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# Cross-validation of IASI/MetOp derived tropospheric $\delta D$ with TES and ground-based FTIR observations

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Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion





## 1 Introduction

Water vapour in the troposphere has a central role in the climate system (Pierrehumbert et al., 2007; Sherwood et al., 2010). Yet there are important uncertainties associated with the mechanisms controlling tropospheric water vapour distribution throughout the globe, leading to systematic biases in actual representations (Soden and Brether-  
ton, 1994; Brogniez and Pierrehumbert, 2007; Allan et al., 2003; Bates and Jackson, 1997; Pierce et al., 2006) and an important spread in future climate predictions (Soden and Held, 2006; de Forster and Collins, 2004). In particular, the cloud feedback is responsible for most of the spread in the different climate models (Cess et al., 1990; Dufresne and Bony, 2008) because of the various representations of associated processes in the different models. Recently, Sherwood et al. (2014) showed that, among 43 climate models, the different ways of simulating convective mixing between the lower and middle tropical troposphere was responsible of about half of the variance in climate sensitivity. It is thus crucial to improve representation of hydrological processes.

Observations of water vapour isotopologues have the potential to reveal information on the processes controlling humidity. The different water isotopologues are indeed characterized by distinct vapour pressures and are therefore sensitive to phase changes: the heavy isotopologues ( $\text{H}_2^{18}\text{O}$ , HDO) preferentially condense while the light ( $\text{H}_2^{16}\text{O}$ ) preferentially evaporates. Hence, the heavy to light isotopologue ratio provides useful information on the air mass history and can be used to constrain hydrological processes (Strong et al., 2007; Worden et al., 2007; Samuels-Crow et al., 2014; Risi et al., 2012a, b; Noone, 2012). The ratio is commonly expressed in  $\delta$  notation:

$$\delta D = 1000 \left( \frac{\frac{\text{HDO}}{\text{H}_2\text{O}}}{\text{VSMOW}} - 1 \right), \quad (1)$$

where VSMOW (Vienna Standard Mean Ocean Water) is the reference standard for water isotope ratios (Craig, 1961).

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



**Cross-validation of  
IASI/MetOp  $\delta D$   
retrievals**

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Among the different methods to determine the isotopic composition of water vapour, it has been shown that remote sensing instruments can be used to infer estimates of  $\delta D$  at a sufficient precision for scientific applications (Risi et al., 2012b), with the advantage that they provide measurements over regions and at altitudes that are not easily accessible. Space sounders also have the potential to provide global distributions (Worden et al., 2007; Frankenberg et al., 2009, 2013; Boesch et al., 2013). The Infrared Atmospheric Sounding Interferometer (IASI) (Clerbaux et al., 2009) onboard the MetOp meteorological satellite is particularly suited for measuring  $\delta D$  owing to its unique sampling characteristics (Schneider and Hase, 2011; Lacour et al., 2012). Indeed, IASI samples the atmosphere almost everywhere on the globe two times a day with a ground pixel size of 12 km at nadir.

Because of their inherent lack of vertical sensitivity, measurements derived from remote sounding instruments constitute a more or less complicated function of the quantity of the interest (Rodgers and Connor, 2003) and can not be regarded as true values. The regularization procedure used in the retrievals is in fact often such that they constitute the most probable estimate given the measurement and some a priori statistical information. Moreover retrieved quantities depend also on several parameters of the inversion such as the a priori, the spectroscopic line database, the spectral range etc. For all these reasons, the validity of quantities derived from remote sensing instruments always needs to be evaluated against other observations. It is at the same time crucial to document how different remote sensing products compare between them. In this paper we assess the validity of  $\delta D$  vertical profiles retrieved from IASI at ULB by comparing them with other available profiles of  $\delta D$  in the troposphere. We use the term “cross-validation” according to von Clarmann (2006) for this exercise as we compare IASI vertical profiles against profiles from other remote sounding instruments which do not constitute absolute values of the state of the atmosphere. Our study is similar to the recent cross-validation of IASI  $\delta D$  retrievals from KIT with ground-based FTIRs (Wiegele et al., 2014). We note that there has been recently an increasing number of absolute measurements of tropospheric  $\delta D$  (Schneider et al., 2014; Herman et al., 2014), which

**Cross-validation of  
IASI/MetOp  $\delta$ D  
retrievals**

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



will be essential to validate  $\delta$ D profiles retrieved from the remote sounders and thus to ensure the optimal use of the latter which are for now often limited to relative variations analyses (Risi et al., 2012b). In this study, although we do not use the absolute measurements, we perform the cross-validation with respect to instruments which have been evaluated against them. This allows us to infer some preliminary conclusions on how our retrievals would compare to these references.

