

## ***Interactive comment on “New temperature and pressure retrieval algorithm for high-resolution infrared solar occultation spectroscopy: analysis and validation against ACE-FTS and COSMIC” by K. S. Olsen et al.***

**K. S. Olsen et al.**

ksolsen@atmosp.physics.utoronto.ca

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### **1 Anonymous Referee 2**

#### **1.1 General Comments**

The paper describes a new retrieval scheme for temperature and pressure originally destined to be used for MATMOS, a discontinued Mars orbiting instrument. The paper is very well written and its scope fits well into C5460

AMT. However, the paper has some shortcomings listed below, which must be addressed before publication. These relate mostly to the mathematical description of the new method in Section 2.3, which should be straightforward to address.

The Referee makes several strong comments about the clarity of the mathematical basis for the algorithm. We understand that our presentation may not be clear enough to another reader, and thank the referee for identifying cases where clarification is needed. Parts of the discussion were made purposefully brief to decrease the length of the manuscript, which was not the best approach. We have addressed each comment with changes to the manuscript which improve the readability and value of the work presented, and we thank the Referee for their time and effort.

At the end of this Response, there is a list of changes. Line numbers refer to the AMT Discussions paper published online at doi:10.5194/amtd-8-10823-2015.

#### **1.2 Specific Comments**

##### **Page 10828, lines 6f**

What characteristic of MATMOS is decisive for this? spectral resolution, SNR, or both? I.e. will the TIRVIM replacement not be able to fulfill this?

It would be a combination of its operation mode and instrument design, the benefits of which are listed on on page 10826, lines 10-17. The spectral resolution TIRVIM will achieve is ten-times coarser than MATMOS, and when it is not operated in solar occultation mode, it has a much shorter optical path through the atmosphere, and lower signal strength. We feel that it is not the place of this manuscript to comment on the capabilities of ACS and NOMAD since this paper focuses on a technique, MATMOS is not flying at this time, and ACS has not published detection limits at the time of writing.

C5461

This equation, while also present in the Stiller paper, has exchanged the order of the sum and the exponential function. As written, more radiation than emitted by the sun would usually measured.

Yes, it should read as the exponent of the sum of contributions from each layer. This has been corrected.

Eq. (2) is highly confusing. Following the argument in the text, it is reasonable to arrive at  $\chi'_i = S(T)\chi_i PT'/(S(T')P'T)$ , which is consistent with Stiller *et al.* I do not see how the VSF enters the picture unless something along the lines of  $\chi'_i = VSF\chi_i \Rightarrow VSF = S(T)PT'/(S(T')P'T)$ , was intended. The usage of VSF in Eq. (3) is also not helpful as it is not clear what "Column" is or what the integration range is. Does this refer to the full column from ground to atmosphere? The full path of one spectral measurement through the atmosphere or just through one layer? Does this text and the following paragraph relate to the fact that the radiative transport model likely does not assume each atmospheric layer to be homogeneous? Incidentally, if my line of reasoning were correct, the quotient of  $\chi_i/\chi'_i$  in Eq. (5) is incorrect. While this would not affect the derived temperatures, it would affect the pressure computation by means of the intercept. As this paper is about describing this new method, all those question must be clarified.

Much of what the Referee asks about is described following each equation. However, in a later comment, the Referee notes that the acronym VSF is used prior to its definition, which happened when the list of steps on page was added between earlier versions.

C5462

To address this comment, we have moved the definition of VSF earlier in the paper, rearranged the discussion of VSF to address the specific question in this comment, and made changes to the list.

What we intended to convey was that in our case, after making some assumptions about geometry and goodness of fit, the *retrieved* VMR can be represented by  $VSF\chi'$ . If Eq.(1) represents the spectral feature being fitted, then, after fitting, we can represent our calculated spectral feature with a version of Eq. (1) where all the quantities have prime symbols, representing that they are a priori quantities, *except* the VMR of CO<sub>2</sub>, which has now been modified by the VSF in order to obtain a spectral fit. To make this description more clear, the prime notation is now stated earlier, how the VSF comes out of the spectral fitting code is clarified, and the order of the discussion has been reorganized.

