Dear Editor,
Dear Authors,

Please find attached my review report.

Best regards,
Matthias Schneider

General comment:

The manuscript presents HDO/H2O data obtained from the space-based sensor GOSAT. The authors describe the retrieval, perform error estimations, and compare the new product to HDO/H2O data obtained within the TCCON. The paper is well written and the topic is of great interest for atmospheric science, therefore it is well-suited for publication in AMT.
Atmospheric HDO/H2O is very difficult to measure. Concerning remote sensing techniques, HDO/H2O is a very complex product and an error study is very important. In this context, I very much acknowledge the efforts of the authors, however and at the same time, I would like to encourage them to further expand their GOSAT HDO/H2O uncertainty studies. In my opinion there are some aspects about the sensitivity of GOSAT with respect to the real atmospheric H2O and HDO variations that need further attention. Furthermore, I am not convinced by the empirical validation study that uses TCCON HDO/H2O data as a validation reference. I think that my concerns could be easily addressed by some few modification of the manuscript.

Major comments:

(1) I think that the response of the GOSAT retrieval on atmospheric H2O and HDO variations should be better documented:
In your current manuscript version you examine how uncertainties in the used HDO a priori profile affect the retrieved HDO/H2O product (Section 2.2, test (5)). But what about uncertainties in the used H2O a priori profile? The ECMWF profile certainly differs from the actual atmospheric profile. Sure, this will not affect your a priori HDO/H2O profile (per definition in your retrieval setup), but it might affect the retrieved HDO/H2O values. This effect might be even more important than uncertainties in the HDO profile, since the H2O signatures are much stronger than the HDO signatures. Moreover, your test (5) assumes that there is a very small HDO error in the lower troposphere and a large error in the upper troposphere. I understand that this is motivated by the fact that your used SMOW HDO profile typically differs like this from the real atmospheric HDO profile, but what happens if there is a large error in HDO in the lower as well as the upper troposphere? I would very much acknowledge if you documented in detail how the GOSAT HDO/H2O product responds to atmospheric H2O and HDO variations.
Here we are actually talking about the averaging kernels. However, the problem is that HDO/H2O kernels are complex and cannot be calculated in a straight forward manner (I guess that this is the reason why you decided to address this issue by your

sensitivity tests). Other authors present at least kernels for H2O and HDO, which is also not sufficient, since there are cross-correlations between H2O and HDO. In Schneider et al. (2012) we have very recently presented a method for calculating proxies for the HDO/H2O kernels. This method can also be very helpful for your GOSAT paper. The fundamental idea is that you transfer your atmospheric {H2O, HDO} state (or {ln[H2O], ln[HDO]} state) into a {0.5*(ln[H2O]+ln[HDO]), (ln[HDO]-ln[H2O])} state. Both states are equivalent for representing the atmospheric H2O and HDO composition. The advantage of such transformation is, that we now have states that are very good proxies for the δD state, (ln[HDO]-ln[H2O]), and for atmospheric Humidity levels, 0.5*(ln[HDO]-ln[H2O]). In this context please have a look on APPENDIX (I). It shows the kernels in the {ln[H2O], ln[HDO]} and {0.5*(ln[H2O]+ln[HDO]), (ln[HDO]-ln[H2O])} states calculated for a retrieval that is very similar to your retrieval (scaling of prescribed H2O and HDO profiles). Among others we observe a strong Humidity interference on δD. These shown simulations are for retrievals of IASI spectra. However, I can well imagine that for GOSAT the humidity interference is even stronger, due to the difference in the H2O and HDO line strengths. I would like to recommend that you complement your GOSAT retrieval paper with a short additional Subsection showing such Humidity and δD kernels for a typical GOSAT retrieval. These kernels would then allow discussing the δD sensitivity of your retrieval as well as the importance of the Humidity interferences in a comprehensive manner.

(2) I have some concerns about your GOSAT / TCCON δD inter-comparison:

My concerns are based on the fact that the GOSAT and the TCCON retrieval setups have some similar shortcomings, e.g., (1) both scale prescribed H2O and HDO profiles taken from analysis data (ECMWF and NCEP, respectively), (2) both apply a fixed HDO/H2O profile shape, (3) both fit very weak HDO lines, compared to much stronger H2O lines. Therefore, the observed agreement between GOSAT and TCCON might be partly artificial and caused by a common artifact in both datasets. The problem is that δD variations are very small and already small artifacts can significantly affect the results.

