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A sensitivity study on spectroscopic parameter accuracies for a mm/sub-mm limb sounder instrument

C.L. Verdes[a,*], S.A. Buehler[a], A. Perrin[b], J.-M. Flaud[b], J. Demaison[c], G. Wlodarczak[c], J.-M. Colmont[c], G. Cazzoli[d], C. Puzzarini[d]

[a] *Institute of Environmental Physics, University of Bremen, Germany, Otto-Hahn Allee 1, D-28359 Bremen, Germany*
[b] *Laboratoire de Photophysique Moléculaire, UPR CNRS 3361, Université de Paris-Sud, Bât 350, 91405 Orsay, Cedex, France*
[c] *Laboratoire de Physique des Lasers, Atomes et Molécules, UMR CNRS 8523, Bât. P5, Université de Lille I, 59655 Villeneuve d'Ascq Cedex, France*
[d] *Dipartimento di Chimica "G. Ciamician," Universita' di Bologna, I-40126 Bologna, Italy*

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Abstract

The purpose of this paper is to perform a detailed error analysis for a mm/sub-mm limb sounding instrument with respect to spectroscopic parameters. This is done in order to give some insight into the most crucial spectroscopic parameters and to work out a list of recommendations for measurements that would yield the largest possible benefit for an accurate retrieval. The investigations cover a variety of spectroscopic line parameters, such as line intensity, line position, air and self broadening parameters and their temperature exponents, and pressure shift. The retrieval process is performed with the optimal estimation method (OEM). The OEM allows one to perform an assessment of the total statistical error, as well as of the model parameter error, such as the error coming from spectroscopic parameters. The instrument parameters assumed are those of the MASTER instrument studied by the European Space Agency, one of the candidate instruments for a future atmospheric chemistry mission. However, the same principle and method of analysis can be applied to any other millimeter/sub-millimeter limb sounding instrument, for instance the Japanese instrument JEM/SMILES, the Swedish instrument Odin, and the Earth Observing System Microwave Limb Sounder. We find that an uncertainty in the intensity of the strong lines give an error of similar magnitude on the retrieved species to which the lines belong. Uncertainties in the line position have overall a small impact on the retrieval, indicating that the line positions are known with sufficient accuracy. The air broadening parameters and their temperature exponents of a few strong lines dominate the error budget. On the other hand, the self broadening parameters and the pressure shifts are found to have a rather small impact on the retrieval.

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1. Introduction

The quantity measured by a satellite borne radiometer contains implicit information on the atmospheric state, e.g., molecular species volume mixing ratio profiles (VMR) and temperature profile. Millimeter wave remote sensing techniques have unique properties compared to infrared and UV–Vis techniques, such as less sensitivity to cloud contamination and independence of external sources as the thermal radiation emitted by molecules is measured. Furthermore, the thermal emission depends almost linearly on temperature as opposed to a non-linear relationship in the infrared region. The millimeter wave range contains, among many others, spectral features of ozone, water vapor, nitrous oxide, chlorine monoxide, and bromine monoxide, all of which are species of major importance for ozone chemistry or

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[*] Corresponding author. Fax: +49 421 2184 555.
E-mail address: cverdes@uni-bremen.de (C.L. Verdes).

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for the greenhouse effect. An accurate retrieval of the quantities of interest requires accurate knowledge about the measurement and retrieval system. This includes knowledge of the spectroscopic data, such as the line strength, line position, pressure broadening parameters, and pressure shifts. An uncertainty in the spectroscopic parameters will lead to a systematic retrieval error. Therefore a thorough and careful investigation on the current accuracy of the spectroscopic parameters and their impact on the retrieval is necessary.

This paper is organized as given in the followings. Section 2 presents the basic equations and introduces the main quantities involved in the analysis. The instrumental and retrieval setup used is presented in Section 3. Some assumptions on the spectroscopic parameters are given in Section 4. The results are presented in Section 5. Section 5.1 presents the results of a detailed error analysis with respect to spectroscopic parameters for a mm/sub-mm limb sounding instrument. This analysis is done in order to give some insight into the most crucial spectroscopic parameters and to work out a list of recommendations for measurements that would yield the largest possible benefit for an accurate retrieval. Possible improvements of the retrieval scheme in order to reduce the retrieval error are also discussed (Section 5.2). Based on the error analysis results, measurements of the line parameters found to be the most critical were carried out at two laboratories in the University of Bologna, Italy, and the University of Lille, France. Moreover, theoretical calculations of some spectroscopic parameters were performed at the University of Paris-Sud. Using the new experimental and theoretical results, an updated database was created. Furthermore, the error analysis is carried out again in order to see the benefits of the updates (results presented in Section 5.3). The main findings and conclusions of the analysis are presented at the end of this paper.

2. Background

A brief description of the basic equations and of some practical considerations is given in the following. For more details please refer to [1,21].

