

Water vapor line parameters: Some feedback from atmospheric users

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Despite recent major improvements of water vapour (wv) databases, the insufficient quality or consistency of the H₂O spectroscopic parameters has been reported many times and line parameters are often manually adjusted to minimize residuals and improve the quality of the fits. Atmospheric observations allow assessing the quality of databases through their simulation using the different line parameters reported in those databases.

This work presents four concrete examples of the spectroscopic problems and proposed improvements in various spectral regions.

1. Ground-based H₂O retrievals by Fourier transform infrared (FTIR) spectroscopy at the high altitude research station Jungfraujoch, Swiss Alps

In order to maximize the information content in the largest altitude range, several micro-windows encompassing strong and weak lines (**figure 1**) are often fitted simultaneously. But to find the best combinations among numerous possibilities in the 700-4300 cm⁻¹ range is not trivial. A lot of micro-windows have been investigated

but preliminary results show that the quality of the multi-micro-window fits is poor, in particular poorer than single micro-window fits (see details in [1]). To lower residuals, it is necessary to modify HITRAN lines parameters, which point to inconsistencies of spectroscopic parameters between different spectral regions. Tuned line parameters have to be adopted until improved and more consistent parameters are made available.

2. Ground-based H₂O retrievals from differential-absorption lidar (DIAL) at Zugspitze, Germany

A high-power DIAL is installed at the Schneefernerhaus high altitude research station (Zugspitze) in order to measure the vertical distribution of wv in the troposphere (3-12 km) with high spatial and temporal resolutions. The system comprises a unique widely tunable narrow-band laser system, whose technical details are described in [3]. A careful choice of 3 lines in the spectral region around 12240 cm⁻¹ (817nm) has been made [3], but one question arises: which dataset among literature data [4-11] is the best? Comparison of line strengths for some

lines highlights substantial differences between the different databases among which HITRAN [4-5] and Ponsardin and Browell [6]. These large inconsistencies could be linked to the measurement technique. This was further investigated by simulating a laboratory spectrum recorded by Fourier transform spectroscopy using different datasets (**figure 2**). This figure confirms inconsistencies between databases, and it shows moreover that the strongest line simulates worse than the two weaker ones, meaning that inconsistencies also exist within a given database.

3. Impact of H₂O on CH₄ retrievals from nadir spectra recorded by SCIAMACHY onboard ENVISAT

The study of the impact of wv spectroscopy on CH₄ retrievals was initiated because of an unresolved seasonal bias in the southern hemisphere. A change in wv spectroscopic parameters not only largely eliminated this bias but also had a substantial impact in tropical regions. The results of this study are published in [12], and will be briefly summarized here. Methane is retrieved in a near-IR micro-window (5990-6130 cm⁻¹). Retrievals from two ground-based solar absorption FTIR spectra (Paramaribo, Suriname; Bremen, Germany) are first performed. **Figure 3** clearly show systematic residuals of up to 6% at Paramaribo using HITRAN [4-5], which mostly vanish using a modified Brussels-Reims (BR) list [13]. Very strong residuals occur for few strong transitions using the BR list due to unallocated or very low broadening parameters, and a modified BR list is proposed consequently. Overall, systematic errors are substantially reduced using the BR list as compared to HITRAN. Then, the impact of wv on SCIAMACHY CH₄ retrievals is evaluated. In **Figure 4**, a positive correlation and no correlation of retrieved methane with wv abundances are obtained using HITRAN and the BR list respectively. This leads to a systematic overestimation by about 60 ppb of tropical methane abundances (**Figure 5**) and of

tropical emissions estimates which are reduced from 260 to ~201 TgCH₄/yr [12].

4. Spectroscopic needs for H₂O retrievals from SOIR onboard VENUS EXPRESS

New simultaneous H₂O and HDO measurements are necessary to answer the key questions about Venus, among which “why Venus and Earth evolved so differently in spite of their similarities in terms of size, mass, density, volume and distance to the Sun?”, and “which scenario can explain the very high atmospheric isotopic ratio D/H (150 x terrestrial)?” SOIR performs solar occultations in the 2250-4360cm⁻¹ infrared region (**Figure 6**) allowing H₂O and HDO retrievals between 70-110 and 70-95 km respectively [14-16]. Spectral fits (**Figure 7**) show broader simulated lines which could be due to incorrect CO₂ broadened widths γ_{CO_2} for wv. In the absence of γ_{CO_2} measurements or calculation in the covered region, a scaling factor to convert air to CO₂ broadening was applied [16]. However accurate values of γ_{CO_2} would be very useful to reduce uncertainties.

Conclusions

Specific spectroscopic problems in the regions 700-4300 and around 12300 cm⁻¹ have been described for water vapor. Systematic errors in methane retrievals due to inaccuracies in water vapor spectroscopic parameters were presented in the 5990-6130 cm⁻¹ range. Ad-hoc improvements to databases are proposed in some cases, in particular for the 700-4300 and 5990-6130 cm⁻¹ regions. Finally, specific needs of CO₂ broadened widths in the 2250-4360 cm⁻¹ region for the study of the Venus atmosphere have been mentioned. More generally, this work demonstrates the importance of high quality laboratory work both for wv retrieval itself and for interfering species, and of collaborations between the spectroscopy and the remote-sensing community through inter-comparisons, cross-validations, and various synergies.

