Authors' Response
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First of all, we would like to emphasize that we are grateful to the GI(D) journal for considering our work and allowing us to express our views. Many thanks to the referees for the time spent on reading and commenting the manuscript. In the following sections, all responses and reasoning will be presented. If the Editor would encourage submission of a revised manuscript, we will incorporate the corresponding comments and suggestions into the revised manuscript that will hopefully address the concerns in the reviews, to which we detail our responses below. The reviewer comments are in sans-serif and our responses are in normal type.

1 Anonymous Referee #4

- Summary and Comments: The paper by Xu et al. is a sensitivity study of the OH retrieval from TELIS data using the PILS retrieval code. The inversion methodology, the software used, the instrument and channels used for the observations are presented. Then, a study of the sensitivity of the inversion to the different sources of error (instrumental and physical – temperature and density profiles) is performed. Finally, this work studies the advantages of using a multi-band inversion scheme for HCl, and studies its sensitivity, showing improvements over older techniques. This paper is a clear explanation of the model and the inversion/sensitivity study scheme used for this instrument. It gives an explanation of the different sources of uncertainties that need to be studied in such observations. However, the reader should be aware that, in more general cases, the physical uncertainties (uncertainty in the molecular energy levels) can also have an important contribution. Based on these observations, I recommend this paper for publication in GI.

  We appreciate the referee's summary and general comments. Energy levels and transition frequency/wavenumber (essentially $\hat{\nu} \propto \Delta E$) are known with an accuracy in the kHz range, and therefore are not relevant for the error budget in this study.

- Detailed comments: p 252 L 22: "emission observations are independent of sunlight" should be replaced by "the considered emissions observations are independent of sunlight". (Since this is not true when NLTE emissions are considered).

  Corrected.

2 Anonymous Referee #5

Clearly, we regret the referee's recommendation to reject the manuscript. We sincerely appreciate many concerns raised by the referee and are confident that in a revised manuscript a more thorough discussion of, e.g. pointing errors and retrieval, will clarify the issues and clearly improve the manuscript (see details below). However, we strongly feel that some of the referee's statements violate the *General Obligations for Referees* and are not appropriate for an *objective judgment of the quality of the manuscript.* An "advice" such as "kill your darlings" is in our opinion in conflict with the *respect the intellectual independence of the authors* obligation and reminds of the Inquisition where heretics were executed. The insinuation of "deliberately ignored efforts by others" is not explained and therefore in contradiction to *Any statement that an observation, derivation, or argument had been previously reported should be accompanied by the relevant citation.*

2.1 General comments

- The title sets up a clear aim, but the manuscript fails to reach it. In fact, I found the discrepancy between aim and the actual content of the manuscript so high that I must suggest to reject the paper. This in contradiction to the other open review here at GID by "Anonymous Referee #4". However, I agree with this referee in that Discussions the actual work done is nicely presented, it is just that I don't find it relevant for the stated aim. In the initial review phase (where I did not participated), Anonymous Referee 3 expressed basically the same criticism as I will do here. The authors wrote a long answer to Referee #3 but did not much to actually fix the problems raised.

  We firmly believe that our paper is still a valuable study for the TELIS 1.8 THz channel which has not been done by anyone else. Furthermore, the referee mentioned the questions raised by Referee #3 in the initial review. In fact, the title was modified and all technical corrections were made according to his suggestions after the initial review. We have also stated the reasons why this sensitivity study based on synthetic data is necessary. In response to the rating for scientific and technical significance, we have listed the novel and unique aspects of our work in our previous response letter. We will revise the conclusions in the manuscript by taking these aspects better into account.

- If I should try to summarise my criticism, I see two main points:
  1. The work seems to have been performed in "isolation", or efforts by others are ignored deliberately. Examples are given below. I don't say that this sensitivity study must be performed following exactly the pattern of all earlier similar studies, new approaches shall of course be investigated, but if related work is ignored it is not possible to judge the merits of a possibly alternative approach.