Extraction of the quantities of interest from a satellite measurement requires a forward model **F**, containing an absorption and a radiative transfer model, and an inversion model (or retrieval model) **I**. The forward model used here is the Atmospheric Radiative Transfer Simulator (ARTS) [3]. The forward model calculates the absorption coefficients k_ν by summing up the contributions of the individual lines, but also non-resonant terms of water vapor, oxygen, and nitrogen, the so-called absorption continua (details about the continua can be found in, e.g. [8,9,17,19,25]).

The absorption coefficient of a specific line, k_ν^l, is given by the line intensity (or strength) S, the line shape $f(\nu,\nu_0)$, describing the distribution in frequency ν, and its position given by the center frequency ν_0:

$$k_\nu^l = nS(T)f(\nu,\nu_0), \tag{1}$$

where n is the number of molecules of the species per unit volume.

The line intensity at a reference temperature T_0, $S(T_0)$, is obtained from a spectroscopic database. The values at other temperatures are obtained by the interpolation relation [26]:

$$S(T) = S(T_0)\frac{Q(T_0)}{Q(T)}\frac{\mathrm{e}^{-E_f/kT} - \mathrm{e}^{-E_i/kT}}{\mathrm{e}^{-E_f/kT_0} - \mathrm{e}^{-E_i/kT_0}}, \tag{2}$$

where E_f and E_i are the two energy levels involved in the transition (obtained from the database), and $Q(T)$ is the so-called partition function [24].

In the microwave region, where the width of the rotational lines is not negligible compared to the center frequency of the line ν_0, a good approximation of the lineshape is the Van Vleck–Weisskopf lineshape [20]:

$$f(\nu,\nu_0) = \left(\frac{\nu}{\nu_0}\right)^2 \times \frac{\gamma}{\pi}\left[\frac{1}{(\nu-\nu_0-\delta\nu_0)^2+\gamma^2} + \frac{1}{(\nu+\nu_0-\delta\nu_0)^2+\gamma^2}\right], \tag{3}$$

where γ is the pressure broadening linewidth and $\delta\nu_0$ is the shift in the line center frequency due to the pressure (hereafter called the pressure shift).

The linewidth γ depends on temperature T, and on the colliding molecules (or the broadening gas), which can be separated into foreign (air) broadening and self broadening parts using the semi-empirical law [7]:

$$\gamma(p,p_s) = \underbrace{\mathsf{agam}(p-p_s)\left(\frac{T_0}{T}\right)^{\mathsf{nair}}}_{\text{air broadening}} + \underbrace{\mathsf{sgam}\,p_s\left(\frac{T_0}{T}\right)^{\mathsf{nself}}}_{\text{self broadening}} \tag{4}$$

where p is the total pressure of the sample, p_s is the partial pressure of the species in question, agam and nair are the air broadening parameter and its temperature dependence, respectively, and sgam and nself are the self broadening parameter and its temperature dependence, respectively.

The inverse model used here is Qpack [6], which uses the Optimal Estimation Method (OEM) described in [15,16].

The forward model **F** generally depends on the (atmospheric) state $\mathbf{x}$ and other parameters $\mathbf{b}$. In a broader sense, the choice of which of the input parameters to **F** belong to $\mathbf{x}$ and which to $\mathbf{b}$ is up to the user. The difference between the two is that $\mathbf{x}$ is retrieved, whereas $\mathbf{b}$ is assumed to be well known. We treat spectroscopic parameters as part of $\mathbf{b}$.

To perform a retrieval and a basic error analysis, the Jacobian of the measurement with respect to $\mathbf{x}$, $\mathbf{K}_x = \partial\mathbf{F}(\mathbf{x}, \mathbf{b}_a)/\partial\mathbf{x}|_{\mathbf{x}_a}$, and with respect to $\mathbf{b}$, $\mathbf{K}_b = \partial\mathbf{F}(\mathbf{x}_a, \mathbf{b})/\partial\mathbf{b}|_{\mathbf{b}_a}$, and the Jacobian of the inverse (retrieval) model with respect to the measurement, $\mathbf{D}_y = \partial\mathbf{I}(\mathbf{y})/\partial\mathbf{y}$, the so-called contribution function matrix, have to be calculated.

In the context of retrieval error characterization important quantities are various error covariance matrices (ECM). These are the measurement noise ECM $\mathbf{S}_\epsilon$, the a priori ECM $\mathbf{S}_a$ (containing the information on $\mathbf{x}$ before the measurement is made), the model parameter ECM $\mathbf{S}_b$ (containing the uncertainties in model parameters), the total retrieval ECM $\mathbf{S}$, the retrieval measurement ECM $\mathbf{M} = \mathbf{D}_y\mathbf{S}_\epsilon\mathbf{D}_y^T$, the smoothing ECM $\mathbf{N} = (\mathbf{A} - \mathbf{I})\mathbf{S}_a(\mathbf{A} - \mathbf{I})^T$, and the retrieval model parameter ECM $\mathbf{P} = (\mathbf{D}_y\mathbf{K}_b)\mathbf{S}_b(\mathbf{D}_y\mathbf{K}_b)^T$. The $\mathbf{S}_\epsilon$, $\mathbf{S}_a$, and $\mathbf{S}_b$ ECMs are input to OEM while the others are output to OEM. Beside these, another important quantity is the averaging kernel matrix $\mathbf{A} = \mathbf{D}_y\mathbf{K}_x$ which gives an impression on the vertical resolution. For more details on the above quantities please refer to [21,23]. The quantities of most interest here are $\mathbf{S}$ (note that $\mathbf{S} = \mathbf{M} + \mathbf{N}$) referred as retrieval precision, and $\mathbf{P}$ which contains error coming from the uncertainties in the model parameters, such as spectroscopic parameters.