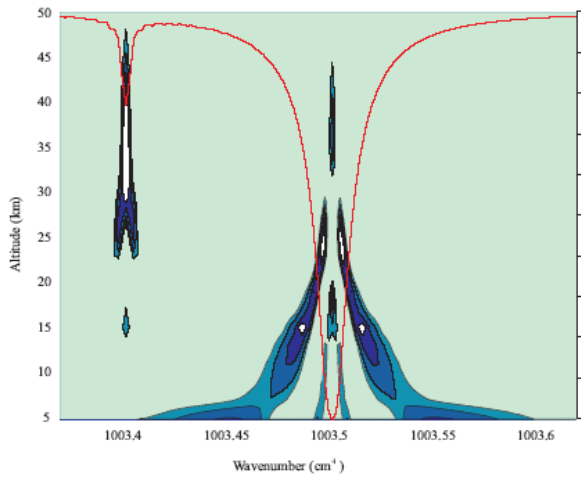


Figure 1: Matrix of the contribution functions for O₃ profile inversion. From [2].

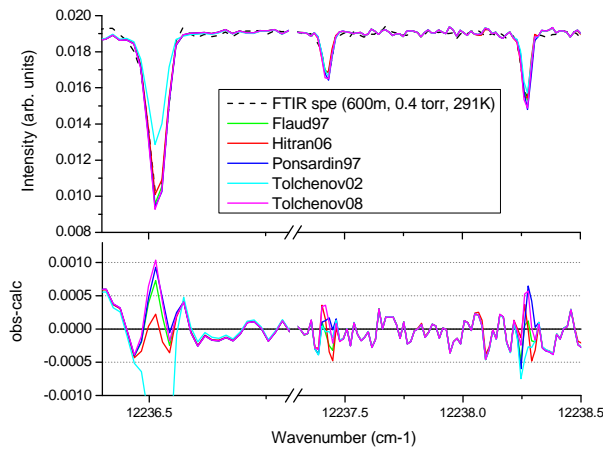


Figure 2: Comparison between measured FTS spectrum (black dots) and simulated spectra with different datasets (colored lines).

Figure 3 (below): Spectral fit of a Paramaribo spectrum (top), corresponding residual (middle), and residual of a fit using a Bremen spectrum (bottom). Colors are contributions from individual gases. The methane $2\nu_3$ Q branch ($5998\text{--}6006\text{ cm}^{-1}$) to which SCIAMACHY is most sensitive is shown in more detail. From [12].

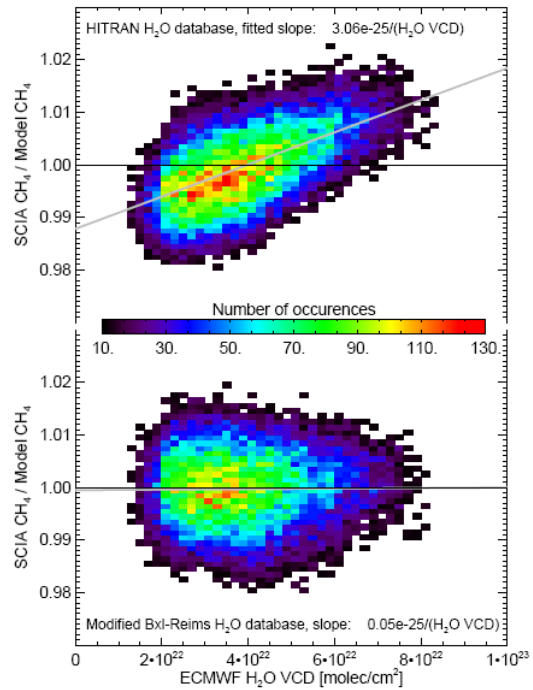
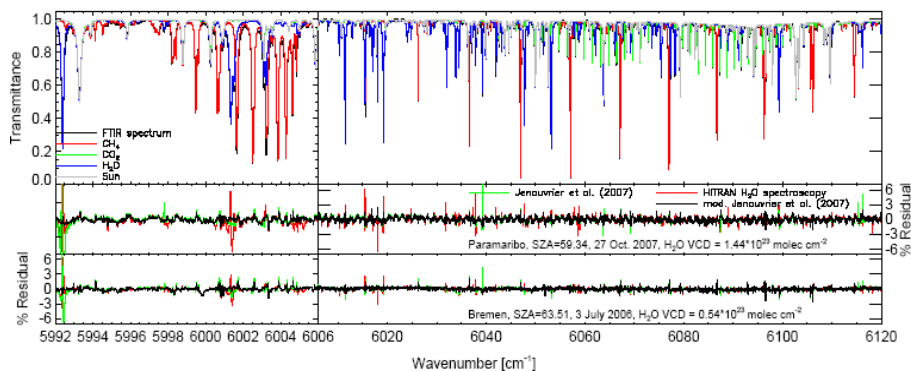


Figure 4: Frequency distribution of the ratio of SCIAMACHY methane retrievals and TM5 model columns over the Sahara in 2004 as a function of water column, using the HITRAN database (top) and a modified version of the BR database [13](bottom). From [12].