  We acknowledge the referee's point, but respectfully disagree for the following reasons. We have to clarify that we are NOT working in isolation. Our team is part of the TELIS project team, which in turn is part of the TELIS/MIPAS-B balloon campaign team. Accordingly we regularly attended the project meetings and presented/discussed our retrieval methodology and results. Moreover, as indicated in the original manuscript, we contributed to the SMILES ozone validation (Kasai et al., 2013) and are currently also involved in the validation of further SMILES products (e.g. HCl). A study of first intercomparison results of HCl between TELIS-THz and SMILES can be found in Xu et al. (2013a).

  Efforts by others are NOT ignored deliberately as well. There are 49 references (although we do not consider the number alone as a quality criterion), and we might have "forgotten" an important feasibility study (although to the best of our knowledge there is no study on OH retrievals from the 1.8 THz complex). In this paper, we try to analyze the error sources from instrumental and atmospheric point of view which could be dominant in far infrared (FIR) and submillimeter limb sounding measurements, especially in view of the real TELIS measurements. In case of the 480–650 GHz channel, the sensitivity paper by de Lange et al. (2009) studied the influence of major instrumental parameters on the retrieval of isotopic water profiles. Furthermore, de Lange et al. (2012) stated that nonlinearities in the calibration procedure that have been found in both channels, can bring about major effect on the retrieval. Both papers have been cited in our manuscript and to our best understanding these two papers are the most related studies. Nevertheless, we have cited similar studies for IR and submillimeter limb sounding, such as Baron et al. (2011) for SMILES, Urban et al. (2005) for Odin/SMR. Carli et al. (1989); Carlotti et al. (2001); Jucks et al. (1998); Pickett and Peterson (1993); Minschwaner et al. (2011) for OH FIR observations have also been included. Certainly, some papers could be missing, and we will consider to add a few more references (Carli et al., 2007; Pickett and Peterson, 1996; Takahashi et al., 2010) to the revised manuscript, but we did not aim for a review with a *complete* literature list.

- 2. Advantages of Tikhonov regularisation over "OEM" is a popular topic for at least one of the co-authors. Here I give the advice to "kill your darlings". This topic is of no relevance for this study, and discussion of the topic is just distracting. If the choice of inversion method has an impact of a basic sensitivity study of this type, then one or both of the methods is used wrongly. To continue on point 2, it seems that the authors considers to find the lambda parameters as part of the sensitivity study and shows that this step is successfully performed by showing example retrievals. This part constitutes a large fraction of the manuscript, but I found it irrelevant. If there exists still an uncertainty in selecting lambda, this is in fact a reason to not use Tikhonov regularisation. There should be no doubt about that the actual inversions can be performed without problems, as much more complex retrievals are performed routinely (by eg. satellite limb sounding groups).

  Indeed, there are several papers discussing the pro's and con's of both approaches, e.g. in geophysics and seismology (Gouveia and Scales, 1997; Scales and Snieder, 1997). Admittedly, the Optimal Estimation Method (Bayes's theorem) is the prevailing approach used in atmospheric remote sensing, but this cannot be used to rule out other methods altogether. Accordingly, "empirical Bayesian methods" are used frequently in practice (Allmaras et al., 2013).

  In fact, Tikhonov regularization has gained increasing attention in recent years, e.g. Eriksson (2000); Hasekamp and Landgraf (2001), and more recently, Schepers et al. (2012) for analysis of spaceborne nadir IR spectra, von Clarmann et al. (2009) for analysis of MIPAS-Envisat limb emission measurements, and Landgraf and Hasekamp (2007) for ozone retrieval from the thermal IR (TIR) and ultraviolet (UV) combination using simulated measurements. Detailed discussions and comparisons of both methodologies in the context of ground-based FTIR measurements were given by, e.g. Hase et al. (2004); Senten et al. (2012). In a blind test retrieval experiment (AMIL2DA) for infrared limb emission spectrometry (von Clarmann et al., 2003) with retrieval codes from six European groups participating (including a predecessor of GARLIC-PILS), it was concluded that "…none of the regularization or discrete sampling approaches chosen by the participating groups significantly distorts the retrieval …".