"Column" represents the total column of gas along the slant path  $s$ , it is the total amount of a gas along the line of sight, from the sun to the instrument. This is now better stated.

Regarding the Referee's final comment about Eq. (5) and the homogeneity of atmospheric layers, there is a further simplification that we make that should also be clarified. GGG assumes that the atmosphere is divided into several homogeneous layers that the observed ray passes through. For each spectral window, when fitting, the contribution from each layer is taken into account and we obtain a VSF value for each observation in the occultation, and they are given at the tangent altitudes, as are  $T$  and  $P$ . Eq. (5) is applied at the tangent altitudes, layers which are no longer homogeneous, but for which we want vertical profiles of temperature and pressure at specific locations of the tangent points. We have expanded the discussion to include the two different altitude grids and to clarify that Eq. (5) is only used for a single layer.

Page 10834, line 19 to page 10836, line 6 now reads:

1. Spectral fitting of CO<sub>2</sub> lines is performed for ten CO<sub>2</sub> vibration-rotation bands with around 40 lines each.

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2. Data quality criteria are imposed on resulting VMR scale factors (VSFs).
3. Temperature and pressure are computed for each band at each altitude.
4. Weighted means of  $T$  and  $P$  are calculated for each altitude to produce vertical profiles of  $T$  and  $P$ .
5. The altitude with the highest quality pressure retrieval is estimated.
6. The vertical profile of temperature is integrated above and below the altitude with the highest quality pressure retrieval.
7. A vertical profile of pressure is computed using the equation of hydrostatic equilibrium.

When GGG fits a computed spectrum to a measured spectrum over a spectral window, it varies the VMR of the target gases until a best fit is achieved. The result is the VSF for each target gas at each altitude, defined for some target gas, by the equation:

$$Column = VSF \int \chi' n_a ds, \quad (1)$$

where the left-hand side is the total column of the target gas along the slant path through the atmosphere, between the sun and the instrument, taking into account bending due to refraction.  $\chi'$  is the VMR of the target gas, the prime notation indicates that it is an a priori quantity,  $n_a$  is the total number density, and  $s$  is the path variable. VSF is therefore the ratio between the true total column of gas, and that calculated by GGG. In solar occultation geometry, once fitting has been performed, and if the altitude, pressure, and temperature are correct, then the slant paths of the actual column and the a priori column are the same. GGG divides the atmosphere into homogeneous layers, calculates the optical path for an observation,

C5464

and accounts for the contributions from each layer. Therefore, the VSF is the ratio between a priori and true gas amounts averaged over the slant path, and we express the retrieved VMR as  $VSF\chi'$ .

For transmission spectra, we can describe the depth of an absorption feature with the Beer-Lambert law:

$$I(\tilde{\nu}) = I_o(\tilde{\nu}) \exp \left[ \sum_i -S(T_i) f(T_i, P_i, \tilde{\nu}) \chi_i (P_i/kT_i) l_i \right], \quad (2)$$

where  $i$  is an atmospheric layer,  $I(\tilde{\nu})$  is the transmitted intensity at wavenumber  $\tilde{\nu}$ ,  $I_o(\tilde{\nu})$  is the incident intensity,  $S(T_i)$  is the temperature-dependent line strength defined in ?,  $f(T_i, P_i, \tilde{\nu})$  is the line shape function,  $k$  is the Boltzmann constant, and  $l_i$  is the optical path length. After fitting, we assume that the measured transmittance,  $I(\tilde{\nu})/I_o(\tilde{\nu})$ , is equal to the calculated transmittance,  $[I(\tilde{\nu})/I_o(\tilde{\nu})]'$ , computed by GGG using a priori quantities and the VSF. We also assume that the line shape function, optical path length, and incident intensity for  $I(\tilde{\nu})$  and  $I'(\tilde{\nu})$  are equivalent ( $f_i \equiv f'_i$ ,  $l_i \equiv l'_i$ ,  $I_o(\tilde{\nu}) \equiv I'_o(\tilde{\nu})$ ). We further simplify the expression for  $I(\tilde{\nu}) = I'(\tilde{\nu})$  by assuming GGG has already accounted for the contributions from each layer  $i$  and obtain an expression for the retrieved VMR,  $VSF\chi'$ , at the altitude of the observation:

$$VSF_j \chi'_j = \frac{S(T_j)}{S(T'_j)} \chi_j \frac{P_j T'_j}{P'_j T_j}, \quad (3)$$

where  $j$  represents the altitude of the tangent point of the optical path for an observation.

*Most of the reasons given for the method of integration could be easily achieved with simple numerical integration schemes (e.g., trapezoidal rule), even exactly taking variations in  $g$  into account. The major aspect seems to be the implicit smoothing of the  $T$  profile, which indeed might benefit the computed  $P$ . On the other hand polynomials of higher degrees have the tendency to overshoot. How do you prevent this?*

There are two, somewhat related, reasons that fitting is done here. The primary reason is that the retrieved  $T$  values are uncertain. There may be outliers with very large deviations from the profile, and there may be unphysical oscillations in the profile. Fitting provides a function for integration that is not forced to pass through each point, and provides some smoothing. The other reason is that the altitude grids are not uniform, making a numerical integration method computationally complicated, while simplifying the interpolation scheme between points. Numerical integration over a non-uniform grid that takes into account the uncertainties of each point can be done, but it still integrates a function that passes through outliers at the cost of increased complexity. Since the integral will be of a function passing through the outlying points, the result will have higher error, and will only be compensated for with a higher uncertainty, assuming the uncertainty of the outlying values are truly representative of their error.

The issues noted in the manuscript cannot be overcome using a simple numerical integration scheme. A simple numerical integration scheme will integrate the area exactly bounded by the data set, and requires a uniform spacing of data points.

Preventing an overshoot is done by dividing the retrieved  $T$  profile into four layers (troposphere, stratosphere, mesosphere, thermosphere) at each inversion point and not fitting a polynomial over the inversion points. We had larger problems with overshooting when interpolating the data to a 1-km grid when there were errors in tangent altitude.

C5466

This section deals with the sensitivity of the proposed retrieval scheme to employed a priori information. While it certainly argues that the available a priori information is likely sufficient (with some exceptions), it fails to quantify the reliance and thus the claim to be "minimal" with respect to a priori knowledge. For example, what effect does the a priori  $\text{CO}_2$  VMR profile has on the retrieved temperature profile? This could be quantified as a Jacobian  $dT_i/d\text{CO}_{2i}$  profile (neglecting the potential impact of different layers) or as an relative or absolute error for a prescribed perturbation. The same is true for temperature and pressure information.

Quantifying the dependence on a priori  $\text{CO}_2$  VMR is tricky because you do not know (and cannot know) the difference between the a priori or retrieved  $\text{CO}_2$  VMRs and the true  $\text{CO}_2$  VMR. We say that the quality of the a priori  $\text{CO}_2$  VMR has minimal impact, because GGG varies that quantity. While an a priori  $\text{CO}_2$  VMR close to the true state of the atmosphere is desirable, spectral fitting specifically assumes we do not know the true state of the atmosphere and needs to work regardless. When fitting spectra to determine the VMR of a target gas, there really should (not necessarily the practice) be no reliance on the a priori (see page 10840, lines 9–20).