3. Instrumental and retrieval setup

The Millimetre-wave Acquisitions for Stratosphere/Troposphere Exchange Research (MASTER) instrument [13,14] studied by the European Space Agency, one of the candidate instruments for a future atmospheric chemistry mission, is used as a realistic example for a state-of-the-art limb sounding instrument. However, the same principle and method of analysis could be applied to any other millimeter/sub-millimeter limb sounding instruments, for instance JEM/SMILES [10], Odin [5], and EOS/MLS [27].

The MASTER instrumental requirements have been investigated in depth and optimized in a series of studies (e.g. [2,13,22]). Global measurements will be performed with a spectral resolution $\Delta\nu = 50$ MHz in five spectral bands, namely: 294.00–305.50 GHz (Band B), 316.50–325.50 GHz (Band C), 342.25–348.75 GHz (Band D), 497.00–506.00 GHz (Band E), and 624.00–626.50 GHz (Band F). The instrument is characterized by a system noise temperature T_{sys} of approximately 6000 K. The main target species are O_3 (in Band B, Band C, Band E, and Band F), HNO_3 (in Band B and Band C), N_2O (in Band B and Band E), CO (in Band D), ClO (in Band E), BrO (in Band D and Band E), H_2O (in Band C and Band E), and HCl (in Band F). The absorption spectra, at an altitude of 25 km, for each species included in the forward calculation, and the total absorption in each spectral band are shown in Fig. 1. The target species in each spectral band are outlined in bold.

For an atmospheric scenario, simultaneous retrievals of molecular species VMR profiles (100% a priori, retrieved on a grid of 2 km) and temperature profile (5 K a priori, retrieved on a grid of 3 km) are performed using simulated measurements of an entire elevation scan cycle (0–50 km). No correlations between the retrieved layers are assumed.

Only the thermal noise is included in the measurement noise, and no interchannel correlations are considered, i.e., a diagonal $\mathbf{S}_\epsilon$ matrix with the diagonal elements set to $(T_{\text{sys}}/\sqrt{\Delta\nu\tau})^2$—(the so-called radiometric formula)—where $\tau = 0.3$ s is the integration time.

4. Spectroscopic database and assumptions

The information on the spectroscopic parameters is taken from the MYTRAN database [11], which was developed in the context of the MASTER instrument study. The present database is mainly based on the HITRAN database [18] but with some additional lines and species (e.g., BrO) from JPL [12]. It includes the values of the spectroscopic parameters, such as the intensity $S(T_0)$ (see Eq. (2)), pressure broadening parameters agam, sgam, nair, and nself (see Eq. (4)), line position ν_0, and pressure shift parameters.[1] Their accuracies, except for the self broadening parameters and pressure shifts, are also contained in the database. For the case of self broadening parameters sgam and nself, a default value of 200% was assumed. An exception to this is the parameters connected to O_2, where the assumed accuracies in the self broadening parameters are the same as for the air broadening parameters (10% for sgam, and 20% for nself, respectively). For the pressure shifts, since they are very difficult to measure, an estimated uncertainty for all lines belonging to the same molecular species is assumed. This is a poor approximation as it is well known that the pressure shift is usually very different (with possible change of sign) from one given transition to the next. Thus, the investigated pressure shift uncertainties were 300 kHz/Torr for H_2O and CH_3Cl lines, 20 kHz/Torr for O_3, N_2O, and CO lines, 50 kHz/Torr for O_2 lines, and 200 kHz/Torr for HCl lines. For the other molecular species, for the sake of simplicity, an uncertainty of 1 MHz/Torr in pressure shifts is assumed. However, the uncertainty of 1 MHz turns out to be exaggerated, especially for HNO_3 lines for which the pressure shifts are very small, as shown in [4] . The analysis are carried out without assuming correlations

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[1] Pressure shift parameters are denoted as the pressure shifts $\delta\nu_0$ per unit pressure.

