented as a black star, while Syrtis Major, Terra Sabae and Nili Fossae (Mumma et al., 2009) are included in the black rectangle.

By taking into account the thermal inertia observed by Mars Global Surveyor (Putzig and Mellon, 2007) to set the thermal properties of the upper layer in our subsurface model and then increasing the thermal conductivity of the second layer to correspond to dry basalt, we found that the stability zone of CH_4 -rich clathrates is the deepest in regions where methane has been locally reported, especially in the area observed by Mumma et al. (2009) where it is located from ~68 m deep (Fig. 16). At this depth, clathrates cannot be affected by seasonal changes in temperature. However, the addition of other gas species in clathrates can shift their stability zone closer or further away from the Martian surface depending on the guest composition. For example, the addition of CO_2 in CH_4 clathrate hydrates decreases the dissociation pressure in the same temperature conditions, allowing them to be stable at shallower depths.

Clathrate composition

We investigated the guest abundance in clathrates as a function of the pressure at which they form Fig. 17 presents the CH_4 and CO_2 mole fractions in binary sI clathrate for a pressure range varying from their dissociation pressure P_{diss} to 10 MPa. Calculations were made at 270 K for an initial gas phase including 50% CH_4 and 50% CO_2 . The intriguing result is that with growth of pressure, the carbon dioxide fraction in clathrate decreases, while the methane content increases consequently. Considering this, binary CH_4 - CO_2 clathrates that would form at depth in the Martian crust would contain a larger fraction of methane than shallow clathrates formed from a similar gas phase.



Figure 17: Mole fraction of CO_2 and CH_4 in binary sI clathrates at T = 270 K as a function of pressure. The gas phase consists of 50% CO_2 and 50% CH_4 . The guest-clathrate interaction model is based on the Kihara potential.

Diffusive transport of methane and water vapour

We simulated methane and water vapour transport through the Martian regolith via a diffusive-adsorptive model. By taking into account only molecular and Knudsen diffusion in our gas transport model, methane that would be emitted from depths showed in Fig. 16 would give a surface flux duration consistent with observations (Mumma et al., 2009). Using this surface flux pattern as an input in a general circulation model (GCM) allows us to obtain a better match with observations for the latitudinal distribution of methane than the one simulated with an instantaneous surface release (Temel et al., 2019). We use different local source regions near the equator and we determine four surface release scenarios occurring over a period of 15 to 60 sols around solar longitude $L_s = 155^\circ$. Among the different tested scenarios, the best agreement is found for a surface emission of 45 sols during which a total amount of about 90,000 metric tons of methane are released over an area of 22,000 km² centred on (0°N, 50°E). Longer surface emissions would also be consistent but would require to increase the total amount of emitted methane in order to reproduce the equatorial CH_4 peak of 50 ppbv (Mumma et al., 2009). In our subsurface model, a 45-sol emission duration corresponds to a source depth of ~ 27 m, which places it outside the stability field of CH₄-rich clathrates showed in Fig. 10, but remains consistent with CO₂-rich clathrates (including small CH₄ fraction) stability zone.

Including adsorption in the model considerably slows down the transport process and increases the surface release duration making the simulations unable to produce short-lived methane plumes, even from shallow depth. As a result, diffusive transport is likely not the dominant process that generated the CH_4 plumes observed by Mumma et al. (2009) and advection will thus be considered in future studies. Taking into account this last process should allow the methane source corresponding to the best GCM scenario, defined above, to be deeper than the 27 m estimated with the diffusive model. Moreover, we showed that with the growth of the pressure formation, and thus the increase of the depth formation, methane content in binary CO_2 - CH_4 clathrate increases. Therefore, CH_4 -rich clathrates that would presently form from a source in the Martian crust would be more likely to occur at a large depth. Short surface releases implying methane liberated from those deep clathrates cannot be explained by our diffusive transport of methane, even if adsorption is neglected, which is consistent with results obtained by Stevens et al. (2017).