  The goal of our work was and is not a comprehensive assessment of Tikhonov regularization and the Optimal Estimation Method, but rather the analysis of TELIS 1.8 THz channel measurements. To this end, an appropriate inversion approach has had to be chosen and the inversion performance should also be briefly discussed.

  From a mathematical point of view, we would like to extend the reasons for discussing Tikhonov regularization and iterative regularization methods with a variety of points:

  - The Optimal Estimation Method is the widely used inversion method in atmospheric remote sensing. The main problem of the Optimal Estimation Method is the selection of the a priori covariance matrix in order to guarantee small solution errors. In most studies, this choice is done empirically, without formulating an objective selection criterion for the solution error. The choice of the a priori covariance matrix is performed by analyzing the averaging kernel, the information content or the degree of freedom. These quantities reflect only some components of the solution error, e.g. the smoothing error or the noise error, and the main problem of balancing the smoothing error and the noise error is not addressed.

- If the a priori covariance matrix is factorized in a suitable manner, then the method of Tikhonov regularization is algebraically equivalent with the Optimal Estimation Method. In this case, the choice of the a priori covariance matrix reduces to the selection of the regularization parameter. The benefit of Tikhonov regularization is that a large class of regularization parameter choice methods can be used to compute the optimal value of the lambda parameter. This fact is well known by mathematicians but it is rarely known by the majority of scientists working in atmospheric remote sensing.
- The merit of our sensitivity analysis is that it introduces a rigorous procedure for selecting the regularization parameter. This selection criterion is based on the minimization of the solution error and can be recommended for atmospheric remote sensing.
- In our analysis we investigate two iterative regularization methods (the iteratively regularized Gauss-Newton method and the regularizing Levenberg-Marquardt method) together with Tikhonov regularization for solving nonlinear inverse problems. The iterative methods are new approaches; they are superior to the method of Tikhonov regularization because they are insensitive to overestimation of the regularization parameter, but they are inferior to the method of Tikhonov regularization from the point of view of computational speed.

In conclusion, our sensitivity study has a very important theoretical merit. It describes a correct regularization parameter choice method in the framework of Tikhonov regularization, and analyzes several regularization solvers for the retrieval problem under examination. In our opinion, this theoretical contribution cannot be ignored.

- Anyhow, to show "successful" single retrievals is still no prove on that the retrieval set-up is sane. To prove this, an ensemble of cases, spanning all real conditions, must be inverted and the statistics of the results be analysed.

  As we stated in the original manuscript, our data analysis operates in a semi-stochastic setting in contrast to most stochastic data models. Sect. 3.2 focuses the retrieval performance from spectra assuming a limb scan with worst signal-to-noise ratio, but otherwise perfect instrumental knowledge. This section aims to compare direct and iterative regularization methods, and to analyze the vertical sensitivity of OH without an accurate a priori knowledge of O_3 and H_2O. Then in Sect. 3.3, the influence of imperfect instrumental knowledge and atmospheric profile is studied by estimating the possible error source individually.

- Despite the above, the authors end up with an inversion set-up that is relatively simple, probably too simple. The inversions deal only with species abundances, while it is today standard to retrieve instrumental variables in parallel. For example, a simultaneous retrieval of a pointing correction is performed for all satellite limb sounders, and I don't see why not this methodology could be applied for here. This would result in a lower sensitivity to pointing uncertainties than estimated in the manuscript. In addition, if I understand it correctly, both OH and O3 have transitions in both sidebands, and this fact should make it possible to retrieve the sideband ratio. Hence, a more final retrieval set-up should be used/considered, to obtain more final estimates of retrieval errors.

Our objective was to study the feasibility to retrieve OH from 1.8 THz balloon-borne observations along with the dominant error sources. In Sect. 3.3 we estimate potential error sources which may be influential in the real data analysis and are suggested by de Lange et al. (2009, 2012). A *complete* analysis of *all* error sources, as for example provided for MIPAS-Envisat or SMILES (Stiller et al., 2002; Baron et al., 2011) space missions were beyond the scope of this study. In the sensitivity study for isotopic water profile retrievals from the TELIS GHz-channel de Lange et al. (2009) considered pointing, sideband ratio, local oscillator frequency, field-of-view, and instrumental line shape. Note that for the present feasibility study using synthetic spectra some instrument parameters were assumed to be known, whereas for analysis of real measurements some instrument parameters are included in the state vector to be fitted. All given uncertainties are based on the expertise from the TELIS instrument team. In contrast to the sensitivity study by de Lange et al. (2009), we have also modelled the TELIS calibration process and successfully analyzed the nonlinearity effect.