A common artifact might be that both the GOSAT and TCCON retrieval suffer from similar humidity interferences on δD. In order to avoid that such artifacts affect the inter-comparison, I suggest eliminating all the variations in the retrieved δD that are correlated to ln[H2O] variations. Furthermore and very important: these δD residuals document that δD actually adds information to H2O. The part of δD that varies in parallel to H2O provides no additional information and its measurement is of limited scientific value. In this context please have a look on APPENDIX (II), where the δD residuals are called “δD deviations” (deviations from a typical δD-ln[H2O] curve). The APPENDIX (II) shows comparisons between our ground-based NDACC FTIR, space-based IASI, and surface in-situ δD products. Furthermore it discusses the advantages of inter-comparing “δD deviations” instead of raw δD data. I encourage you to make a similar inter-comparison between the “δD deviations” of GOSAT and TCCON. Such an inter-comparison would be significantly more convincing than your current study and it could show that your δD data add effectively new information to the ECMWF humidity data.

(3) TCCON δD as reference?

TCCON has been established for highly precise measurements of total column averaged CO2 and CH4. Due to TCCON’s importance for CO2 and CH4 there is a strong collaboration between the GOSAT and the TCCON communities. I fully

understand that this collaboration is now expanded to HDO/H2O. However, I would like to remark that the TCCON δD product can hardly serve as a reference for validation studies, since the spectral range covered by TCCON is not optimal for measuring HDO/H2O. The H2O signatures of TCCON are strong, but the HDO signatures are rather weak and significantly interfere with strong H2O and CH4 lines. These differences in the H2O and HDO signal present severe difficulties for obtaining HDO/H2O at high quality. It is certainly interesting that TCCON has the potential to measure HDO/H2O, but if you need a HDO/H2O reference, I honestly think that you should work with the HDO/H2O data produced from NDACC spectra. These NDACC mid-infrared spectra are of higher spectral resolution than the TCCON near infrared spectra and the corresponding H2O and HDO signatures are of similar strength and well-isolated from signatures of interfering absorbers. These are strong advantages for obtaining a high quality HDO/H2O product. Furthermore, within the project MUSICA there have already been significant efforts for theoretically and empirically assessing the quality of the NDACC δD product (by the way: a very complex work that is still ongoing, some recent results are shown in APPENDIX (II)).
I would like to suggest adding NDACC HDO/H2O data to your inter-comparison study. The MUSICA NDACC δD product is freely available for the scientific community and for ten globally-distributed NDACC sites (Schneider at al., 2012). Among the six sites you use in your inter-comparison study there are three sites with MUSICA data: Ny Alesund, Bremen, and Wollongong. So adding a comparison to MUSICA data would not require too much additional work.

Other comments:

Page 6645, line 24:
Actually Worden et al. (2012) use a very similar retrieval recipe as Schneider and Hase (2011): fit of a broad microwindow, simultaneous fit of interference absorbers, fine model atmosphere gridding, etc. The main differences are that Worden applies TES spectra instead of IASI spectra (slightly higher spectral resolution) and that he uses a much weaker HDO/H2O constraint. This weaker constraint is the main reason for the increased sensitivity as reported in Worden et al. (2012). It increases the theoretically estimated sensitivity of the system, but at the same time it increases the uncertainty of the product. With IASI we could also achieve a similar sensitivity as Worden et al. (2012) for TES, if we used a weaker constraint. Please consider this when you describe the possibilities of TES and IASI.

Page 6648, line 18:
A correlation (or constraint) between HDO and H2O is implicit in your retrieval setup. If you calculate the a priori HDO profile from the a priori H2O profile (ECMWF) by assuming SMOW throughout the atmosphere you assume rather unrealistic HDO/H2O profile shape. This is a strong constraint for your HDO/H2O retrieval. Since it is implicit in your retrieval setup and since there is no flexibility it can be called a hard constraint. What you describe at the beginning of page 6656 is an effect of this constraint.