Another issue with quantifying the retrieval uncertainty is the small number of occultations analyzed. This would be a long-term project for when this algorithm is used as the primary retrieval scheme for a live mission. The method is mainly sensitive to two things: a  $\text{CO}_2$  feature was not fitted very well, and our assumption that  $I = I'$  is wrong; or the a priori are wrong, so we cannot compute  $T$  and  $P$  from the slope and intercept of a  $\ln(VSF)$  vs.  $E''$  relationship. In the first case, we want to know why the fit was bad. Most likely, the feature is not well resolved among interfering lines or noise, or the absorption is too strong. It could also be because of the a priori. We assume  $T$ ,  $P$ , and  $z$  are accurate, and vary only  $\text{CO}_2$  to fit the line, which is why retrieving those

C5467

quantities is critically important. In the second case, we currently rely on statistics to do our best - an occultation has 30 to 100 spectra, we observe 10 CO<sub>2</sub> vibrational-bands, each with 30 to 40 microwindows, so a temperature retrieval uses 9,000 to 40,000 fits, far too many to evaluate by hand, especially when an occultation takes place every 90 minutes. The manuscript suggests future steps that can be taken to improve this on page 10842, lines 5–7.

On the other hand, the quantity  $\chi/\chi'$  is assumed to be close to 1 when used to compute pressure. The impact of a bad CO<sub>2</sub> a priori is very easy to see, provided you know the true CO<sub>2</sub> a priori. CO<sub>2</sub> is used because it is a major species with strong absorption features, and its VMR and vertical profiles are well known. For retrievals on Earth, we assume  $\chi \approx \chi'$  up to around 75 km. The ACE-FTS temperature retrievals, developed for over ten years, have very specific ways to deal with different regions of the atmosphere where our assumption break down. For Mars, we have a lot less certainty about the shape of the CO<sub>2</sub> profile and at what altitude it falls off. Producing a priori CO<sub>2</sub> VMR profiles for Mars, understanding how far they deviate from the true CO<sub>2</sub> VMR vertical profile, and what impact that has on real Mars retrievals is future work for when, and if, this instrument has another chance.

**Page 10840, line 1ff, continued**

Further, the text notes that a temperature profile deviation of more than 10 K would seriously degrade the quality of the final temperature product. For altitudes from the upper stratosphere upwards, this would be worrying on Earth (a worrying that seems to be justified as for some profiles, where the a priori profile differed by 30 K from the ACE-FTS result, which consequently could not be reproduced by the new scheme). How does this relate to expected temperature uncertainties on Mars, which most readers (as am I) are probably not an expert in?

C5468

This is an exceptionally large worry for Earth and Mars. However, there are other assumptions that we make that have a larger impact. One thing we focused on in this paper was retrievals at Earth, where we understand our assumptions best, and where we are actually qualifying our retrievals. On Earth, we have very accurate temperature a priori up to 60 or 70 km, because of the complexity of models and extent of our observing network. Above 70 km, we expect to have differences in our a priori temperature greater than 10 K, and our retrievals there become more dubious. Above 70 km, three other things occur: the CO<sub>2</sub> VMR begins to fall off and our assumption that  $\chi \approx \chi'$  is no longer valid, CO<sub>2</sub> absorption weakens and our assumption that  $I \approx I'$  breaks down, the atmosphere is no longer in local thermodynamic equilibrium and Boltzmann statistics can no longer be used to define temperatures. While these are touched on on page 10842, lines 1–2, and page 10832, lines 17–19, they are not explicit and out of context, so we have added the line:

At Earth, a priori errors on the order of 10 K are expected to occur only at very high altitudes, above 70 km. At such altitudes, the retrieval algorithm presented is impacted by weaker absorption by CO<sub>2</sub> as density decreases, loss of accuracy in the a priori CO<sub>2</sub> VMR as it falls off, and the departure from local thermodynamic equilibrium.

at page 10841, line 15.