The retrieval of some instrumental parameters is considered by the authors for analysis of the real observations. However, according to the laboratory and in-flight measurements, the oxygen spectral microwindow in the 1.8 THz channel selected for the pointing and temperature retrieval showed extremely high noise temperatures, revealing that it can be very difficult to derive pointing and temperature profiles. Alternatively, for the analysis of observed spectra we rely on the MIPAS-B pointing information and temperature retrievals, as both instruments were installed on the same gondola during the flight, and the corresponding retrieval studies have been published in de Lange et al. (2012) and Kasai et al. (2013) in case of retrievals of HCl, ClO, and O_3. For the 1.8 THz channel the sideband ratio measurements vary from 0.95 to 1.05 and have been consolidated in the latest laboratory campaign. Hence uncertainty for the THz channel is much lower than that for the GHz channel (0.6–1.4). In our case, OH lies only in the upper sideband, and the information is insufficient so that the retrieval of the sideband ratio is not possible in the real data analysis, which was also noticed by de Lange et al. (2012) for HCl and ClO retrieval from the submillimeter measurements obtained by the 480–650 GHz channel.

- The option of a joint pointing retrieval is discussed at the end of Sec. 3.3.3, but the text does not reflect the general knowledge totally. The comments hint that it is possible to retrieve a pointing correction for each individual spectrum, but that should be a rare case. If the pointing must be fitted in this manner there exists so called "pointing jitter" and a substantial level of such jitter is known to "kill" useful retrievals (at least as long not oxygen is covered).

As already mentioned previously, the a priori pointing information is taken from the equipment installed on MIPAS-B and the accuracy is rather reliable (Friedl-Vallon et al., 2004). Similar studies (e.g. Baron et al. (2001)) suggest that pointing offset is not necessary to be retrieved in case of sufficient accuracy. Also, the pointing correction is correlated to the retrieval of instrument baseline offset and "greybody" profile (see also the response after next). de Lange et al. (2012) concluded that for the HCl retrievals from TELIS GHz-channel observations uncertainties due to pointing are less severe due to the high performance of the MIPAS-B attitude and heading reference system.

- Here I suggest the authors to take a closer look at similar work elsewhere, to get input for an improved study. Beside the actual inversion set-up, it should then be clear that it is standard to also consider other errors, maybe most notably spectroscopic errors. Such errors are fundamental for Sec. 4, treating multi-channel retrievals. If perfect spectroscopic information is assumed, then such retrievals seem to work very well, but in practice the situation is very different.

Consistent spectroscopic input data are well known to be a serious problem for synergistic retrievals exploiting infrared and ultra-violet observations, see e.g. (Flaud et al., 2006). As mentioned previously, Landgraf and Hasekamp (2007) analyzed joint retrievals for a combination of a TIR (TES or IASI like) instrument and UV (GOME and OMI type) instrument using simulated measurements, but they did not even discuss spectroscopy issues. On the other hand, Natraj et al. (2011) emphasized that "one important source of systematic error that will need to be addressed when combining TIR and UV spectral measurements is the current discrepancy between UV and TIR spectroscopic parameters." Regarding our synthetic measurements, the consistent spectroscopic information over two different spectral ranges is not an issue, as we only took line parameters from the HITRAN 2008 spectroscopic database. As checked in the HITRAN database, the spectroscopic information over 1.8 THz and 619 GHz ranges is consistent (Manfred Birk and Georg Wagner, personal communication, 2013). In support of the Microwave Limb Sounder Drouin (2004) has measured pressure-induced broadening and shift of the lowest rotational transition of hydrogen chloride (HCl) and confirmed "best agreement" with the transitions in the infrared fundamental vibrational transition (Pine and Looney, 1987). The consistency of the J=1-0 broadening data for pure rotation and fundamental is not surprising since the vibrational dependence of pressure broadening in case of simple diatomic molecules is expected to be small. It furthermore shows that systematic error sources are well controlled for both data sources. The results from the vibrational band can thus be used for all rotational transitions. Line strength uncertainties of 2% (as used by de Lange et al. (2012)) can be seen as a conservative estimate, as these values are very well determined from electric dipole moments.