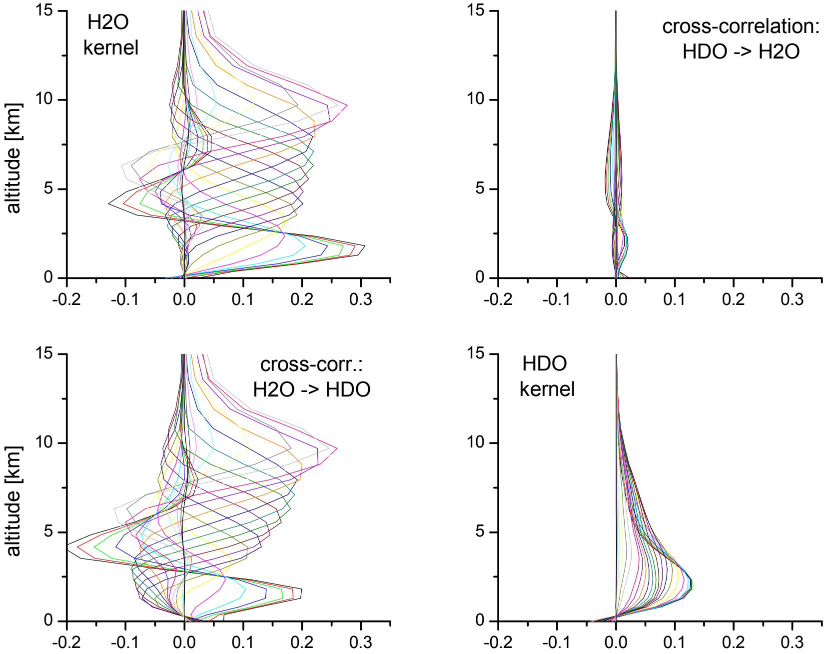
Page 6651, line 2:
Here Schneider et al., (2006) is not a good reference. Better would be to cite pioneering works in the field of atmospheric δD profile measurements and modeling, e.g., Ehhalt (1974) and Joussaume et al. (1984).

Page 6657, line 27:
MUSICA will provide a high quality tropospheric δD dataset using ground- and space-based remote sensing and in-situ measurement techniques. Concerning the ground-based remote sensing component, MUSICA works with NDACC and not with TCCON spectra. A quality assessment for TCCON δD is no MUSICA task, but of course we would be happy to support respective activities of TCCON colleagues. Please correct this in your conclusion section.

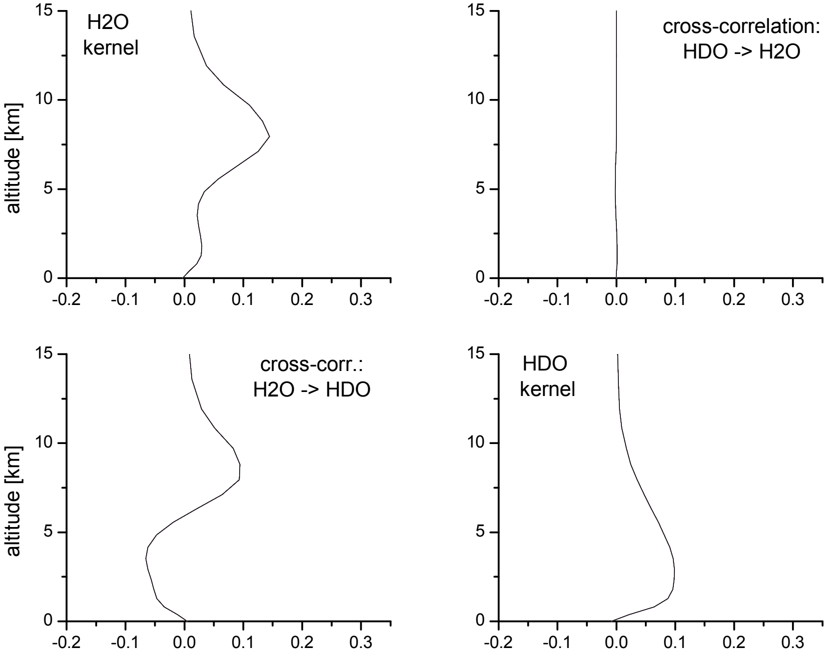
APPENDIX (I)

H2O and HDO kernels

IASI profile retrieval of Schneider and Hase (2012)



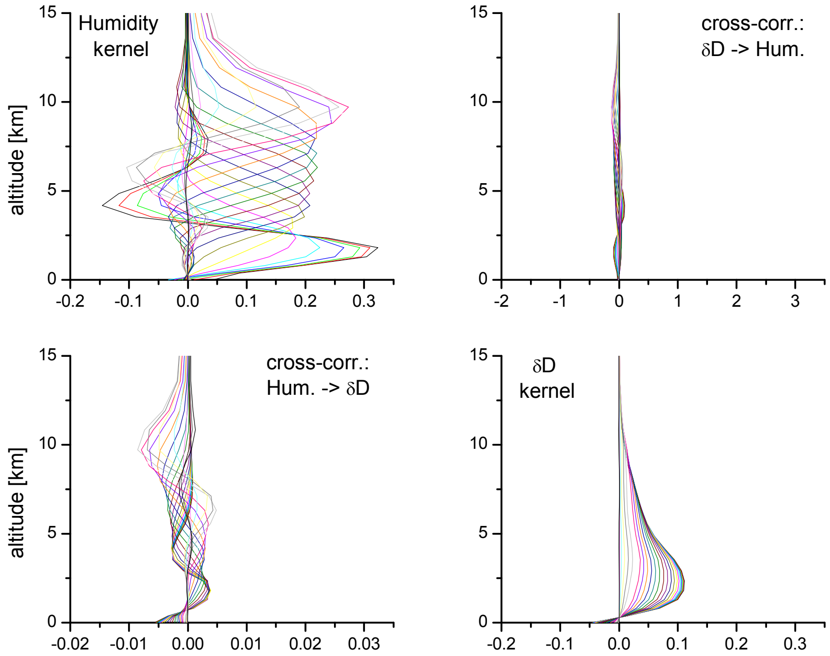
IASI profile scaling retrieval (for a rough estimation of GOSAT kernels)