Our diffusive gas transport model has been also used to estimate an upper limit to the CH₄ steady-state release rate employed in the Mars Regional Atmospheric Modelling System (MRAMS) to simulate the transport and mixing of methane in Gale crater and to test whether the results are consistent with in situ observations made by the Mars Curiosity rover (Pla-García et al., submitted). For these simulations, sources located at 45 m deep (black star on Fig. 10) and release regions outside and inside Gale crater have been considered. In the steady state release experiment inside Gale crater, the methane values at the source location fluctuate from 0.1 to ~1 ppbv. This is comparable with the TLS-SAM low background methane abundances but still ~1 order of magnitude lower than the methane spikes (~7 ppb). For the steady-state methane release scenarios outside of Gale crater, modelled abundances at MSL are ~100 times lower compared to TLS-SAM spikes during all seasons. Thus, to match the observations, the steady state fluxes would need to be increased by two

orders of magnitude. However, the surface flux has been determined with "ideal" parameters and already presents an upper value for diffusive methane surface flux from shallow sources. So, although diffusive transport is consistent with low background levels of methane at Gale crater, clathrate dissociation and subsequent methane diffusion through the regolith cannot be responsible for CH_4 spikes observed by MSL (Webster et al., 2015, 2018).

Finally, in the simulations related to water vapour, near-surface ice is not stable at MSL landing site and at 30° N. However, the water vapour exchange between the subsurface and the atmosphere at these locations is plausible up to 12×10^{-3} kg m⁻² day⁻¹. The results showed also that the water vapour flux at the surface varies with amplitude around 10 times larger when adsorption is taken into account. At Phoenix landing site, a permanent ice table close to the surface can be observed but its location depends on the initial ice content of the subsurface. When pore spaces are filled with ice at depth where it is stable, the ice table depth become shallower. To match the observed water ice depth of ~5 cm (Smith et al., 2009), simulations showed that pores must be filled with 70% volume fraction of ice.

4.3 Conclusions and Recommendations

The network brought together partners with expertise in modelling the subsurface atmosphere interactions, in spectroscopic remote sensing of the composition and structure of planetary atmospheres, in the development of radiative transfer codes, in the dynamics of the upper atmospheres through the investigation of airglow and in developing theories and models to explain atmospheric data and to decipher atmospheric processes.

An important synthesis of current knowledge on the Venus thermal structure and dynamics has been made; it consists in tabular compilations of the vertical and latitudinal structure of the temperature in the Venus atmosphere as a function of altitude from the available observations and guidance from the atmospheric models. Temperature and density measurements from different VEX instruments have been collected, critically reviewed and compared, with the purpose to build a reference atmosphere encompassing most of the Venus atmosphere.

Three comprehensive reviews of: (1) the clouds and hazes on Venus, (2) the aeronomy of the Venus upper atmosphere and (3) the composition and chemistry of the neutral atmosphere of Venus were published following remarkable progress made in the field after the VEX mission.

The project therefore contributed to a better valorisation of the Venus Express data. While the mission finished in December 2014, the exploitation of the measurements obtained during 8.5 years by the various instruments was far from complete. Five years after the end of the mission and inter-comparisons between the instruments, as well as modelling exercises were necessary to apprehend how much the mission contributed to a better understanding of the Venus atmosphere but also to define the challenges for future missions to Venus.

The NOMAD team was extremely busy to development all the necessary tools for the analysis of the NOMAD data that started to accumulate in April 2018 at an incredible rate compared to what the team was used to with the SOIR data. The whole retrieval procedure

was improved in term of the liability of the derived physical parameters, was adapted to the Martian atmosphere and to several observation geometries, but also importantly was upgraded towards an automated pipeline and to allow a significant decrease of the computation time. Moreover, the possibilities to combine several types of measurements in a synergistic way were studied in view of improving the investigation of the Martian atmosphere and increasing the science return of the ExoMars TGO mission.

SCOOP has been invaluable in the preparation for ESA's ExoMars 2016 Trace Gas Orbiter (TGO) data analysis and exploitation by developing tools and testing them. Some results were also of interest in the definition of the observation strategy.

In addition, we demonstrated the importance of ultraviolet remote sensing to determine the density of CO_2 and O, the two major players in the upper Martian atmosphere. In particular we showed the both constituents exhibit strong seasonal variation between 70 and 140 km. These changes result from the combined effect of the planet's distance to the sun and the atmospheric dust load. Further studies are now needed to discriminate between the two effects by analysing the time response of the atmosphere to the onset of the dust storms. Similarly, the precipitation of energetic electrons and protons is likely an additional heat source that should be quantified in the future by correlating temperature measurements with global observations of the Martian ultraviolet aurora.

Global imaging observations of the NO nightglow has provided a crucial step forward in the understanding of the upper atmosphere circulation and its seasonal changes. They have also demonstrated the presence of a wide variety of tides and waves affecting the atmospheric structure. The exact nature and sources of these perturbations, their local time, seasonal and longitudinal should be further investigated.

