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 #1

Please find below the response to Referee #1’s comments (in bold her/his comments and in italic the authors’ replies).

General comments

The IRWG of NDACC is an international network bringing together more than 20 observational FTIR sites over the world since the 1990s. In comparison to other observational methods used for the investigation of gaseous composition of the atmosphere, FTIR spectrometry provides a unique advantage of simultaneous measurements of the total columns (or even profiles) of a number of climatically active gases. The significant efforts are being made by the IRWG community to develop the unified retrieval strategies for deriving total columns/profiles of atmospheric species including O₃. The main target of these efforts is verifying and harmonizing the results obtained by different groups operating FTIR sites. To get reliable information on O₃ trends in the stratosphere which are currently nearly zero, it is necessary to provide the FTIR products of high accuracy and precision. Achieving this goal requires knowledge of the parameters characterizing the alignment of FTIR spectrometer (instrumental line shape function, ILS) and correct accounting of ILS in the retrieval procedure. Paper by García et al. is devoted to the detailed study of the influence of several ILS approaches (used in the procedure of inverse problem solving) on the O₃ retrieval results (focusing the stratosphere). FTIR instruments having different alignment status are considered.

The manuscript corresponds to the AMT main subject areas and can be recommended for publication (minor revision is required) after a few points are addressed (please, see specific comments section)

Specific comments

1) Results presented in Appendix B deserve to be moved to the main text of the paper as a separate section. But the final decision is up to the authors.

Appendix B aims to document how alternative approaches to evaluate the Instrumental Line Shape (ILS) function from atmospheric trace gas retrievals with well-known vertical distribution (i.e. carbon dioxide, CO₂, and hydrogen fluoride, HF), as suggested by previous works, are not precise enough to evaluate ozone (O₃) retrievals. Both strategies are found to produce unrealistic ILS estimates, therefore these approaches were not included in the main study. We would like to thank the referee for pointing this out. However, we would like to keep these findings in a separate Appendix to allow readers to be focused on the final ILS strategies presented and tested in this work.
2) Authors tested several approaches of ILS for the getting best retrieval results on O3. Is there a “universal” recipe for the processing FTIR observations (for example, archive spectra) in the absence of information on instrument alignment (ILS function)? Is it correct that in the case of the ideal ILS function should be used for overall spectra processing? Is it possible to create a homogeneous O3 row by stitching separate O3 time series obtained as a result of processing FTIR spectra using different ILS approaches? Analysing such a complex time series can be an additional challenge to reveal long-term O3 trends close to zero.

One of the main motivation of this work is indeed that there is no a universal or standard approach to evaluate the ILS function of ground-based FTIR instruments. In this context, this study pretends to assess the impact of the existing ILS treatments within the NDACC FTIR community on the FTIR O3 products, as an exemplary case.

Nevertheless, we believe that the provision of a "universal" optimized recipe would be difficult. The history of site operation as quality of the spectrometer, availability of cell measurements, etc. will in general suggest different specific strategies for achieving the best data product. Although not fully satisfactory from the viewpoint of network traceability, the construction of appropriate schemes will certainly involve considerable amount of operator knowledge, so even if spectra would be archived, important auxiliary information would probably not be forwarded and might be finally lost. Whether an ideal ILS should be assumed also needs to be decided by the site operator, as this will depend on specific factors.

The results of the current work point to the optimal approach to deal with the FTIR instrumental characterisation is the continuous monitoring of the ILS function by means of independent data, such as the low-pressure N2O-cell measurements. Nonetheless, if independent information on the instrument alignment is not available, an intermediate approach could be the simultaneous ILS retrieval together with the atmospheric temperature profile fit. The combined (ILS, O3 and temperature) approach is found to be superior with respect to assuming an ideal ILS function. It improves the precision of the FTIR O3 retrievals as well as reduces the cross-interference between the atmospheric temperature and instrumental performance for the IFS 120/5HR spectrometers. For more unstable instruments, such as the IFS 120M, the temperature retrieval exhibits a drastic negative impact on O3 products even though the ILS fit is simultaneously performed.

Therefore, the strategy of TCCON to use HCl cells in the solar beam for achieving a complete documentation of the ILS performance is a step ahead (NDACC might in future achieve a similar ILS monitoring at least for the InSb detector by using HBr cells).

Regarding the strategy of combining O3 retrievals from different ILS approaches, we fully agree to the referee that this is a challenging task. Nevertheless, stitching the full time series together using different approaches might be unavoidable and without alternative, as we typically face technical progress on the instrumentation and ILS monitoring procedures over the years. It would be good to include such information on sub-periods in the metadata.
3) It is not quite clear whether the AVKs (averaging kernels) were taken into account when comparing the O₃ results obtained by the FTIR and Brewer techniques?

The Brewer technique only provides O₃ amounts in the integrated total column and, so far authors know, information about vertical sensitivity is not available. Therefore, the Brewer and FTIR observations are straightforwardly compared without taking the FTIR vertical sensitivity (i.e. retrieved averaging kernels) into account.