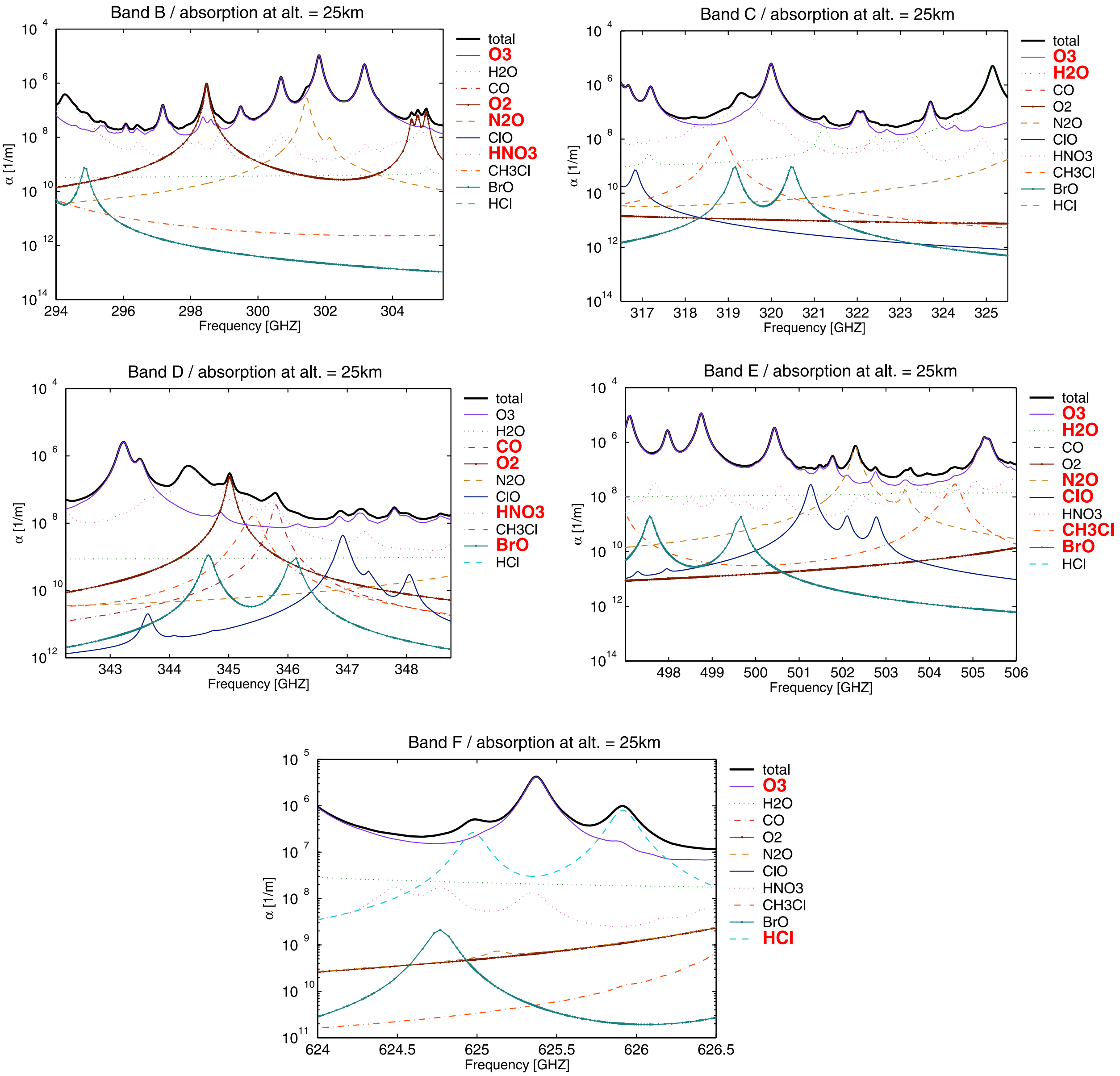

Fig. 1. MASTER spectral bands. Displayed are the species absorption and total absorption spectra at an altitude of 25 km. The target species are outlined in bold.

between the different parameters and lines. An exception to this is the case of HNO_3, where a correlation of 0.6 between the same parameter of different lines is assumed.

5. Results and discussions

For the instrumental and retrieval setup presented in Section 3, an assessment of the retrieval error on the target species of MASTER coming from the spectroscopic parameters uncertainties stated in the MYTRAN database is made. The steps of the analysis are discussed in details in the followings.

5.1. Assessment of spectroscopic parameter impact

For the first step, retrieval simulations are carried out for an initial database containing the best available information on the spectroscopic parameters found in the literature, as collected in the MYTRAN database. The main purpose of this is to give an insight into the most crucial parameters whose accuracy will most strongly affect the retrieval performance for a limb sounding instrument like MASTER. This also allows to work out a list of recommendations for measurements that would yield the largest possible benefit for the MASTER instrument. The data are also of direct relevance for the analysis of the spectra to be observed by MARSCHALS, the airborne demonstrator for MASTER.

Regarding the uncertainties in intensities, the retrieval simulations show that the retrieval error is mainly dominated by the error coming from uncertainties in a few strong lines. As expected, an uncertainty in the intensity of the strong lines gives an error of similar magnitude on the retrieved species to which the lines belong. For instance, 10% uncertainty in the intensity of the N_2O line at 301.443 GHz, the strongest N_2O line within Band B, generates an error of 10% on the retrieved N_2O (Fig. 2, left plot), 5% uncertainty in the strong H_2O line at 325.153 GHz generates an error of 5% on the retrieved H_2O in Band C (Fig. 2, right plot), and 2% uncertainty in the strong O_3 lines generates an error of about 2% on the retrieved O_3. However, an uncertainty in the intensity of the strong lines (usually these are O_3 lines) turns into a much higher error on a retrieved weak species, such as BrO. Possible improvements of the retrieval scheme for the weak species are discussed in Section 5.2.