We use for the cross-validation of IASI,  $\delta$ D profiles from the TES instrument on-board Aura (Worden et al., 2012) and from ground-based FTIRs from the MUSICA network (Schneider et al., 2012) which are both sensitive to  $\delta$ D in the same part of the troposphere as IASI. We do not perform the comparison with other space sounders, which provide  $\delta$ D retrievals in the upper troposphere or near the surface where IASI is generally less sensitive (Lacour et al., 2012; Schneider and Hase, 2011).

The main purpose of the cross-validation exercise presented here is to verify that two profiles from two different remote sounding instruments agree within their respective limitations (Rodgers and Connor, 2003) that is to say that the estimated profiles are well characterized by their error and sensitivity matrices. In Sect. 2 we introduce the methodology employed to adequately intercompare the different instrument products. Specifics of the  $\delta$ D retrievals (also referred as HDO / H<sub>2</sub>O ratio retrieval) are also documented in this section. We then give a brief overview of the different instruments in Sect. 3. In Sects. 4 and 5 we detail the results of the comparison between IASI and TES and between IASI and the ground-based FTIRs respectively.

## 2 Methodology to inter compare $\delta$ D profiles

In this study we mainly follow the Rodgers and Connor (2003) methodology developed to inter-compare indirect measurements. Its application to  $\delta$ D retrievals is described below.

## 2.1 Retrieval of the HDO / H<sub>2</sub>O ratio

Retrieving the HDO / H<sub>2</sub>O ratio at a sufficient quality from remote sounding instruments is challenging since the retrieval needs to be precise enough to capture the fine isotopic variations and sensitive over the large dynamical range of water vapour concentrations in the troposphere. This requirement is antagonist with the general formulation of the optimal estimation as the precision of the retrieval highly depends on the applied statistical constraint which itself limits the range of possible states. One way of overcoming this limitation is to introduce an inter constraint between the two water isotopologues and to perform the retrieval on a logarithmic scale (Schneider et al., 2006; Worden et al., 2006). The different retrieval products we use here (Lacour et al., 2012; Worden et al., 2012; Schneider et al., 2012) have been obtained applying this constrained approach. One difficulty introduced by the constrained retrieval is the posterior characterization of the  $\delta D$  profiles as the averaging kernels and error covariance matrices obtained are indeed representative of the retrieved states  $\log(H_2O)$  and  $\log(HDO)$  and can not be directly applied to  $\delta D$ .

Schneider et al. (2012) have developed an elegant method to characterize the vertical profiles of H<sub>2</sub>O and  $\delta D$  for retrievals which constrain the ratio  $\log(HDO / H_2O)$ . This methods allows to transform the products obtained in the  $\{\log(H_2O), \log(HDO)\}$  space into a proxy state  $\{\log(\text{humidity}), \delta D\}$ . It is then possible to provide proxy error covariance matrices and averaging kernels for the  $\delta D$  profile which in turn facilitates its use for geophysical analyses.