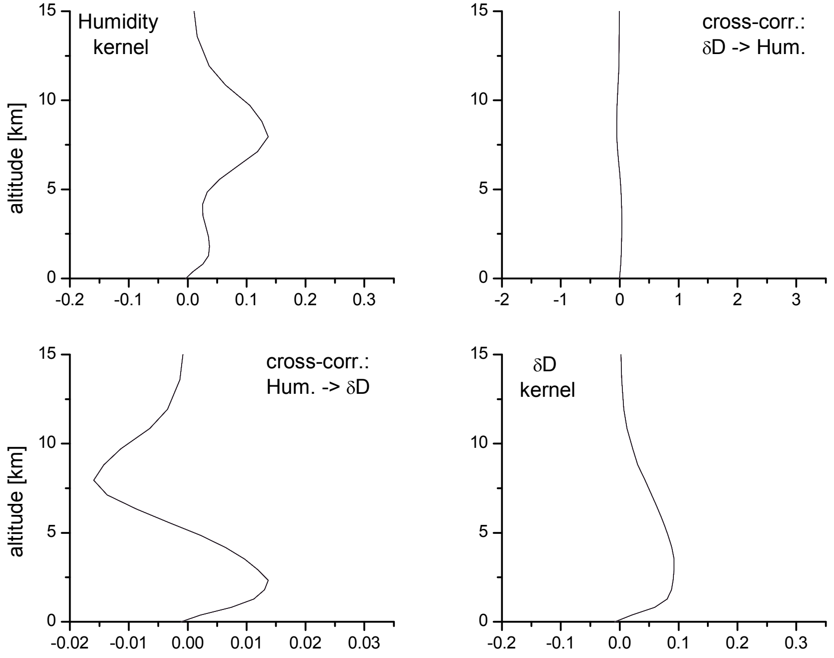


Here we present row kernels for the {ln[H2O], ln[HDO]} state for a typical IASI retrieval. There are strong cross-correlations between ln[H2O] and ln[HDO]. The particularly strong cross-correlation (or interference) of ln[H2O] on ln[HDO], is due to the fact that there is more info in the H2O lines than in the HDO lines (H2O lines are stronger than HDO lines). This effect might be even stronger for GOSAT retrievals.

APPENDIX (I)

Proxies for Humidity and δD kernels


IASI profile retrieval of Schneider and Hase (2012)


IASI profile scaling retrieval (for a rough estimation of GOSAT kernels)

Here we present the kernels for the 0.5*(ln[H2O]+ln[HDO]) and the (ln[HDO]-ln[H2O]) states. These kernels are good proxies for Humidity and δD kernels (for more details please refer to Schneider et al., 2012). In case of a profile scaling retrieval (the GOSAT retrieval setup), the interferences of Humidity on are particularly strong δD (left Figure).

Please note that the x-axis of the cross-correlation plots are scaled by a factor of ten in order to account for the different natural variability of Humidity and δD.

APPENDIX (II)

(1) Comparison of IASI and ground-based FTIR water isotopologue data for coincidences at Izaña observatory: δD and „δD deviations“

- Comparison period: Oct./2007 – March/2011
(extension of the Schneider and Hase, 2011 study)