Overall, uncertainties in the line positions have a small impact on the retrieval, indicating that the line positions are known with sufficient accuracy.

The air broadening parameters, agam, and their temperature exponents, nair, of a few strong lines are found to dominate the error budget. These are generally the strongest O_3 lines within each MASTER spectral range, i.e., the O_3 lines at 300.685, 301.813, and 303.165 GHz in Band B, at 317.195 and 319.997 GHz in Band C, at 343.506, 343.238, and 343.181 GHz in Band D, and at 625.372 and 623.688 GHz in Band F. In the spectral range of Band E the N_2O line at 502.296 GHz is the most important for an accurate retrieval, but also some impact from a few strong O_3 lines is seen. However, the investigated agam uncertainty for N_2O line (the one quoted in the initial database) is much larger (50%) compared to the ones for the strong O_3 lines found in Band E spectral range (20% or even better). The parameters of the strong lines have a much higher impact on the retrieval of the weak species, like BrO.

Similar findings as for agam parameters apply for the temperature exponent nair parameters. Overall, the impact is smaller than the one generated by agam, but still non-negligible. The parameters connected with the same strong O_3 lines listed above have the greatest impact on the retrieval.

On the other hand, the self broadening parameters are found to have little impact on the retrieval. This is even true for species with high self broadening coefficients and high volume mixing ratios, such as water vapor and oxygen (Fig. 3, left plot).

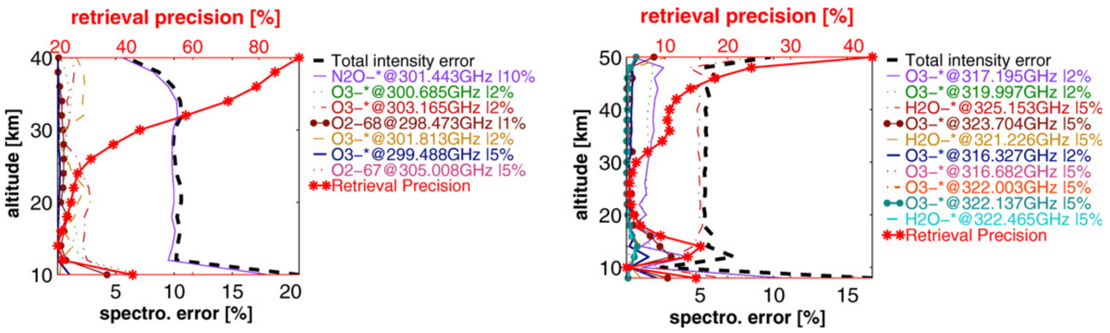

Fig. 2. N_2O retrieval in Band B (left) and H_2O retrieval in Band C (right): individual line intensity error and total intensity error. Only the individual terms which have a contribution larger than 5% to the total error are displayed. The retrieval precision is also displayed (x-axis for this is shown at the top).

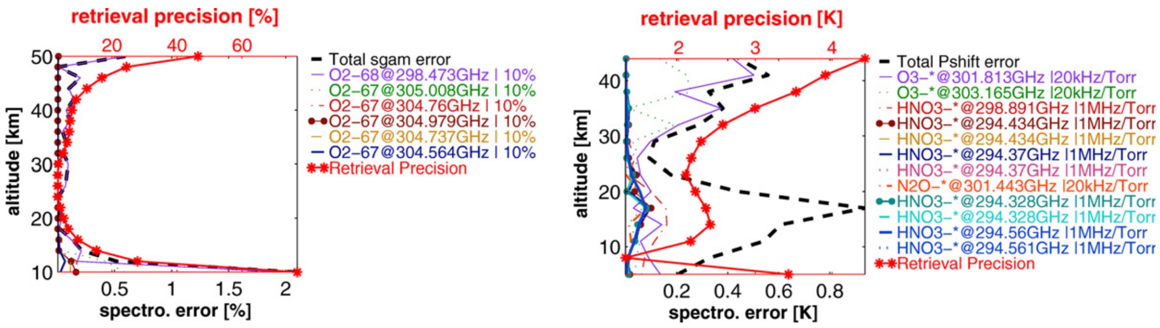

Fig. 3. Left: O_3 retrieval in Band B. Individual and total sgam error. Right: temperature retrieval in Band B . Individual and total pressure shift error. Displayed are the same quantities like in Fig. 2.

Generally, the pressure shifts are found to have a rather small impact on the retrieval. The only non-negligible impact comes from the parameters associated with the HNO_3 lines (Fig. 3, right plot). When looking at this result one has to keep in mind the very large number of the HNO_3 lines and the assumed uncertainty for the HNO_3 lines pressure shift of 1 MHz/Torr which is an extremely conservative value. The individual errors coming from individual lines are rather small, but the cumulated error is rather large. Recent laboratory measurements showed that the HNO_3 lines have very small pressure shift (see [4]), and therefore, this parameter is not a problematic one.