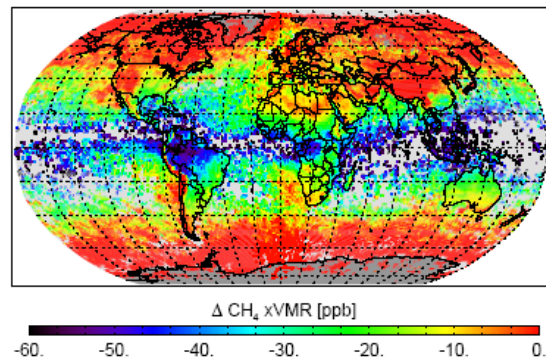


Figure 5: Difference of SCIAMACHY column averaged mixing ratios of CH₄ using HITRAN and the modified BR list (HITRAN-BR). From [12].

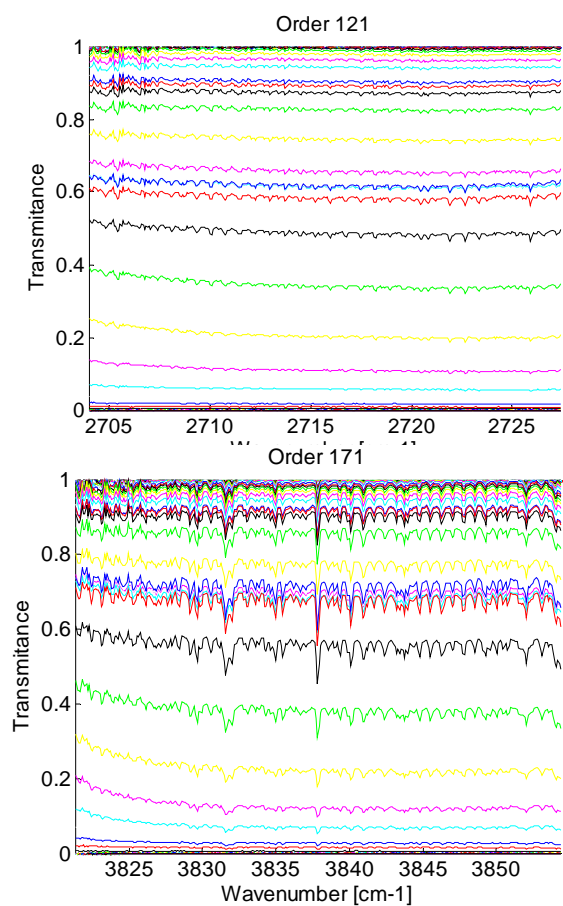


Figure 6: Evolution of one occultation at sunset Aug. 20th 2007: Transmittance spectra in specific ranges of HDO (top) and H₂O (bottom) absorptions. From [16].

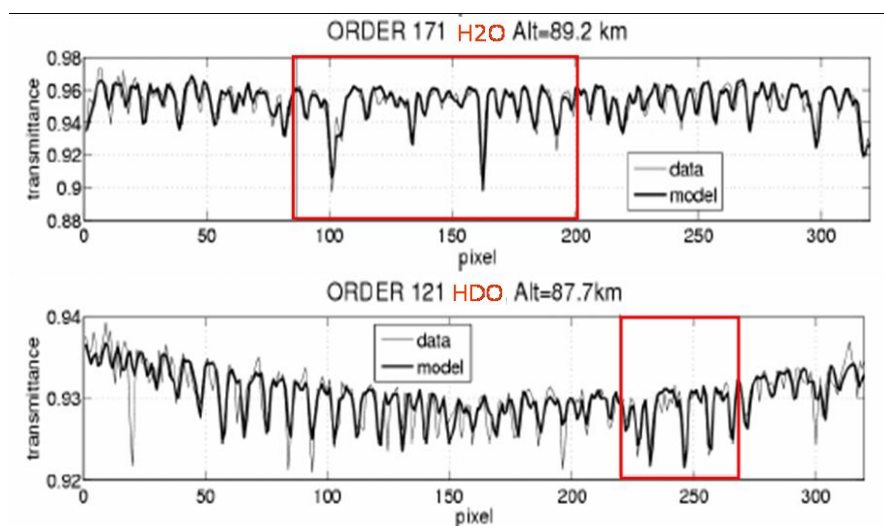


Figure 7: Examples of best data fitting for HDO (top) and H₂O (bottom) at 86-89 km on July 27, 2007. The boxes relate to the chosen ranges for the retrievals. From [14].

Acknowledgments

Support from the Belgian Federal Science Office (SSD & ESA-Prodex programmes), the National Fund for Scientific Research (FRFC program), the European Space Agency, and the Communauté française de Belgique (Actions de Recherche Concertées) is acknowledged.

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