In order to give a better accurate estimation of the methane clathrate occurrences on Mars, a physical model such as the one developed during the SCOOP project needs to be coupled with topography/geological analysis to determine possible regions within the clathrate stability zone where sufficient CH_4 supplies could exist.

Although Trace Gas Orbiter is currently not detecting any Martian methane (Korablev et al., 2019), this does not prevent potential future observations, especially if the methane is outgassed only episodically. From the point of view of diffusion, a higher surface flux of methane should be observed in warmer regions and periods. Also, gas accumulation being a process spread over time, Martian regions that already have been recognized as CH_4 emission areas in the past would be expected to repeat that episodic releases through time (Etiope and Oehler, 2019). The region observed by Mumma et al. (2009) or Gale crater seem therefore to be good locations for follow-up methane studies. In addition, it is important to note that methane outgassing scenarios are strongly dependent on the subsurface environment. The Mars InSight Lander should provide new data to constrain seismicity and tectonism on Mars and thus new clathrate destabilization scenarios linked to pressure changes.

We showed that clathrate dissociation and subsequent methane diffusion through the regolith cannot be responsible for CH_4 spikes observed by MSL (Webster et al., 2015, 2018) or short-live methane plumes (Mumma et al., 2009). Other potential subsurface methane sources that would imply gas diffusion through the regolith, and thus are subject to the same physics, are also unlikely. In order to explain these high and sporadic CH_4 levels, other gas transport processes such as advection should be investigated.

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5. DISSEMINATION AND VALORISATION

Products

The results obtained during the course of the SCOOP project were reported at international conferences and in international peer-reviewed journals. The list of publications in which SCOOP is acknowledged, is provided below in Section 6.

The references in bold therein will be published as three chapters of the Venus III book (ed. Bézard, B., Russel, C., Satoh, T., Smrekar, E. and Wilson, C.).

The two references in italic in Section 6 are important contributions for the update of the Venus International Reference Atmosphere (VIRA) based among others on the wealth of new information on the Venus atmosphere, from the surface up to the highest layers of the atmosphere, obtained with the Venus Express mission.

All density, volume mixing ratio, extinction and temperature profiles from SOIR that have been validated and published elsewhere are now available on the open access Virtual European Solar and Planetary Access (VESPA) infrastructure (Trompet et al., 2017) under the label 'Venus atmospheric profiles From SPICAV-SOIR/VEx' (http://vespa.obspm.fr/planetary/ data/). VESPA (http://www.europlanet-vespa.eu/) aims at building a Virtual Observatory for Planetary Science, connecting all sorts of data in the field, and providing modern tools to retrieve, cross-correlate, and display data and results of scientific analyses (Erard et al., 2018). Figure 18 is an example of VESPA capability, it represents on each hemisphere the position in terms of latitude and longitude of all SOIR H₂O and HDO observations during the VEX mission and it also gives an overview of all colocated measurements of both trace gases.



Figure 18: Positions on the surface of Venus of all H_2O (red squares) and HDO (blue crosses) vertical profiles accessible in the SOIR database. Panel A is the northern hemisphere and panel B is the

southern hemisphere. Concentric circles represent the latitude and the position on the circles gives represents the longitude.

Workshop

The SCOOP partners organized an international workshop entitled 'Mars: From the Ground to the Upper Atmosphere'. It was held at IASB-BIRA on 21-23 June 2017 and welcomed 32 participants from five Belgian and six International organizations. The themes of the workshop have covered two different aspects of the study of the Mars atmosphere: (i) thermal structure and dynamics, (ii) surface-atmosphere interaction and atmospheric chemical composition. The participants also had a brainstorming discussion about possible outreach activities. The details of all contributions are given in Table I.