- Temporal coincidence criteria: 1h

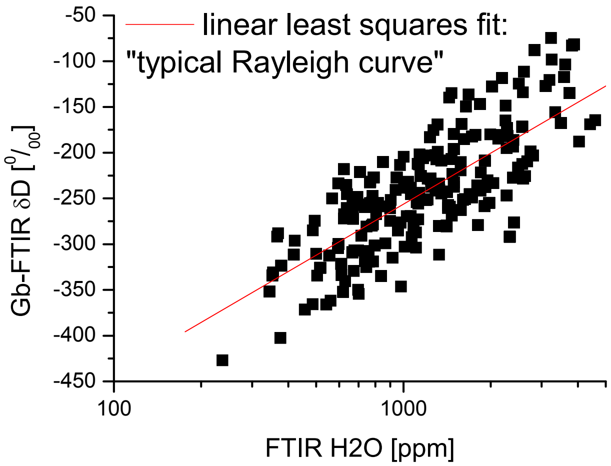
- Spatial coincidence criteria: 1° x 1°

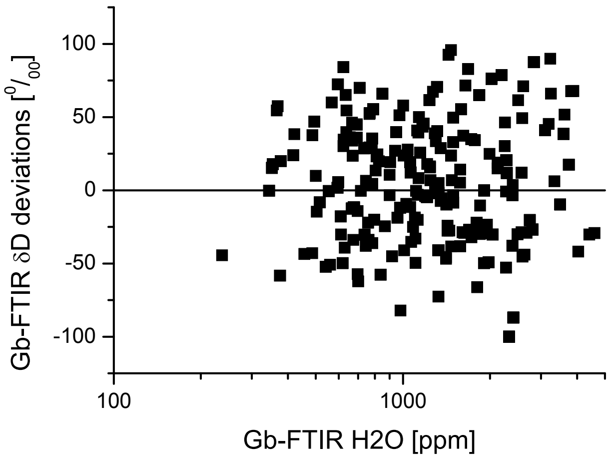
- Number of valid coincidences: 481

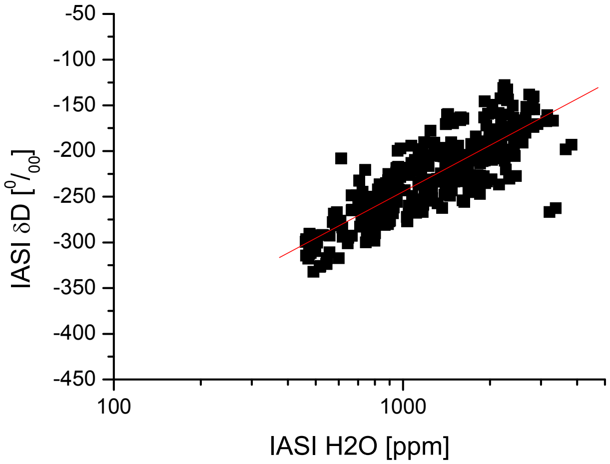
<u>Acknowledgement:</u> This work has been performed within the MUSICA project. MUSICA is funded by the European Research Council under the European Community's Seventh Framework Programme (FP7/2007-2013) / ERC Grant agreement n° 256961.

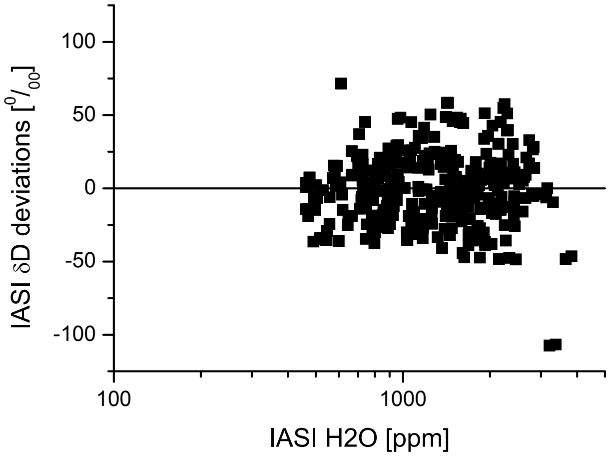
APPENDIX (II)

H2O – δD plots and „δD deviations“









For calculating the „δD deviations“ we remove the „typical Rayleigh curve“ relation from the δD variability.

APPENDIX (II)