5.2. Optimization of retrieval scheme

The assessment of the line intensity errors shows that the retrieval of the weak species is very much affected by the uncertainties in the intensity of a few strong lines, usually O_3 lines. A cause of this could be the interference of weaker O_3 lines with the weak species, as in the standard retrieval scheme all O_3 lines are simultaneously fitted. The problem is that the spectroscopic parameters of the different O_3 lines might be inconsistent, and the fit residual would interfere with the retrieval of other species. Therefore, it is investigated whether a modification of the retrieval scheme could reduce this error. It turns out that the intensity error on the retrieved weak species is much reduced if the intensities of a few lines (lines found to have the highest impact) are fitted separately. For instance, by fitting separately the intensities of three strong O_3 lines (at 497.098, 498.798, and 505.369 GHz) found to have the highest impact on the retrieved BrO in Band E (see Fig. 4, left plot), the total error is significantly reduced from 200 to 60%, (see Fig. 4, right plot). The error connected with the three lines in question has practically vanished. Moreover, the modification of the retrieval scheme has no negative effects on the retrieval of other quantities; on the contrary, it positively affects the retrieval quality of the other quantities, as well. For instance, the error on the retrieved temperature, where the same lines yield the largest error in the standard retrieval scheme, is also significantly reduced. It is interesting to see that good information on the O_3 is obtained either from each of the three mentioned lines or from the remaining lines if the three ones are excluded from the database. Fig. 5 shows the O_3 general retrieval performance results from O_3 lines at 497.098 GHz (left), at 498.798 GHz (middle), and at 505.369 GHz (right).

However one should keep in mind that there is an upper limit for the number of the fitted parameters, and therefore the proposed approach would work only

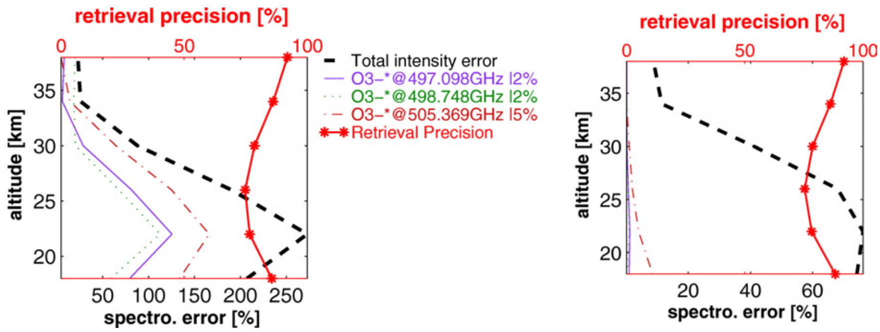

Fig. 4. Band E, BrO retrieval. Left: error terms for the standard retrieval scheme (all the O_3 lines are fitted simultaneously). Right: error terms for the case when three O_3 lines are treated separated. For the sake of clarity, only the individual error terms connected with the lines in question are displayed. The total error for each of the retrieval schemes is also displayed.

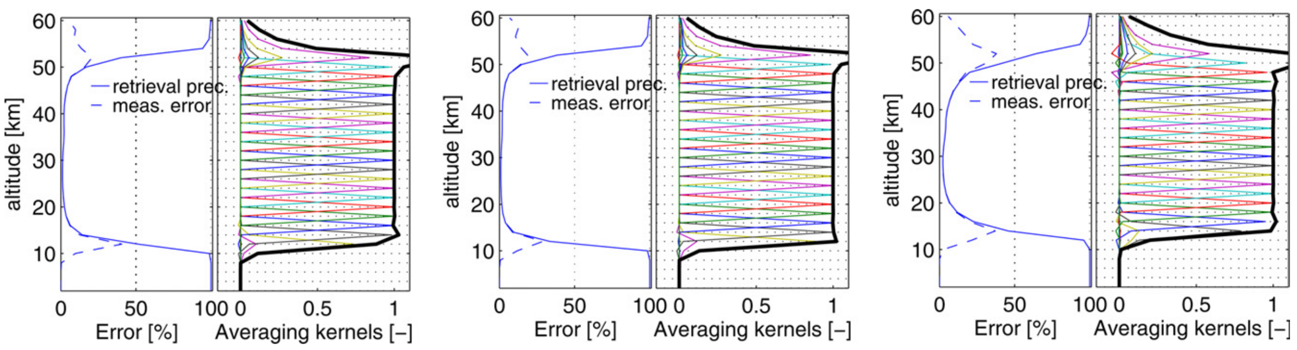

Fig. 5. Band E, O_3 retrieval from O_3 line at 497.098 (left), from O_3 line at 498.798 GHz (middle), and from the O_3 line at 505.369 GHz (right). For each retrieval scheme, the set of two plots displays the retrieval precision and the measurement error on the left, and the averaging kernels and measurement response on the right.

in the case that only a few lines dominate the total error budget.