- Maybe the most problematic part of microwave measurements is so called baseline distortions. This issue is not discussed at all. Neither how this can be handled by the retrievals and to what extent the real measurements are affected.

  Our retrieval code PILS can deal with the retrieval of instrument baseline offset. When dealing with the real measurement obtained by TELIS, not only the instrument baseline offset, but also the "greybody" profile accounting for the broad continuum-like contributions that are important for lower altitudes and not depicted by current continuum models (Woiwode et al., 2012; Castelli et al., 2013), should be retrieved. The retrieval of the baseline offset and the greybody profile has been implemented in the real TELIS data analysis (see also Kasai et al. (2013); Xu et al. (2013b,a)). A brief discussion related to the issues of baseline and "greybody" will be added into the manuscript.

- This brings us to the actual measurements. The manuscript gives the impression that this part of the TELIS observations has been totally ignored. I could not find a single reference to earlier studies dealing with these inversions. At least I found it hard to believe that this "channel" was included in TELIS without any inversion simulations during the design phase. I am not familiar with TELIS so I could be wrong, but then the lack of relevant citations shall be expressed clearly. In summary, older work should be acknowledged, and it should be discussed of these results are consistent with older ones.

  The synthetic measurements and uncertainties in error sources used for this study is actually based on TELIS characterizations, in-flight and laboratory measurements, including observing altitude, tangent spacing, FoV, and uncertainties in instrument parameters (e.g. hot load measurements, sideband ratios, pointing information, etc.). We have cited de Lange et al. (2009, 2012) with respect to the retrieval studies of the 480–650 GHz channel. But concerning the 1.8 THz channel, we are not aware of any retrieval study by others conducted for this channel. Moreover, the selection of the 1.8 THz channel for detecting OH was based on hardware considerations during the design phase, which has been stated in the original manuscript. For both channels the selection of error sources to be considered were defined in discussions with the instrument team.

2.2 Some other comments

- The estimation of smoothing error is not clear. I assume you use S_x-matrices as defined in Eq 4. Eq 4 corresponds to a 100% (1 sigma) natural variation of the gases. Do you really assume this high variability? And I don't find the values you apply for l_i and l_j.

  In this case, we set $l_i = l_j = 100\,\mathrm{km}$, so that $\mathbf{L} \approx \mathbf{L}_1$ with $\mathbf{L}_1$ being the discrete approximation to the first-order derivative operator. We will add the values in the revised manuscript.

- You end up with low values of lambda. In Sec 4 even lambda = 0 for O3. This means that you are close to, or actually doing, least squares. In this case, the level of regularisation is effectively implemented by the grid spacing. Are you using a too coarse grid, and the smoothing error could in fact be lower?

  Here we implemented the joint retrieval of OH and O_3 with the help of multi-parameter regularization scheme. The employed regularization scheme is the partial multi-parameter regularization to retrieve some components of the state vector, i.e. joint fit of main target HCl and one auxiliary molecule O_3 as a contamination. In this case, the ozone profile is not meant to be data product, but is simply included to improve the fit and the HCl profile. The result that we found is in agreement with a general recommendation concerning the regularization strength of auxiliary parameters: a small regularization parameter for O_3 implies that the joint retrieved O_3 profile is unrealistic, but the residual is small. The retrieval grid in our study is identical to the tangent spacing below the observer, which is not a coarse grid.

- Eq 9: This definition is only useful if the emission line covers only a single frequency channel. Anyhow, seems to a very indirect way to say that you set T_{sys} to 3800 K.

  $T_{\mathrm{sys}} = 3800\,\mathrm{K}$ is given by the instrument team and based on previous in-flight observations.

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