In addition, the method allows for a minimization of the cross dependence of the H<sub>2</sub>O retrieval on the  $\delta D$  retrieval and vice versa (Schneider et al., 2012). As retrieved H<sub>2</sub>O and  $\delta D$  exhibit different vertical sensitivities (the sensitivity to  $\delta D$  being limited compared to H<sub>2</sub>O) and are thus not fully representative of the same air mass, Schneider et al. (2012) recommend to distinguish two types of products. A product (type 1) for an optimal use of H<sub>2</sub>O vertical profiles alone and a product (type 2) for consistent H<sub>2</sub>O and  $\delta D$  data which are likely to be used together and need to be representative

## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



of the same air mass. This is achieved by reducing the  $H_2O$  profile to the  $\delta D$  retrieval sensitivity. In this paper we use this proxy state (type 2) to characterize  $\delta D$  profiles in terms of averaging kernels and error covariance matrices and all retrievals have therefore been a posteriori corrected to obtain a product of type 2. Specifically, according to Schneider et al. (2012) this is done by:

$$\hat{\mathbf{x}}^* = \mathbf{P}^{-1} \mathbf{C} \mathbf{P} (\hat{\mathbf{x}} - \mathbf{x}_a) + \mathbf{x}_a, \quad (2)$$

with  $\mathbf{x}_a$  the a priori state vector,  $\hat{\mathbf{x}}$  the estimated state vector  $\{\log(H_2O), \log(HDO)\}$  the profiles originally retrieved and  $\hat{\mathbf{x}}^*$  the corrected state vector  $\{\log(H_2O), \log(HDO)\}$  that is used to compute the  $\delta D$  ratio of type 2. For the description of  $\mathbf{P}$  and  $\mathbf{C}$  matrices we refer to Schneider et al. (2012). These matrices ensure the reduction of vertical sensitivity and resolution of the  $H_2O$  profile as well as a correction of the cross dependence. Averaging kernels and error covariance matrices from the different retrievals have all been transformed into the  $\{\log(\text{humidity}), \delta D\}$  proxy space.

## 2.2 Transformation between grids

A cross-validation exercise should compare like with like and consists of applying corrections to make the different retrievals comparable. A first step required for the cross-validation involves the adjustment of the different vertical grids on which the retrievals are performed. The state vectors, the error covariance matrices as well as the averaging kernels matrices need to be represented on the same grids to be comparable. The state vector and the error covariance matrices can be transformed into a coarser or a finer grid. Indeed, following Rodgers (2000) the state vector  $\mathbf{x}$  on a fine grid is related to a reduce vector  $\mathbf{z}$  on a coarser grid as:

$$\mathbf{x} = \mathbf{W} \mathbf{z} + \epsilon_{\mathbf{W}} \mathbf{x} \quad (3)$$

with  $\mathbf{W}$  the interpolation matrix and  $\epsilon_{\mathbf{W}} \mathbf{x}$  the error induced by the interpolation (Calisesi et al., 2005). The transformation of the state vector on a fine grid to a state vector on















## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



analysis. For each TES measurement, a backward trajectory was computed with HYS-PLIT (Draxler and Hess, 1998). The data was rejected if the position of the airmass four hours before the TES measurement was too far ( $2.5^\circ$ ) from the IASI measurement. This  $2.5^\circ$  threshold has been defined by analysing the statistical differences between the TES and IASI integrated 3–6 km column and the distance of the airmass. We found that a spatial mismatch above  $2.5^\circ$  led indeed to significant differences.

### Comparison of one TES observation vs. several IASI observations

Generally, intercomparison studies are carried out by comparing one observation vs. another observation. Because the observational error on the IASI retrieval is relatively important (38% in the free troposphere, Lacour et al., 2012) compared to TES, to the FTIR and also compared to the expected natural variability of  $\delta D$ , the comparison between a couple of  $\delta D$  profiles could have limited utility. To cope with that, we chose to average all the IASI measurements fulfilling the collocation criteria with one TES  $\delta D$  observation. By doing so, the IASI observational error is lowered by the squareroot of  $N$ , the number of observations. Likewise, the error covariance matrix of the IASI error of Eqs. (8) and (10) is divided by  $N$ . Generally the number of IASI observations available around one TES observation ranges from 1 to 15.

### 4.2 Retrieval characteristics

Figure 2 shows typical averaging kernels for IASI and TES at tropical latitudes. These averaging kernels correspond to  $\delta D$  proxy averaging kernels (Schneider et al., 2012). For IASI, the resolution of the averaging kernels is quite coarse, about 4–5 km and the information of the retrieval comes mainly from the 0–3 and 3–7 km layers. The peaks of the averaging kernels are not perfectly located at their nominal altitude especially above 6 km indicating that the retrieved state above that altitude is mainly sensitive to variations of the real state at lower altitude. The degrees of freedom (DOFS) for this typical retrieved profiles of IASI is 1.7. Compared to IASI, TES averaging kernels



sensitivity to  $\delta D$ , we thus smoothed TES retrieved profiles with IASI averaging kernels for the more like with like comparison.