While ACE-FTS can technically produce vertical profiles from < 5 km to 150 km, it has a “sweet spot” for trace gas retrievals. Below  $\approx 10$  km there are problems with strong refraction, total absorption within microwindows, strong inter-species interference, and clouds. Above  $\approx 80$  km, it runs into the same issues mentioned above. For Mars, we are not ready to make any statements about the quality of retrievals at different altitudes. We presume that refraction and clouds at low altitudes will allow lower altitude retrievals, we also presume the assumption of local thermodynamic equilibrium will break down at a lower altitude and that absorption by all gases will be weaker than for

C5469

Earth at all altitudes.

As an aside, judging the quality of these retrievals at high altitudes the difference from ACE-FTS retrievals assumes that those from ACE-FTS represent the true state of the atmosphere, when they face the same problems as this method. ACE-FTS temperature retrievals do not have associated uncertainties.

**Page 10840, line 1ff, continued**

As the method is in effect a kind of linearization around the a priori  $\text{CO}_2$ /temperature/pressure profile, could it not be employed iteratively; that is use the derived  $T/P$  profile as “a priori” and repeat the process? In fact, Stiller et al. used this to reduce the impact of a priori and applied some damping factor for the iterative updates to compensate for over-correction. Did you follow such experiments, especially with the aspect of reducing the impact of required a priori information? One might combine this with a trust region-like approach that'd limit the amount of temperature correction to the 10K where the linearization seems to hold up quite well.

It can be, and we tried this. We never saw that it improved the retrievals though. There are dangers with an iterative approach, and we mention these on page 10833, lines 20-23 with regards to tangent altitude retrievals. In theory, a first pass may underestimate the temperature, a later pass may overestimate it, and so on, hopefully converging. However, convergence is not guaranteed, and too many iterations tended to introduce oscillations in the temperature profile, especially above 70 km, where our assumptions break down. The tangent altitude retrieval was shown to need a few iterations, and converged rapidly. Temperature retrievals between 10 and 60 km or so only needed a single iteration to produce an accurate profile, and further iterations would actually degrade the accuracy about 60 km in some cases. A brief description of this experience has been added:

C5470

After a vertical profile for  $T$  and  $P$  has been found, the method can be applied iteratively, using the retrieved vertical profiles as refined a priori. This was originally done by *Stiller (1995)* for ATMOS. While there can be convergence issues with an iterative approach, as noted in Section 2.2, it may be used for a MATMOS-like mission. The ACE-FTS retrievals presented here were not done iteratively because of the high-quality of the a priori. Iterating the retrieval too many times for ACE-FTS tended to introduce oscillations in the temperature profile, especially above 70 km, where our assumptions break down. For Mars, where the a priori will be less accurate, iterating the temperature retrieval may be beneficial.

Lastly, many of the given arguments for the increasing quality of Martian a priori information could also be brought forward to justify the use of the ACE-FTS retrieval scheme. At which point is the proposed scheme more robust?

This is true. There were several reasons the ACE-FTS retrieval scheme was not going to be used, at least for the first version of the MATMOS data product. All of the a priori information that goes into the ACE-FTS retrieval can be eventually developed for Mars, and has changed over time for the ACE-FTS algorithm. Please refer to page 10829, line 14. Practically, the ACE-FTS personnel working on temperature retrievals would not be working on MATMOS, and adapting the ACE-FTS to work at Mars would require a similar amount of effort as adapting GGG to retrieve temperature.

C5471

### 1.3 Minor Remarks

#### Page 10828, line 28f

Fixing parameters makes the retrieval simpler, obviously. But I do not understand the notion that fixing parameters is “advantageous since gas absorption coefficients depend on  $T$  and  $P$ ”. I assume that some elaboration would be helpful in respect to what is going to be fixed and what the added advantages are beyond making the originally ill-posed problem well-posed.

If we allowed  $T$  and  $P$  to vary, then for every calculation we would need new gas absorption coefficients, then new line shapes. It is just that they are the component of the spectral calculation that would require the most complexity and computation.

#### Page 10830, line 3

I assume that 129 profiles of spectra were analyzed?