Wednesday 21 June 2017							
13:00 – 13:30 Welcome and coffee							
Session 1. Thermal structure and dynamics (TSD)							
Part 1. Chair: Jean-Claude Gérard							
13:30 - 13:50	Results from the MAVEN/IUVS Occultational Experiment	R. Yelle (LPL)					
13:50 - 14:10	Highlights of MAVEN/IUVS Results in Mars' Middle and Upper Atmosphere	N. Schneider (LASP)					
14:10 - 14:30	Seasonal Transport in Mars' Mesosphere revealed by Nitric Oxide nightglow	A. Stiepen (ULg)					
14:30 - 15:30	Discussion	all					
15:30 - 16:00	Coffee break						
Part 2. Chair: Roger Yelle							
16:00 - 16:20	Martian neutral density and temperature from MAVEN/IUVS observations and general circulation modeling	A. Medvedev (MPI-SSR)					
16:20 - 16:40	A 1D radiative transfer model at the terminator: Comparison with SOIR/VEx temperature profiles $% \mathcal{A} = \mathcal{A} = \mathcal{A} + \mathcal{A}$	A. Mahieux (IASB-BIRA)					
16:40 - 17:00	Role of small-scale gravity waves on the formation and variations of high- altitude carbon dioxide ice clouds in Martian atmosphere	E. Yiğit (GMU)					
17:00 - 18:00	Discussion	all					
	Thursday 22 June 2017						
9:00 - 9:20	Coffee						
Session I. Theri Part 3 Chair: Er	nal structure and dynamics (ISD) (continued)						
9:20 - 9:40	Modelling the effects of gravity wave in the GEM-Mars GCM	L. Neary (IASB-BIRA)					
9:40 - 10:00	Simulations of gravity waves, dust storms and water cycle on Mars using DRAMATIC MGCM	T. Kuroda (NICT)					
10:00 - 10:20	Global distribution of gravity wave activity in Mars' lower thermosphere derived from MAVEN/IUVS stellar occultations and analyzed using two Martian General Circulation Models	H. Nakagawa (TU)					
10:20 - 11:20	Discussion	all					
11:20 - 11:50	Coffee break						
Session 2. Surfa	ce-atmosphere interaction and atmospheric chemical composition (SAI / ACC)						
Part 1. Chair: Aı	ın Carine Vandaele						
11:50 - 12:10	Spectral properties of the Martian dust in the VNIR range	F. Altieri (INAF)					
12:10 - 12:30	Mars observations by SOFIA/ EXES	S. AOKI (IASB-BIKA)					
12:30 - 12:50	The NOWIAD Spectrometer Suite On The EXOMATS 2016 Orbiter	(PMI)					
12.30 - 14.00 14.00 - 14.20	Retrieval and characterization of carbon monovide (CO) vertical profiles in the	S Bauduin (LUB)					
14.00 14.20	Martian atmosphere from observations of PFS/MEX	o. Datatur (OLD)					
14:20 - 14:40	Synergistic atmospheric retrievals : Martian CO as a test-case	S. Robert (IASB-BIRA)					
14:40 - 15:40	Discussion	all					
15:40 - 16:10	Coffee break						
16:10 - 17:40	Session 3. Outreach	all					

Table I: Program of the SCOOP Workshop

Friday 23 June 2017							
9:00 - 9:20	00 – 9:20 Coffee						
Session 2. Surface-atmosphere interaction and atmospheric chemical composition (continued)							
Part 2. Chair: Hiromu Nakagawa							
9:20 - 9:40	GEM-Mars atmospheric chemistry simulations	F. Daerden (IASB-BIRA)					
9:40 - 10:00	Clathrate hydrates and possible methane outgassing scenarios on Mars	É. Gloesener (ROB)					
10:00 - 10:20	Formation of layers of methane in the atmosphere of Mars after surface release	S. Viscardy (IASB-BIRA)					
10:20 - 10:50	Coffee break						
10:50 - 11:10	Modelling of the atmospheric methane transport with a GCM coupled with a subsurface model	O. Temel (VKI)					
11:10 - 11:30	The Mars atomic oxygen dayglow: predictions based on the OI 297.2 nm MAVEN/IUVS observations	L. Gkouvelis (ULg)					
11:30 - 12:30	Discussion	all					
12:30 - 13:30	2:30 - 13:30 Sandwich lunch in the canteen of the Royal Meteorological Institute (RMI)						

Outreach activities

Information about our activities was given to the public during the Space Pole open doors (September 28-30, 2018) to which partners from ROB and BISA participated.

Large audience publications:

- Limaye, S., V. Wilquet, and A.C. Vandaele, Ce que Venus Express nous a appris et ce que nous ignorons toujours après la première mission de l'ESA vers notre plus proche voisine. Ciel et Terre, 131(1), 2-8 (2015).
- Wilquet, V. and M. Kruglanski, Le plongeon de la sonde Venus Express dans l'atmosphère de Vénus. Ciel et Terre, 131 (1), 9-14 (2015).
- Vandaele, A.C. Du méthane sur Mars? Ciel et Terre, 131(1), 15-21 (2015).
- Vandaele, A.C. Des champs de lave chauds observés sur Vénus. Ciel et Terre, 131(3), 82-84 (2015).
- Vandaele, A.C. Le site d'atterrissage de Schiaparelli. Ciel et Terre, 132 (4), 117 (2016).
- Vandaele, A.C. Exomars en route vers Mars. Ciel et Terre, 132 (2), 54-55 (2016).
- Vandaele, A.C. Exomars à peine arrivé observe déjà Mars avec succès. Ciel et Terre, 132 (6), 181-183 (2016).
- Stiepen, A. Avec NOMAD à bord d'ExoMars. <u>http://reflexions.ulg.ac.be/cms/c 429858/fr/avec-nomad-a-bord-dexomars?part=2</u> (2016)
- Ritter, B. and J.-C. Gérard. Des aurores à protons observées pour la première fois sur Mars! https://www.recherche.uliege.be/cms/c_9942571/fr/des-aurores-a-protons-observees-pour-la-premiere-fois-sur-mars (2018)
- Robert, S. Metingen van de atmosfeer van Mars bij beperkte zichtbaarheid, Heelal (2018)
- Robert, S., A. Piccialli, I.R. Thomas, Y. Willame Mesures de l'atmosphère martienne sous visibilité réduite, Science Connection 58, p28-31 (2018)
- Vandaele, A. C., A. Piccialli et S. Robert. Les atmosphères planétaires sous la loupe de la spectroscopie spatiale, Zenit (2018)

Press releases, TV and radio interviews, public events:

- (March-September 2016) Exhibition at the Euro Space Center in Redu, Belgium: 'Focus op/sur Mars', Official opening with the press, March 10. A. C. Vandaele presented the scientific goals of the ExoMars mission.
- DailyScience (4 January 2016) AC Vandaele by DailyScience on NOMAD and ExoMars : <u>http://dailyscience.be /2016/01/04/exobiologie-en-mars-leurope-met-le-cap-sur-mars/</u>
- A press release (5 November 2015) was issued by ESA on the study of the Martian aurora with Mars Express (<u>http://www.esa.int/Our Activities/Space Science/Mars Express/Shining a light on the aurora of Mars</u>). About 6700 readers connected to this web page.
- Invited talk for the 'Extension de l'ULB', Nivelles (Sept. 2015), Vandaele, A.C., Exomars: la future mission de l'ESA vers Mars.
- Space News (19 May 2015): "La Belgique à la recherche de traces de vie sur Mars", <u>http://www.space-news.be/2015/mai-jun/190515a.html</u>
- Le Soir (25 March 2015) V. Wilquet: NOMAD and ExoMars: "La Belgique va chercher des traces de vie sur Mars", Le Soir
- RTBF (24 March 2015) "NOMAD, futur instrument d'étude de l'atmosphère martienne, testé à Liège", <u>http://www.rtbf.be/info/regions/detail_nomad-futur-instrument-d-etude-de-l-atmosphere-martienne-teste-a-liege?id=8939736</u>
- BIRA-IASB Press Release on NOMAD (20 March 2015): <u>http://www.aeronomie.be/fr/nouvelles-presse/2015-03-24-mars-nomad.htm</u> <u>http://www.aeronomie.be/nl/nieuws-pers/2015-03-24-mars-nomad.htm</u>
- (March 2015) Two important press releases issued by NASA covered the discovery and analysis of Martian diffuse aurora by A. Stiepen and collaborators, as well as the impact of solar flares on Mars' atmosphere, and reported in international and Belgian press (e.g. <u>http://mars.nasa.gov/news/whatsnew/index.cfm?FuseAction=ShowNews& NewsID=1789</u> and <u>http://dailyscience.be/2015/11/06/de-surprenantes-aurores-martiennes-identifieespar-trois-chercheurs-liegeois/</u>)
- ExoMars 2016 Launch, Baikonour, Kazakistan 12-3-2016 O. Karatekin and A. C. Vandaele
- RTBF (March 14, 2016), le JT: "La mission ExoMars 2016 a quitté l'orbite de la Terre", Interview of Élodie Gloesener by Lucie Dendoven.
- RTBF La Première (March 14, 2016), "Mars, des jeunes et des robots", Interview of Élodie Gloesener by Françoise Baré.
- Expo "Focus op/sur Mars", at the Euro Space Center, Redu, Belgium, March-Sept. 2016
- National Geographic, 16/10/2016. Interview with Özgür Karatekin for the TV series Mars.
- 'Le satellite MAVEN révèle la complexité de l'atmosphère de Mars', 19 Octobre 2016, <u>https://www.ulg.ac.be/cms/c_8048815/fr/le-satellite-maven-revele-la-complexite-de-l-atmosphere-de-mars</u>
- <u>http://www.aeronomie.be/fr/nouvelles-presse/2016-10-10-exomars-arrivee.htm</u> including a press event on 19 and 20 October 2016 at ORB-KSB:
- RTBF La Première (October 20, 2016), Soir Première: "Schiaparelli sur Mars", Interview of Élodie Gloesener by Arnaud Ruyssen.
- RTBF (October 19, 2016), le JT: "ExoMars : A l'assaut de la planète Mars", Interview of Élodie Gloesener by Lucie Dendoven.
- BX1 (October 19, 2016), #M Le Mag de la rédac, Interview of Élodie Gloesener by Jean-Christophe Pesesse about ExoMars 2016.