The direct comparison (no smoothing) is shown on the left panel of Fig. 4 and the smoothed comparison on the right panel. The total expected difference (black curve) of the direct comparison ranges from 120‰ at the lowest layer to 55‰ at 4.5 km, increasing again up to 68‰ at 7.5 km. The total expected difference is largely controlled by IASI observational error in the 0–2 km layer and above 6 km. In the free troposphere the difference of vertical sensitivities (smoothing error) between the two sounders also has an impact in the direct comparison. Note that IASI’s observational error exceeds the  $\delta D$  global variability above 7 km and at 0.5 km, and this is because the a priori covariance matrix ( $\mathbf{S}_a$ ) used in the IASI retrieval is larger than the  $\mathbf{S}_c$  used for the comparison. This error budget indicates that the direct comparison is relevant in the free troposphere when it refers to the expected natural variability of  $\delta D$  at global scale (dark blue bold line). However at a more regional scale (here the tropical variability given by the light blue bold line) the direct comparison is less significant since the total expected difference (55‰) is very close to the expected natural variability of  $\delta D$  ( $\sim 70$ ‰).

The right panel of Fig. 4 shows a similar error budget but accounting for the difference in sensitivity between instruments. One can see that the smoothing contribution is significantly reduced compared to the direct comparison. TES observational error is also reduced mainly because the fine structures have been removed by the IASI averaging kernels. This does however not affect the total expected difference since this error was already relatively small. The total expected difference is now only controlled by IASI’s observational error and is reduced to 38‰ at 3.5 km.

#### 4.4 Expected vs. real differences

In the previous section we have described the differences expected from the comparison between TES and IASI based on the theoretical error budgets of the different retrievals. In this section we compare the theoretical error budget with the real differences between TES and IASI  $\delta D$  retrieved profiles. Those are taken as the SD of the

## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



5 difference TES-IASI in the  $\delta D$  profiles and are plotted as green line in Fig. 4. For the direct comparison, we find that the real difference is lower than the expected one below 7 km. This indicates that the difference TES-IASI at these altitudes is in agreement with the theoretical error budget. The fact that the real difference exceeds the expected one

10 above 7 km could be due to an underestimation of the IASI's observational error (since all other contributions are mostly negligible). When smoothing TES retrieved profiles with IASI averaging kernels the real differences decrease in the free troposphere where the smoothing error was important. As for the non-smoothed comparison, the real difference remains below the theoretical one over the entire 0–7 km range.

15 While these figures are indicative of the error budget above the Indian and Pacific Oceans, the variations in sensitivity are such that the budget will depend on humidity and temperature conditions. However, we found that the results presented in Fig. 4 are generally representative of all observations above the oceans. In the following subsection we provide a more statistical view on the agreement between TES and IASI.

### 4.4.1 Statistics of the agreement between IASI and TES

20 In this subsection we compare IASI to TES statistically for the MD and PIO datasets. We focus on retrieved  $\delta D$  values at 4.5 km which is the altitude where IASI is the most sensitive above the oceans. For the PIO dataset we document the agreement for both the direct and the smoothed comparisons. For the MD dataset we only consider the direct comparison because the sensitivity of TES – depending on the latitude (Fig. 3) – is sometimes higher and sometimes lower than IASI sensitivity. As we discussed in Sect. 4.2 the direct comparison is meaningful since the expected differences are substantially smaller than the natural variability at a global scale. We summarize the results from the comparison between IASI and TES in Table 1, in terms of  $1\sigma$  SD, slope of the major axis regression ( $m$ ) and Pearson correlation coefficient ( $r$ ).