This is an error, thank you. There are 129 *occultations*, and each occultation will have 30–100 spectra recorded at tangent altitudes between 5–170 km. Changed page 10830, line 3 to:

A set of 129 occultations recorded by ACE-FTS, representing different latitudes and seasons, were analyzed; they are discussed in Sec. 3.2 and results are shown in Sec. 3.3. Each ACE-FTS occultation is a series of 30–130 (mean 53) spectra recorded at tangent altitudes between 5 and 150 km.

C5472

#### Page 10834, line 19

What kind of a priori information is entered here for the retrieval of  $\text{CO}_2$  with respect to  $\text{CO}_2$ ? Is optimal estimation used or some kind of Tikhonov-regularisation?

We are using the TCCON a priori for gas VMRs (Wunch et al., 2011), and we specify this later, while discussing the steps in detail, on page 10836, lines 14–16. Optimal estimation is not used because we have measurements throughout the altitude range.

#### Page 10834, line 21

VSF looks like an acronym, but was not introduced.

Yes it is, and it is now expanded at this point. VSF stands for VMR scaling factor.

#### Page 10835, line 14

It would be clearer to introduce  $I'$  here as  $I'(\tilde{\nu})/I'_o(\tilde{n}u)$ .

We believe you are referring to the placement of the prime symbols, which we had placed outside the parenthesis as:  $[I(\tilde{\nu})/I_o(\tilde{\nu})]'$ . This was done because we hadn't explicitly stated what the prime notation was used for. That is no longer that case, and we agree with you about clarity either way and have made the change.

#### Page 10835, line 16

$I$  and  $I'$  as defined in (1) are not defined on a layer, however, part the sum contained in (1) are, which is probably meant here, but not stated. The

C5473

easiest remedy would be the definition of some variable with an underbrace or similar for the term in between [ and ] in (1).

Added “where the sum is of contributions from each layer of the atmosphere the solar ray passes through,  $i$  is the atmospheric layer...” Note that the current manuscript has “where  $i$  is the optical layer,” which was misleading.

**Page 10835, line 18f**

Dropping the subscripts may enhance the brevity, but not the clarity. While  $\chi'_i$  was a discrete variable previously, it is unclear in what fashion it is used in Eq. (3) where a continuous function in  $s$  is suggested.

As part of addressing the Specific Comments, subscripts have been re-introduced, and the section has been reorganized. Eq. (3) is a continuous integral rather than a discrete sum because we do not compute the total column to obtain the VSF.  $\chi'$  now has a subscript  $j$  denoting it refers to a specific atmospheric layer (it is a function of  $z$ ).

**Page 10836, Eq. (5)**

The physical constants  $h$  and  $c$  are missing. Or simply  $c_2$  could be used.

Fixed, thank you.

**Page 10836, lines 14ff**

The description now mingles the planetary-body agnostic algorithm and the implementation and data used for the tests using ACE-FTS data. It might become more readable with a separation of method and application.  
C5474

This is a description of the method as implemented. A priori for MATMOS are discussed on page 10841, line 1.

**Page 10836, line 17**

It is rather confusing to reuse  $\chi_i$  here for the true CO<sub>2</sub> profile.

All non-primed quantities are defined as the true quantities. A priori quantities, and those computed from them are given primes, the retrieved VMR is  $VSF\chi'$  (although not a true retrieval, since we treat  $T$  and  $P$  as unknown quantities at this time).

**Page 10837, line 1**

“and a th” → “and th”

Fixed, thank you.

**Page 10837, line 10**

What kind of uncertainties are used here? Noise error, or also systematic errors due to background gases?

They are the uncertainty in the fit, the variances that come out of a weighted non-linear least squares Levenberg-Marquart minimization routine. That the fitting is least squares is noted on page 10837, line 9.

**Page 10837, line 12**

What is  $T$  and what is  $\Delta T$ ? You state that you derive one temperature  $T_j$  for each line  $j$ . Is  $\Delta T_j = T_j - T'$ ?

