Comment on amt-2022-44 "Impact of instrumental line shape characterisation on ozone monitoring by FTIR spectrometry" by Omaira E. García et al.

Anonymous Referee #2

Please find below the response to Referee #2's comments (in bold her/his comments and in italic the authors' replies).

General comments

The work by Garcia et al. focus on the impact of the instrumenta line shape of the high resolution FTIR spectrometer on the retrieval of vertical ozone profiles. The authors evaluate ver systematically more than 8 retrieval steregies to use y estimate the instrumental lineshape and evaluate these strategies using the long term measurements of FTIR spectra together with measurements from Brewer and the frequent ozone soundings. These collocated measurements at the Izaña observatorio are an unique posibility to evaluate the different retrieval strategies with respect to the instrumenta line shape and to study the sensitivity of the ozone profile retrieval on the estimation of the ILS.

The optimization of retrieval strategies for vertical gas profiles and especially of ozone by a very focused study is going to improve this remote sensing method towards a more exact measuremet method which is an important step for measurements in the NDACC network. The work fits perfectly in the scope of AMT, the manuscript is well written and clear presented.

In my opinion the manuscript is ready and paper should be published as is.

Specific comments

1) I would recomend to include a headline like "relative difference" in table 1,3,4 and it would be helpfull to see in addition to the infromation with respect to the brewer column measurements, a relative diference between the retrieval sterategies, maybe with respect to the favourite retrieval sterategies of the authors. This would ilustrate clear how sensible the ozone profile depend on the retrieval sterategy with respect to the ILS.

Following the Referee's suggestion, the comparison between the retrieved O_3 products (total columns and profiles) from the ILS retrieval strategies has been included in Section 4. To do so, the following text, table and figure has been added.

The differences between the ILS treatments are transferred to the O_3 TCs and profiles as summarised in Table 1 and Figure 1, respectively. The set-ups not retrieving MEA information provides the largest bias with respect to the cell-derived ILS O_3 TCs (i.e. up to 0.3% for 5B/5C in the 2005-May 2008 period), whereas the most significant variability *is observed for the most refined ILS set-ups (i.e. up to 0.7% for 5F/5G in the 2005-May 2008 period). As expected, the simultaneous temperature retrieval strongly affects the differences between the ILS treatments due to the cross-interference between the ILS, and the O_3 and temperature profiles (especially beyond the lower stratosphere, as illustrated in Figure 1).*

Set-up	1999-2004 M[%], σ[%], R	2005-2008 M[%], σ[%],R	2008-2018 M[%], σ[%], R	1999-2018 M[%], σ[%], R
5B	0.13, 0.12, 1.000	0.27, 0.07, 1.000	0.11, 0.04, 1.000	0.12, 0.08, 1.000
5C	0.10, 0.13, 1.000	0.27, 0.07, 1.000	0.10, 0.04, 1.000	0.12, 0.08, 1.000
5D	-0.05, 0.47, 0.998	-0.01, 0.57, 0.994	0.01, 0.32, 0.999	0.01, 0.38, 0.998
5E	-0.08, 0.47, 0.998	-0.02, 0.59, 0.993	0.01, 0.32, 0.999	0.00, 0.38, 0.998
5F	0.00, 0.53, 0.998	-0.08, 0.70, 0.991	-0.16, 0.64, 0.993	-0.15, 0.64, 0.994
5G	-0.01, 0.53, 0.998	-0.08, 0.69, 0.991	-0.16, 0.64, 0.993	-0.15, 0.64, 0.993
5H	-0.06, 0.05, 1.000	-0.01, 0.01, 1.000	0.00, 0.01, 1.000	0.00, 0.03, 1.000
5BT	0.65, 0.59, 0.997	1.62, 0.39, 0.998	0.36, 0.17, 1.000	0.36, 0.17, 0.997
5CT	0.63, 0.62, 0.997	1.63, 0.40, 0.998	0.36, 0.17, 1.000	0.42, 0.49, 0.997
5DT	0.30, 1.88, 0.976	0.29, 1.82, 0.940	0.11, 0.85, 0.991	0.14, 1.16, 0.982
5ET	0.24, 1.87, 0.976	0.30, 1.74, 0.942	0.11, 0.89, 0.990	0.14, 1.17, 0.982
5FT	0.30, 1.87, 0.976	0.33, 1.65, 0.950	0.25, 1.09, 0.983	0.26, 1.28, 0.977
5GT	0.23, 1.85, 0.976	0.34, 1.76, 0.943	0.25, 1.10, 0.983	0.26, 1.30, 0.977
5HT	-0.18, 0.25, 1.000	0.00, 0.02, 1.000	0.02, 0.03, 1.000	0.01, 0.09, 1.000

Table 1. Summary of statistics for the O_3 TC comparison for the set-ups 5B/5BT, 5C/5CT, 5D/5DT, 5E/5ET, 5F/5FT, 5G/5GT, and 5H/5HT with respect to 5A/5AT: median (M, in %) and standard deviation (σ, in %) of the relative differences (RD, 5X/5XT - 5A/5AT), and Pearson correlation coefficient (R) for the periods 1999-2004, 2005-May 2008 and June 2008-2018, and for the entire time series (1999-2018). The number of quality-filtered measurements is 466, 683, and 3775 for the three periods, respectively, and 4924 for the whole dataset.