25 For the PIO dataset we found a SD of the difference of 43‰ for the direct comparison which decreases to 35‰ when TES retrievals are smoothed with IASI averaging kernels. These value are in line with the theoretical estimations of the error. The correlation





## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



with a majority of points below the Rayleigh distillation curve in DJF. In zone C, both instruments show a clear amount effect (enhancement of the depletion with high water vapour content) although IASI H<sub>2</sub>O values seem slightly drier than TES.

At 3.5 km the seasonal and longitudinal variations are coherent between the two instruments, but the general agreement is less good than at 5.5 km. For example, an amount effect is well observed for each zone for TES while it can only be clearly seen in IASI retrievals in zone C. The reason of these differences is probably due to the better sensitivity of TES at these altitudes and below.

### 4.6 Comparison instrument–model

One of the specific applications of satellite measurements of  $\delta D$  is to evaluate performances of isotopes-enabled GCM. TES observations have for example previously been used to evaluate GCM at a global scale (Yoshimura et al., 2011; Risi et al., 2012b) while IASI observations have been compared to LMDZ at regional scales (Lacour et al., 2012; Pommier et al., 2014). Moreover because of the integrated nature of the isotopologues ratio, models are often useful to interpret the measurements. We take the opportunity of this cross-validation study to briefly investigate the differences that can arise from the comparison of a GCM with TES or with IASI. The goal here is twofold: (1) document how the instruments will differ in instrument–model comparisons and (2) illustrate the impact of IASI sampling in model–observation comparisons.

We use the GCM LMDZ (Risi et al., 2010) that we consider as the reality. We also consider retrieved profiles from IASI and TES as the reality. The model outputs are thus not smoothed with any instrument vertical sensitivity. This is not an usual approach but it allows having an idea of how close observations are from reality. Indeed by not taking the instrument sensitivity into account during the comparison, retrievals are considered as an estimate of the true state with an error contribution due to the smoothing, rather than estimate of a state smoothed by the averaging kernels (which is done when smoothing models outputs with averaging kernels) (Rodgers, 2000). We use the Pearson correlation coefficient as a metric of the agreement between LMDZ

**Cross-validation of  
IASI/MetOp  $\delta D$   
retrievals**

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



and the retrieved  $\delta D$  between 3 and 6 km, and the results are reported in Table 2. We have subdivided the MD dataset in 2 different latitudinal groups according to the TES sensitivity: tropical observations located between  $15^\circ$  S and  $15^\circ$  N and subtropical to mid-latitudes observations located between  $15$  and  $45^\circ$  in both hemisphere. Note also that the comparison TES-LMDZ considers one TES observation vs. one LMDZ cell, and that this results in a worse agreement than previous studies that generally average TES observations over time and/or space.

For the PIO dataset the values found in Table 2 show that the comparison LMDZ vs. TES shows a better correlation coefficient (0.26) than for the LMDZ vs. IASI comparison (0.15). This is also true for the MD dataset at tropical latitudes with slightly higher correlation coefficient of 0.46 and 0.30 for TES and IASI respectively. In contrast, for the subtropical to mid-latitudes observations, we find a better correlation coefficient for the LMDZ vs. IASI comparison (0.42) compared to the LMDZ vs. TES comparison (0.30). The better agreement between LMDZ (reality) and IASI above  $15^\circ$  makes sense since we observe a significant decrease in TES sensitivity at these latitudes (see Fig. 3).

With the PIO dataset we finally investigate how the number of available observations can impact a model–instrument comparison. This is interesting because the number of daily IASI observations in one model cell ( $3.75^\circ \times 2.53^\circ$ ) on a given day can be very large. Indeed, from the histogram in Fig. 7 we see that there is about 25% of the LMDZ cells that contains 1 to 10 observations and about 12% that contains 90 observations or more. The average number of observations available per cell is 46. The correlation coefficient between IASI and LMDZ increases compared to a one to one comparison, due on one hand, to the decrease of the observational error by  $\sqrt{N}$  when averaging several observations and on the other hand to the better sampling of the model cell by IASI that allows to capture the variability of  $\delta D$  within this cell. When including less than 10 observations the correlation coefficient is below 0.25 but it increases up to 0.5 when including more than 90 observations. This is important and suggests that model–observation comparison could be largely improved by exploiting the unprecedented sampling of IASI.