- La Libre Belgique, 19/10/2016 Les cinq minutes à haut risque de l'atterrissage européen sur Mars, Interview of Özgür Karatekin.
- ExoMars 2016 TGO orbit insertion and Schiaparelli arrival at Mars, ESOC, Darmstadt, Germany, 19-20 October 2016, O. Karatekin.
- RTL TV (October 22, 2106), Info, "Le module Schiaparelli a raté son atterrissage et s'est écrasé sur Mars" Interview of Özgür Karatekin
- France 2 (TV) 22/11/2016, Telematin, Poursuit-on le programme spatial européen? Interview of Özgür Karatekin.
- RTBF La Première (February 28, 2017), Soir Première: Interview of Özgür Karatekin
- RTBF TV (28 February 2017), "Envoyer des touristes autour de la Lune, est-ce réellement envisageable? Interview of Özgür Karatekin.
- Jeunesse et Science (invited talk Grand Public), Modave, 25 March (2017). NOMAD, un instrument belge à la découverte de Mars. A.C. Vandaele
- Karatekin, Ö., Talk Cosmic to me #3. Cassini-Huygens: Drop the probes, Brussels, 25-10-2017.
- Interview about Mars aurora in general public magazine 'Ciel & Espace' (December 2017).
- BIRA-IASB Press Release : <u>http://www.aeronomie.be/fr/nouvelles-presse/2018-03-20-instrument-mars-pret.htm</u> (21 mars 2018)
- Interview of AC Vandaele at the radio "Les Eclaireurs" (12 Mai 2018): <u>https://www.rtbf.be/lapremiere/article/detail exomars-cloud-energetique-parcours-de-</u> reussite?id=9911720
- Exhibition 'Verwondering-Emerveillement-Verzauberung-Wonder' (07-09/2018) at 'Royal Palace': http://www.aeronomie.be/fr/nouvelles-presse/2018-07-20-emerveillement.html.
- Interview of A. Piccialli for MEDIA INAF during the European Planetary Science Conference (Berlin, 16-21 September 2018)
- A. C Vandaele gave a talk during the 13eme Nuit des Etoiles, Parentville (13-10-2018): NOMAD, un instrument belge à la conquête de Mars.
- In the frame of 'Space Talks',K. Lefever participated to an evening around Mars and NOMAD (13-11-2018): ExoMars BIRA op verkenning naar Mars
- A. Piccialli conceived and managed a Mars exhibit: Dag van de Wetenschap" at the Planetarium of Brussels (25 November 2018).
- L'Université de Liège associée aux premiers résultats de NOMAD (12 April 2019): <u>https://www.news.uliege.be/cms/c 10894634/fr/l-universite-de-liege-associee-aux-premiers-resultats-de-nomad</u>
- Public defence in LLN of the PhD of Élodie Gloesener entitled "Methane clathrate hydrate stability in the martian subsurface and outgassing scenarios" (3 September 2019)

Websites and Social Media:

We offered information about our activities, as well as a general overview of our field of research, for both large and more scientific oriented audiences. It can be found at (IASB-BIRA), http://planetary.aeronomie.be for the coordinating partner at http://www.lpap.ulg.ac.be and http://reflexions.ulg.ac.be for partner 2 (ULg) and at http://planets.oma.be for partner 3 (ORB-KSB). News about the SCOOP project and related activities also placed project webpage are on the http://planetary.aeronomie.be/en/scoop.htm.

Twitter and Facebook accounts:

https://twitter.com/BIRA_IASB?ref_src=twsrc%5Etfw

https://twitter.com/ExoMars NOMAD

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ANNEXES

Publications on the website: https://www.belspo.be/belspo/brain-be/themes 2 GeoUniClim en.stm