Motivation for looking on „δD deviations“

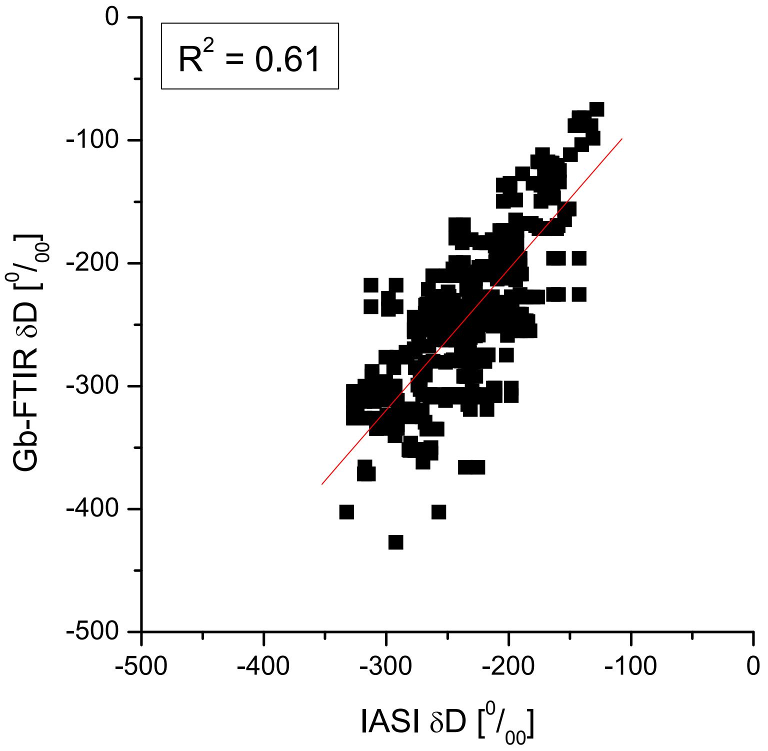
(1) Large part of atmospheric δD variations can be explained by Rayleigh distillation processes, which shows up as a strong linear correlation between δD and ln[H2O]. However, scientifically most interesting are the deviations from the Rayleigh relation or the variabilities in the typical H2O-δD relation. The added value of δD observations can be well documented by looking on the „δD deviations“!

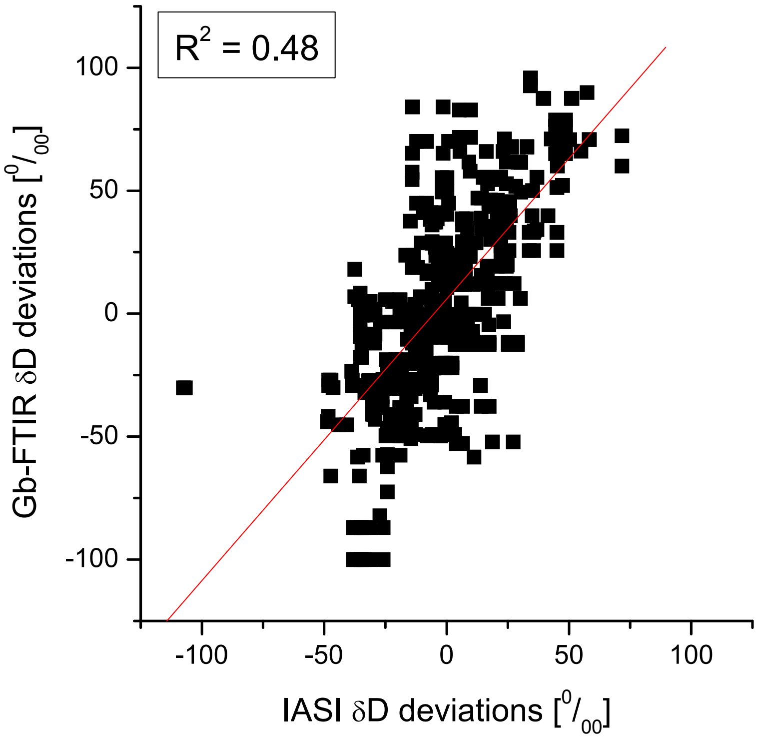
(2) Remote sensing observation of δD might be affected by interferences from H2O (Schneider et al., 2012). These interferences might produce an artificially good correlation of the δD values obtained by two different remote sensors. The „δD deviations“ are per definition not systematically correlated with H2O, i.e. not affected by possible H2O interferences. In this context, validating the „δD deviations“ of remote sensor is much more meaningful than just validating δD.

(3) „δD deviations“ are very usefull when comparing different datasets. An example is the comparison of a remote sensing and a surface in-situ dataset. While the remote sensor detects mainly a free tropospheric airmass, the surface in-situ experiment detects a boundary layer airmass. The systematic differences in the isotopic composition of these airmasses becomes partly visible in the typical H2O-δD relations. Removing these typical H2O-δD relations (by calculating the „δD deviations“), removes large part of systematic differences and allows for a more reasonable comparison of the datasets.

APPENDIX (II)

Comparison IASI vs. FTIR for δD and „δD deviations“





Both the gb-FTIR and IASI see similar „δD deviations“. The differences between both datasets is reasonable (they can be largly explained by the different sensitivities of the two remote sensing systems).