## 5 Comparison IASI vs. FTIR

### 5.1 Datasets description and collocation criterion

Three ground-based NDACC-FTIRs of the MUSICA network have been selected at different latitudes: Kiruna, Karlsruhe and Izana. We consider FTIR and IASI observations collocated when there are no more than three hours between the two measurements and when the IASI observation is located in a radius of  $1.5^\circ$  around the measurement sites. We have applied the same approach than for the IASI-TES comparison to make the comparison the most significant possible and when several IASI observations fulfilled the collocation criteria, we have averaged them to reduce the observational error. FTIRs and IASI  $\delta D$  profiles correspond to the years 2010, 2011 and 2012.

### 5.2 Retrieval characteristics

Representative averaging kernels for the three ground-based FTIR are plotted in Fig. 8 in comparison with the corresponding IASI averaging kernels. The IASI averaging kernels exhibit similar sensitivity profiles from high latitude to subtropical latitudes with degrees of freedom of 1.7, 1.9 and 1.7 at Kiruna, Karlsruhe and Izana, respectively. As discussed before, the IASI retrieval sensitivity to  $\delta D$  is coming from the free troposphere and also from the lowest layers of the atmosphere. At Arctic latitude (Kiruna) the IASI sensitivity close to the surface is the highest, probably owing to a favourable thermal contrast (Pommier et al., 2014). The FTIR averaging kernels exhibit similar sensitivity than IASI in terms of information content with DOFS of 1.5, 1.2 and 1.7 for Kiruna, Karlsruhe and Izana respectively. The profiles of vertical sensitivities however significantly differ: Kiruna and Karlsruhe FTIR are mainly sensitive in the first layers of the atmosphere and at Izana, the FTIR exhibits sensitivity in the 3 to 5 km layer and also above 6 km.

## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



### 5.3 Expected difference

The expected differences for the direct IASI-FTIR comparison are calculated according to Eq. (8) in the same way as for TES comparisons. The same  $\mathbf{S}_c$  covariance matrix was also used. To evaluate the significance of the cross-validation, we compare the expected differences (black curve) in Fig. 9 at the three sites with the global  $\delta D$  variability (dark blue curve) but also with the regional variabilities (respectively green, brown and cyan curves for Kiruna, Karlsruhe and Izana). The variabilities were calculated from LMDZ model profiles within a given  $20^\circ$  latitudinal band. We can see from Fig. 9 that Kiruna and Karlsruhe present very similar error budgets mainly controlled by IASI observational error while at Izana the smoothing error also impacts the expected difference. For this comparison, we found that the smoothing of one instrument averaging kernels with the other was not productive. The comparison can thus not be optimized to take into account the different vertical sensitivities of the two instruments and only the direct comparison is discussed next.

The error difference budgets are shown in Fig. 9, representative of an average of the error budgets of a one month period. We note from Fig. 9 that the observational errors from the FTIR and from IASI are very different. For both sites the FTIR observational error is indeed lower than 20% throughout the vertical profile while IASI observational error ranges from 20% around 3–4 km to 80% in the upper troposphere. It is interesting here that the IASI observational error is significantly smaller in the lower troposphere compared to the error budget discussed previously in Fig. 4. This is mainly due to the fact that the two sites are on the continent, where the sensitivity of IASI to near surface  $\delta D$  is better due to more favourable thermal contrast. It is also interesting to notice that the IASI observational error in the lower troposphere does not exceed the  $\delta D$  variability at global scale and at a regional scale. This indicates that IASI retrievals provide relevant  $\delta D$  measurements in these conditions even in the boundary layer.

For Kiruna and Karlsruhe, the total expected difference is lowest in the free troposphere (about 20% for Kiruna and 35% for Karlsruhe) and highest in the upper

## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



troposphere. Compared to the regional expected variability of  $\delta D$ , the comparison might be considered useful below 5 km since both budgets show expected difference lower than the  $\delta D$  variability at regional level.