5.3. Benefits of new measurements

Based on the results presented in Section 5.1, a list of line species to be studied experimentally in laboratory and new theoretical calculations is set up. These measurements and calculations are performed and results in a new database. The laboratory measurements concern the air broadening parameters of a number of O_3 and HNO_3 lines found to weight the most for an accurate retrieval. These lines are listed in Table 1 together with the experimental value of measured parameter. Beside these, laboratory measurements for pressure shifts of few lines are performed (e.g., for H_2O line at 325.153 GHz) and the new results are included in database. The theoretical calculation includes recalculation of the intensity values for the N_2O, H_2O, and O_3 lines. Furthermore, for the agam parameters of HNO_3 lines for which no experimental data are available, an empirical approach based on existing experimental data is used [4,11]. Regarding nair or nself, when no available information on these parameters are found in the literature, they are set to a default value of 0.7 (e.g., for HNO_3 lines). Beside the mentioned modifications in the database, the best available informations on line parameters found very recent in literature are also considered. For each updated line parameter, the corresponding updated uncertainty is taken into account in the new database. For more details on the database please refer to [4,11].

Using the updated database, retrieval simulations are carried out yet again in order to see the benefit of the measurements and theoretical calculations.

In regards to the intensity error, no significant differences are found, since no major changes in the intensities were made. A slightly different behavior is seen for the N_2O line at 301.443 GHz on the retrieved N_2O at low altitudes (see Fig. 6). Even though the uncertainty in the intensity of the line in concern remains the same, the small difference can be explained by the recalculation of the line intensities for N_2O lines (the recalculated line intensities for N_2O lines are usually approximately 6% lower than the ones quoted in the initial database). When looking at the N_2O retrieval precision (Fig. 6, right plot) for the two sets of simulations, one can see that retrieval precision for the updated retrieval simulations is slightly degraded compared to the initial one (especially at low altitudes), an effect of the change in the line intensity value itself.

Better knowledge of the air broadening parameters of the strong O_3 lines greatly improves the retrieval accuracy. Figs. 7–9 show the agam error budget before (left) and after (right) the updates are performed. The spectral lines associated with different error terms are tabulated in the middle. The corresponding uncertainty is shown on the left (before measurements) and on the right side (after the measurements) of each specific spectral line. For clarity, the same scale has been used in both plots. Overall, the total error on the retrieved quantities is decreased, a consequence of improved knowledge of agam parameters of a few O_3 lines (listed in Table 1), the ones found in the initial retrieval analysis to be the most critical. The current accuracy for the agam of the measured O_3 lines is 2% compared to the initial one of 10%. Thus, the improved knowledge of the agam for the O_3 lines at 300.685, 301.813, and 303.165 GHz, the strongest ones in the spectral range of Band B, drastically decreases the error generated on the retrieved O_3 in Band B (from more than 5% to 1%, see Fig. 7). Furthermore, the new

Table 1
List of the measurements

Line	T	agam	nair
O_3 at 300.685 GHz (B)	238	3.730(18)	
O_3 at 301.831 GHz (B)	296	3.081(19)	0.676(20)
O_3 at 303.165 GHz (B)	296	3.287(19)	0.849(32)
O_3 at 317.195 GHz (C)	296	3.427(29)	0.580(60)
O_3 at 319.997 GHz (C)	296	2.950(6)	0.722(13)
O_3 at 343.238 GHz (C)	240	3.583(26)	
O_3 at 343.506 GHz (D)	240	3.689(30)	
HNO_3 at 316.6114 GHz (C)	298	3.832(77)	
HNO_3 at 316.9019 GHz (C)	298	3.820(57)	
HNO_3 at 319.897 GHz (C)	298	4.192(27)	
HNO_3 at 319.2215 GHz (C)	298	4.282(19)	
HNO_3 at 320.005 GHz (C)	298	4.211(12)	
HNO_3 at 322.348 GHz (C)	298	4.574(14)	
HNO_3 at 344.2417 GHz (D)	298	4.181(41)	
HNO_3 at 470.233 GHz (outside)	298	4.189(43)	
HNO_3 at 544.360 GHz (outside)	298	3.920 (34)	

Tabulated are the spectral lines (the MASTER spectral range within the line is located is given in brackets), the measurement temperature, and the measured air broadening parameter. The statistical error given in parentheses are 1σ of the less-square fit.

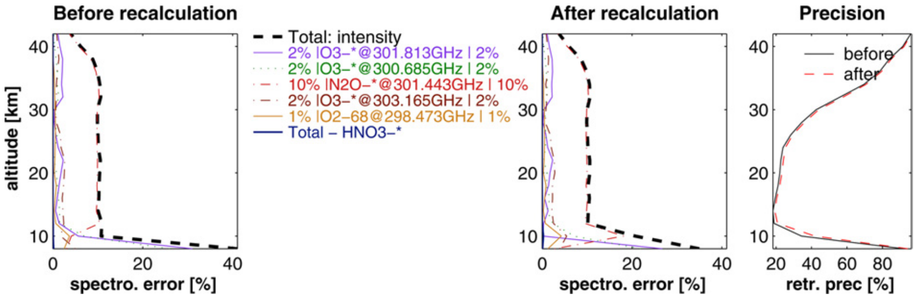

Fig. 6. Band B, N_2O. Left: intensity error terms before the updates. Middle: intensity error terms after the updates. Right: retrieval precision before and after recalculation.