The „δD deviations“ have reduced variability, since they only show the part of the δD variations that are not in common with the ln[H2O] variations. Validating „δD deviations“ is a much stricter validation excercise than validating δD, however, it is the kind of validation that shows that the δD data really provide additional and scientifically very useful information.

APPENDIX (II)

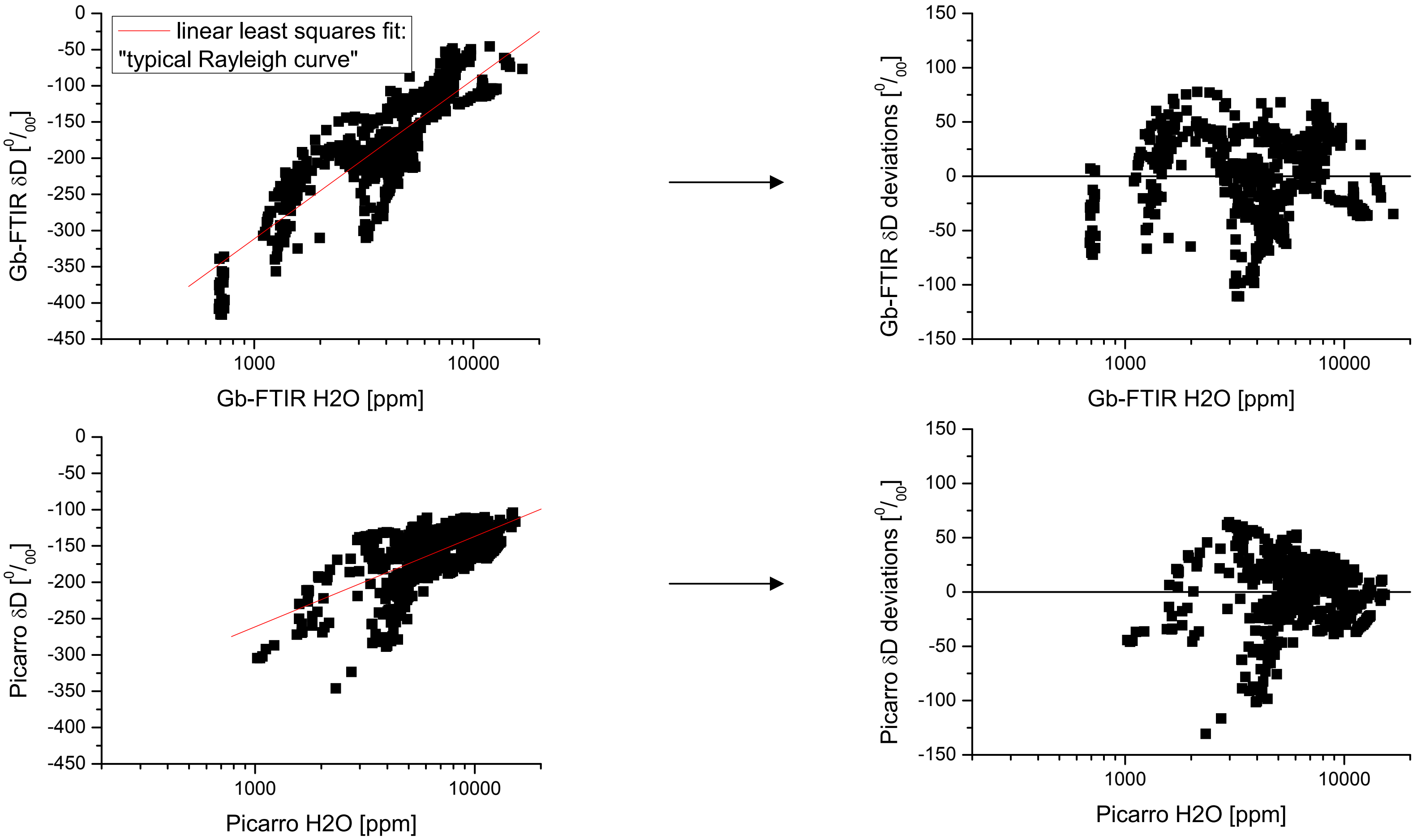
(2) Comparison of ground-based FTIR and Picarro surface in-situ water isotopologue data at Izaña observatory: δD and „δD deviations“

- Comparison period: April/2012 – July/2012
- Temporal coincidence criteria: 1h
- Number of valid coincidences: 596

Acknowledgement: This work has been performed within the MUSICA project. MUSICA is funded by the European Research Council under the European Community's Seventh Framework Programme (FP7/2007-2013) / ERC Grant agreement n° 256961.