At Izana, the total expected difference ranges from 90‰ at 2.5 km to about 60‰ at 4.5 km. At higher altitude the total expected error exceeds the natural variability of  $\delta D$ . In this case it is not only the IASI observational error that dominates the total difference expected. From 2.5 to 4 km the smoothing error is indeed large and contributes with both IASI and FTIR observational error. From 4 to 6 km the FTIR observational error becomes less important while at higher altitude it is the IASI observational error that becomes predominant again. The comparison appears significant with respect to the variability of  $\delta D$  at global scale but not at regional scale.

#### 5.4 Expected vs. real differences

The real difference between the 2 instruments are calculated as the SD of the difference for each level for the corresponding time period of the computed error budgets. As in the IASI vs. TES comparison the SD profiles are plotted (green curves) on the error budget in Fig. 9 for the three sites.

We find that the SD profiles of the difference follow well the error profiles expected from the theoretical error (although with small deviations at Karlsruhe and Izana). This indicates that the error budget and sensitivity characterization are realistic and correct.

#### 5.5 Statistics of the agreement between FTIRs and IASI

Figure 10 gives a scatter plot of IASI vs. FTIR observations for the three different sites. The data refer to the  $\delta D$  at 2.5 km for Kiruna and Karlsruhe and at 5.5 km for Izana, which are the altitudes for which the two instruments share the most sensitivity. The SD of the difference between IASI and FTIR for all the collocated measurements are 24, 35 and 55‰ for Kiruna, Karlsruhe and Izana respectively which is in very good agreement with theoretical expected difference. The correlation coefficients of 0.75,

### Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



0.77 and 0.68 indicate that  $\delta D$  retrieved from both instruments co-vary well together. The smaller correlation coefficient of 0.68 at Izana compared to Kiruna and Karlsruhe is logical due to the larger difference expected at this site. The slope of the regression curves indicate that the amplitude of  $\delta D$  variations is more important for IASI than FTIR at Kiruna and Karlsruhe. But that the opposite prevails at Izana.

For the three sites, IASI  $\delta D$  are biased low compared to FTIR. The mean bias values (FTIR-IASI) are 107, 72 and 47‰ for Kiruna, Karlsruhe and Izana respectively. Since we are not considering exactly the same atmosphere in the different locations due to the impossibility of smoothing one retrieval with the averaging kernels of the other the values can not quantitatively be compared between them. Qualitatively, this bias appear to decrease with altitude and the value of 47‰ found at Izana is close to what has been found in the recent absolute validation of ground-based FTIR by Schneider et al. (2014) where the authors found a high bias of the Izana ground-based FTIR of +70‰ in the middle troposphere. In Wiegele et al. (2014), the authors used the same FTIR data to cross-validate the IASI/MUSICA product (retrieved at KIT/IMK-ASF) and found for all sites a consistently low bias. A direct comparison between the here presented IASI/ULB product and the IASI/MUSICA product would be interesting, but is out of the scope of this paper.

## 5.6 Variations of the $\log(q)$ - $\delta D$ relation

To analyze the consistency of the humidity- $\delta D$  relation between IASI and ground-based FTIR observations we follow a similar approach than for comparison with TES. The idea is to see if IASI and ground based FTIRs show coherent variations in the  $\log(q)$ - $\delta D$  space. We plot on Fig. 11  $\delta D$  vs. humidity for the three different sites.  $\delta D$  (at 2.5 km for Kiruna and Karlsruhe and at 5.5 km for Izana) are given in terms of relative variations to remove the biases discussed above. In the 3 first panels the different seasons are differentiated by colours. To better visualize spatial variations the comparison is also provided for all sites together but with colours to distinguish each (right

### Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



panel). Since the different retrievals are not considering the same atmosphere this is a qualitative approach.

The extreme right panel of Fig. 11 shows that the three different sites exhibit very different distributions in the  $\delta D$ - $\log(q)$  space. The amplitude of variations are very similar for IASI and the ground-based FTIR. The variability is the largest at Izana with 400% between the minimum and maximum values, due to the fact that the retrieved value refer to the free troposphere (5.5 km) where the true variability is indeed expected to be large. The amplitude of variations is the lowest for Kiruna. At this site for which no winter collocated points were available, we observe a good agreement between the two distributions. The amplitudes of variations (for  $\delta D$  and  $H_2O$ ) for both instruments are similar as well as the seasonal differences although in the case of IASI the seasonal patterns appear to be more scattered. At Karlsruhe the general patterns agree best despite a steeper slope for IASI and shows well differentiated seasonal differences for both instruments. At Izana IASI retrievals are more scattered than the FTIR ones owing to the larger observational error from IASI.