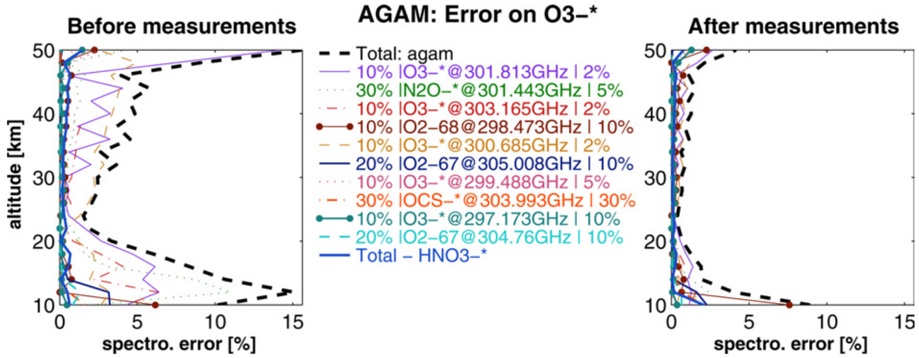

Fig. 7. H_2O retrieval in Band C. Air broadening parameter agam error terms before the measurements (left) and after the measurements (right).

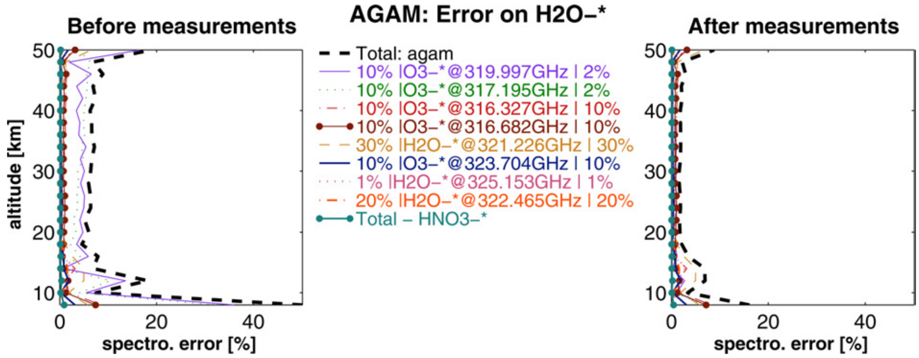

Fig. 8. H_2O retrieval in Band C. Air broadening parameter agam error terms before the measurements (left) and after the measurements (right).

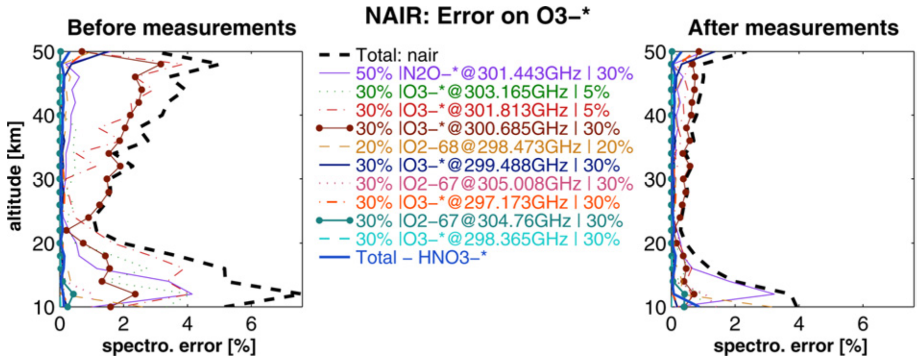

Fig. 9. O_3 retrieval in Band B. Temperature exponent nair error terms before the measurements (left) and after the measurements (right).

measurements within Band C and Band D overall improve the retrieval accuracy. For instance, the error is reduced from 10% to 1% for the retrieved H_2O in Band C (see Fig. 8). The new measurements carried out for the nair parameter also improve the retrieval accuracy. For instance, the nair error on O_3 retrieved in Band B is reduced from 4% to 1% (see Fig. 9).

6. Conclusions

Uncertainties in the intensities of strong lines lead to comparable errors on the retrieval of the species to which the lines belong. The uncertainties in these strong lines are very much amplified in the case of weak species, such as BrO. Further investigations on the retrieval scheme optimization show that this error can be reduced by fitting separately the parameters of a few lines found to account the most for an accurate retrieval. Air broadening parameters, agam, and their temperature exponents, nair, of strong lines (usually O_3 lines) dominate the error budget. Laboratory measurements of the air broadening parameters of these lines lead to great improvements in the retrieval accuracy. The line position, self-broadening parameters, and pressure shifts have a small impact on the retrieval accuracy.

Even though the analysis has been performed for the MASTER instrumental parameters, the compiled conclusions apply to any other similar instrument, such as the Japanese instrument JEM/SMILES, the Swedish instrument Odin, and the Earth Observing System Microwave Limb Sounder.

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