APPENDIX (II)

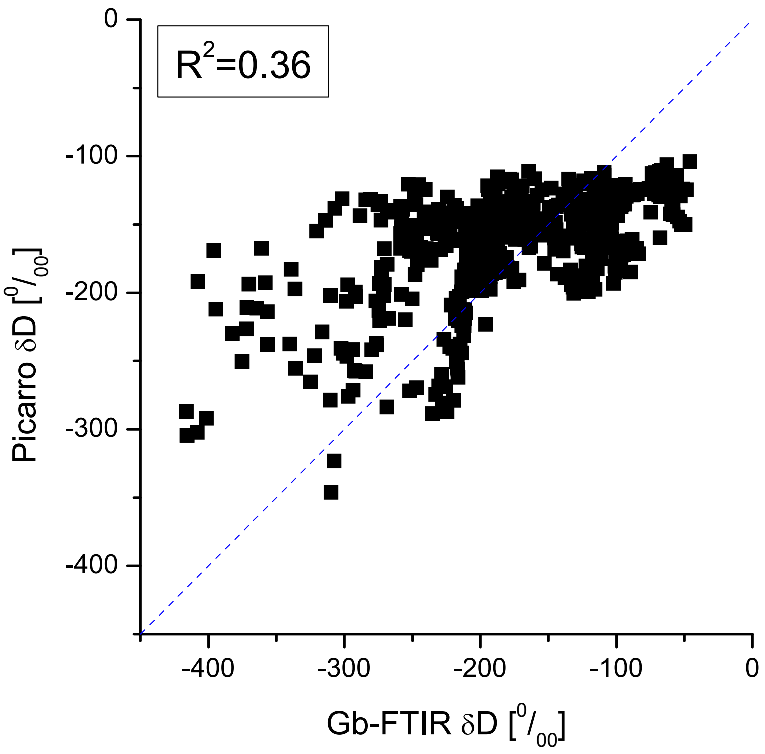
H2O – δD plots and „δD deviations“

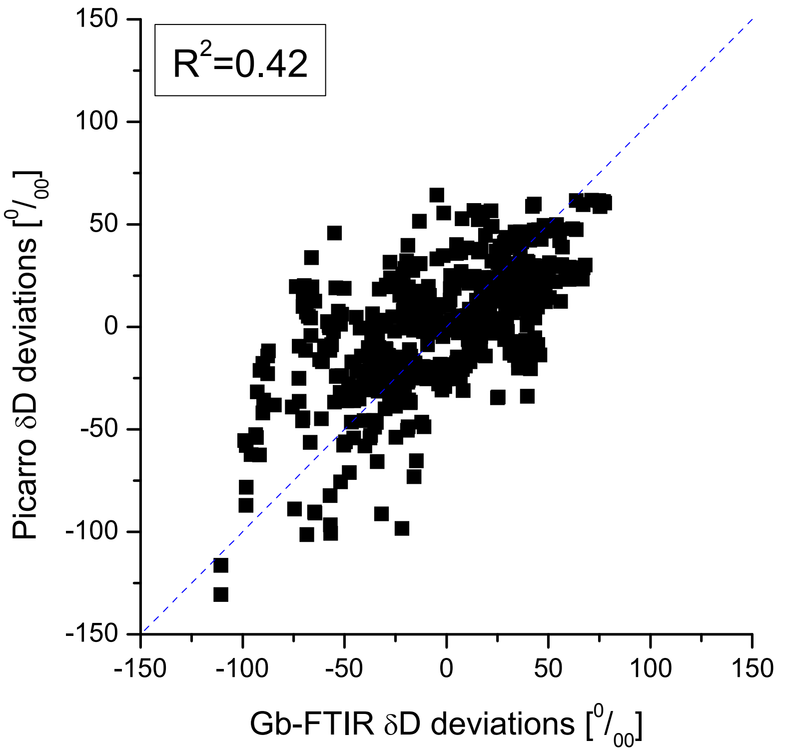


Here the „typical Rayleigh curves“ are systematically different, since Picarro and FTIR detect systematically different airmasses: the Picarro is influenced by the MBL and the FTIR detects free tropospheric air! By calculating the δD deviations we assure that the datasets are better comparable.

APPENDIX (II)

Comparison FTIR vs. surface in-situ Picarro for δD and „δD deviations“





The „δD deviations“ correlate better than the raw δD data, since for the „δD deviations“ the effect of observing systematically different airmasses is reduced.