C5475



$T$  is a temperature value computed from Eq. (5) for one band at a given altitude and  $\delta T$  is its uncertainty. Clarified by changing the sentence to: “At a given altitude, temperature,  $T$ , pressure,  $P$ , and their uncertainties,  $\delta T$  and  $\delta P$ , are computed for each band...”

**Page 10838, line 25**

I do not see how keeping  $M$  and  $g$  constant keeps this more adaptable to other planets than allowing a variation in latitude and altitude for either variable. Obviously it is the simplest solution. To keep it adaptable but more correct, it could be simply implemented as a table to be read in, while an analytical formula would naturally be preferable.

It is not the best, but the simplest at this time. Currently, we don't have reliable substitutes for another planet. The MSIS model, which gives  $M$  as a function of altitude is not developed for Mars, and the gravitational function used was empirically determined for Earth. Essentially, we do not currently have access to an accurate global table of such values for Mars.

**Page 10840, line 20**

Why should the VSF of CO<sub>2</sub> not be unity? Isn't it mostly in the vicinity of unity, especially, if the a priori temperature and pressure are good?

We simply presume the fit using unmodified a priori will not be exact because there is some uncertainty on the CO<sub>2</sub> a priori and tangent altitude, and, more importantly, we have not yet retrieved  $T$  and  $P$ .

C5476

**Page 10845, line 15**

Why was this interpolation scheme chosen, especially in contrast to the perhaps more common four-point cubic spline? Is this consistent with the interpolation scheme that underlies the radiative transfer model?

In early versions of the retrieval, our retrieved tangent altitudes had some errors which resulted in adjacent observations being too close together, or even out of order vertically. Interpolation in these cases sometimes resulted in large, unphysical “bulges” in the vertical profile. In an attempt to prevent these from occurring, we tried a few other interpolation approaches, and the three-point method performed slightly better than others, as measured by the magnitude of the standard deviation of the mean difference between our retrieved temperature and those from ACE-FTS. This is also similar to what ACE-FTS uses in Boone et al. (2005). We discuss the tangent altitude retrievals on page 10833, Sec. 2.2, but they are not the focus of this paper.

## **2 List of Changes**

Page and line numbers refer to the AMT Discussions paper.

- Page 10830, line 3: changed “129 spectra” to “129 occultations.”
- Page 10830, line 4: added the sentence: “Each ACE-FTS occultation is a series of 30–130 (mean 53) spectra recorded at tangent altitudes between 5 and 15 km.”
- Page 10834, line 19 to page 10836, line 6: significant revision, see above. New text reads as:

C5477

1. Spectral fitting of CO<sub>2</sub> lines is performed for ten CO<sub>2</sub> vibration-rotation bands with around 40 lines each.
2. Data quality criteria are imposed on resulting VMR scale factors (VSFs).
3. Temperature and pressure are computed for each band at each altitude.
4. Weighted means of  $T$  and  $P$  are calculated for each altitude to produce vertical profiles of  $T$  and  $P$ .
5. The altitude with the highest quality pressure retrieval is estimated.
6. The vertical profile of temperature is integrated above and below the altitude with the highest quality pressure retrieval.
7. A vertical profile of pressure is computed using the equation of hydrostatic equilibrium.

When GGG fits a computed spectrum to a measured spectrum over a spectral window, it varies the VMR of the target gases until a best fit is achieved. The result is the VSF for each target gas at each altitude, defined for some target gas, by the equation:

$$Column = VSF \int \chi' n_a ds, \quad (4)$$

where the left-hand side is the total column of the target gas along the slant path through the atmosphere, between the sun and the instrument, taking into account bending due to refraction.  $\chi'$  is the VMR of the target gas, the prime notation indicates that it is an a priori quantity,  $n_a$  is the total number density, and  $s$  is the path variable. VSF is therefore the ratio between the true total column of gas, and that calculated by GGG. In solar occultation geometry, once fitting has been performed, and if the altitude, pressure, and temperature are correct,

C5478

then the slant paths of the actual column and the a priori column are the same. GGG divides the atmosphere into homogeneous layers, calculates the optical path for an observation, and accounts for the contributions from each layer. Therefore, the VSF is the ratio between a priori and true gas amounts averaged over the slant path, and we express the retrieved VMR as  $VSF\chi'$ .