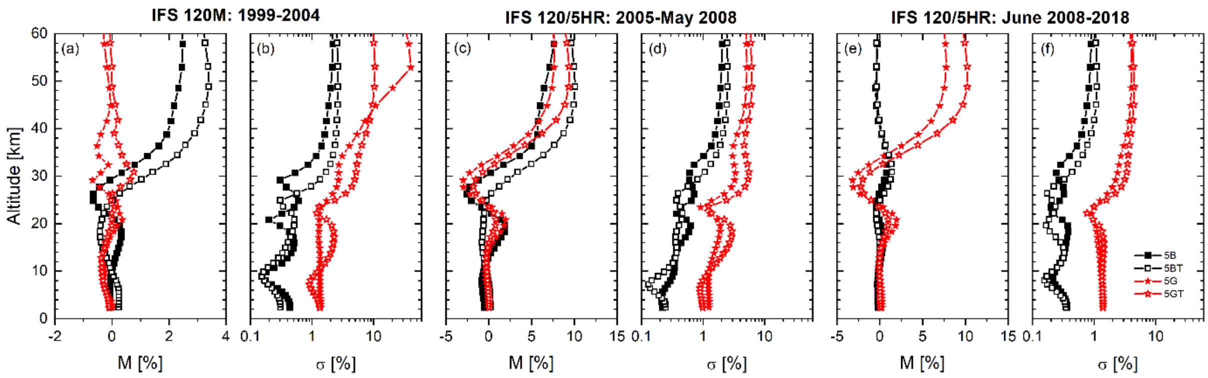

Figure 1. Summary of the O_3 profile comparison for the set-ups 5B/5BT, and 5G/5GT with respect to 5A/5AT for the periods 1999-2004, 2005-May 2008 and June 2008-2018, and for the entire time series (1999-2018). (a), (c), and (e) display the vertical profiles of the median (M) RD (5X/5XT - 5A/5AT, in %) for the three periods, respectively. (b), (d), and (f) same as (a), (c), and (e), but for the standard deviation of RD distributions (σ, in %).

Regarding including the headline of "relative difference" in the tables that summarise the total columns and profiles comparisons, this information is already mentioned in the table captions. In addition, these tables include information not only referred to the relative differences (i.e. Pearson correlation values). Therefore, we would like to keep the table captions as they are to avoid readears to get confused with the information contained.

2) I would recomend to include a little more basic information about the modulation eficiency and the phase error in the begining of the section 3.1, so that the reader get the important information which and how the ILS depends on both parameters without consulting the cited papers.

Following the Referee's suggestion, the following information has been added to Section 3.1:

The ILS function is the Fourier transform of the weighting applied to the interferogram (Davis et al., 2001). In the case of ideal instruments, the ILS is affected only by modulation loss that is due to the self-apodization of the interferometer, accepting a finite field of view, and is symmetric (Hase et al., 1999). For real instruments, the ILS also accounts for misalignments and optical aberrations of the spectrometer and is equivalent to a complex modulation efficiency (ME) in the interferogram. The phase corrected interferogram generated by a spectral line is of the form (Hase et al., 1999):

$IFG(\delta) \sim MEA(\delta) \cdot cos(2\pi\sigma - PE(\delta))$

where $IFG(\delta)$ is the interferogram (with δ as the mirror displacement), σ is the wavenumber, MEA is the modulation efficiency amplitude, and PE is the modulation efficiency phase error.

The MEA and PE are parameters describing the deviations from the expected nominal ILS. Because the measurement process of an FTIR spectrometer is performed in the interferogram domain, this parameterisation refers to the interferogram, LINEFIT uses 20 equidistant grid points up to OPDmax and assumes a smooth variation of MEA and PE along OPD. MEA (normalized to unity at zero path difference, ZPD) is a measure of ILS width, and a decline of MEA towards indicates a broader ILS, while a rise indicates a narrower ILS with stronger sidelobes. A curving PE indicates ILS asymmetry (while a linear rise is equivalent to a spectral shift of the ILS, but does not a distortion of its shape). From the physical viewpoint, interferometric misalignments, deviations from the aspired circular interferometric field-of-view, OPD-dependent vignetting effects, and mismatch between the wavefronts of the reference laser wavefront and the infrared beam are main drivers of ILS imperfections.

Davis, S.P.; Abrams, M.C.; Brault, J.W. Fourier Transform Spectrometry; Academic Press: Cambridge, MA, USA, ISBN 0-12-042510-6, 2001.

3) It is very interessting that the authors recomend to fit the pase error at ZPD, but use the modulation efficiemncy from the cell measurements. It would be very nice if the authors might try to give a possible physical explanation, why a fit of the "pase error" at ZPD from an individual spectrum imporves the retrieval? Does it depend on alignment the temperature of the beamsplitter the phasecorrection duringt the calculation of the spectrum?

This is an interesting question. Ideally, the phase correction should guarantee zero PE at ZPD. However, this phase information is effectively deduced from a rather small number of interferogram points in the centerburst, so there is noise superimposed on the phase spectrum. This problem has been highlighted by the late Luc Delbouille, who suggested to do repeated measurements of the centerburst between the full-resolution scans and use this low-noise phase spectrum for the phase correction [L. Delbouille, priv. comm.]. So far, such schemes have not been realized for operational NDACC work. Besides, as the referee suggests, we cannot rule out the existence of other effects distorting the phase spectrum, as the laser does not use the full beam diameter of the infrared beam and the resulting wavefront errors might depend on temperature (e.g. slight deformations of the cubecorner mirrors).