For transmission spectra, we can describe the depth of an absorption feature with the Beer-Lambert law:

$$I(\tilde{\nu}) = I_o(\tilde{\nu}) \exp \left[ \sum_i -S(T_i) f(T_i, P_i, \tilde{\nu}) \chi_i (P_i/kT_i) l_i \right], \quad (5)$$

where the sum is of contributions from each layer of the atmosphere the solar ray passes through,  $i$  is an atmospheric layer,  $I(\tilde{\nu})$  is the transmitted intensity at wavenumber  $\tilde{\nu}$ ,  $I_o(\tilde{\nu})$  is the incident intensity,  $S(T_i)$  is the temperature-dependent line strength defined in ?,  $f(T_i, P_i, \tilde{\nu})$  is the line shape function,  $k$  is the Boltzmann constant, and  $l_i$  is the optical path length. After fitting, we assume that the measured transmittance,  $I(\tilde{\nu})/I_o(\tilde{\nu})$ , is equal to the calculated transmittance,  $I'(\tilde{\nu})/I'_o(\tilde{\nu})$ , computed by GGG using a priori quantities and the VSF. We also assume that the line shape function, optical path length, and incident intensity for  $I(\tilde{\nu})$  and  $I'(\tilde{\nu})$  are equivalent ( $f_i \equiv f'_i$ ,  $l_i \equiv l'_i$ ,  $I_o(\tilde{\nu}) \equiv I'_o(\tilde{\nu})$ ). We further simplify the expression for  $I(\tilde{\nu}) = I'(\tilde{\nu})$  by assuming GGG has already accounted for the contributions from each layer  $i$  and obtain an expression for the retrieved VMR,  $VSF\chi'$ , at the altitude of the observation:

$$VSF_j \chi'_j = \frac{S(T_j)}{S(T'_j)} \chi_j \frac{P_j T'_j}{P'_j T_j}, \quad (6)$$

where  $j$  represents the altitude of the tangent point of the optical path for an observation.

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The ratio of line strengths is:

- Page 10836, Eq. (5): changed  $E''$  to  $hcE''$ .
- Page 10837, lines 12–14: changed to “. . . unsuitable for retrieving temperature at each altitude. At a given altitude, temperature,  $T$ , pressure,  $P$ , and their uncertainties,  $\delta T$  and  $\delta P$ , are computed for each band and then a data quality filter is applied to  $T$  values from each band. . .”
- Page 10841, line 21: added the sentence: “At Earth, a priori errors on the order of 10 K are expected to occur only at very high altitudes, above 70 km. At such altitudes, the retrieval algorithm presented is impacted by weaker absorption by  $\text{CO}_2$  as density decreases, loss of accuracy in the a priori  $\text{CO}_2$  VMR as it falls off, and the departure from local thermodynamic equilibrium.”
- Page 10837, line 21: added the paragraph: “After a vertical profile for  $T$  and  $P$  has been found, the method can be applied iteratively, using the retrieved vertical profiles as refined a priori. This was originally done by *Stiller (1995)* for ATMOS. While there can be convergence issues with an iterative approach, as noted in Section 2.2, it may be used for a MATMOS-like mission. The ACE-FTS retrievals presented here were not done iteratively because of the high-quality of the a priori. Iterating the retrieval too many times for ACE-FTS tended to introduce oscillations in the temperature profile, especially above 70 km, where our assumptions break down. For Mars, where the a priori will be less accurate, iterating the temperature retrieval may be beneficial.”

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Interactive comment on Atmos. Meas. Tech. Discuss., 8, 10823, 2015.