Overall Fig. 11 shows that IASI and the ground-based FTIR reproduce similar spatial and seasonal variations in humidity- $\delta D$  relationships. We can safely conclude that the two instruments probe the same hydrological processes in the same way.

## 6 Conclusions

In this study we have cross-validated  $\delta D$  profiles retrieved from IASI spectra with profiles from TES and three ground-based FTIRs. We provided a comprehensive and detailed estimation of error differences expected from the comparisons between the different instruments. Generally, we find that the total difference between TES and IASI, and between IASI and the ground-based FTIR is controlled by IASI observational error and by the smoothing error due to the differences in sensitivity of the instruments. In the comparison with the ground-based FTIRs, only a direct comparison was performed because it was not possible to simulate one retrieval with the averaging kernels of the

### Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



other. The relevance of the different comparisons was analysed regarding the expected natural variability of  $\delta D$  at a global scale and also at regional scale. Except at Izana, all the comparisons exhibit differences lower than expected natural variability at regional scales.

5 We have further verified the theoretical consistency of our error estimations and showed that they were consistent with the real differences in  $\delta D$  measured by the various instruments. This successful cross-validation of IASI has been performed at various locations from tropical to Arctic latitudes above sea and land giving us excellent confidence in the retrieved profiles from IASI at global scale. Moreover, spatio-temporal  
10 variations of the humidity– $\delta D$  relation were analysed and show coherent variations among the instruments, indicating that the latter were sensitive to the hydrological processes in the same way.

The cross-validation exercise performed here also allowed us to better characterize IASI retrievals. Above sea, we have shown that IASI retrieval exhibit large error in the  
15 lower and upper troposphere exceeding the expected natural variability of  $\delta D$ . The retrieved profile is on the contrary exploitable in the free troposphere where the error is minimized. Above land, the large thermal contrast reduces the error in the lowest layers and allows retrieving profiles of  $\delta D$  down to the near surface with sufficient precision, as demonstrated with the comparison at Kiruna and Karlsruhe.

20 By analysing the empirical differences between IASI and the other sounders, we found a small bias with TES ( $-3\%$  in the free troposphere) and an important bias with the FTIR ( $-47\%$  in the free troposphere). As TES data are bias-corrected, this suggest that the IASI retrieved profiles presented here are unbiased. Furthermore the TES bias correction is applied to deal with a supposed inconsistency with spectroscopy of HDO, which we cannot confirm after this cross-validation.  
25

Finally, we have investigated the impact of IASI sampling in a model–instrument comparison and showed that the daily agreement between model and IASI was greatly improved when using all IASI observations available in a model cell. This suggests that

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## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

---

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

model evaluation against observations could be optimized with IASI more than with other sounders (in the free troposphere).

## Appendix A: Sensitivity change along the meridional gradient for IASI retrieval

Since IASI presents some sensitivity to surface we expect a change in sensitivity with decreasing surface temperature. This change is not visible on Fig. 3, in this appendix we further investigate this apparent contradiction. In Fig. A1, we used all available IASI data along the meridional gradient and average the degrees of freedom for H<sub>2</sub>O and  $\delta$ D on latitude bins. For H<sub>2</sub>O there is an increase in sensitivity with surface temperature and a small decrease is observed with high water vapour content. For  $\delta$ D we also observe a significant increase in DOFS with latitude but with a more significant drop off in sensitivity with high water vapour content. This could explain why IASI sensitivity is more constant with latitudinal variations than TES.

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## Cross-validation of IASI/MetOp $\delta$ D retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## References

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### Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



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## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



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## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Risi, C., Noone, D., Worden, J., Frankenberg, C., Stiller, G., Kiefer, M., Funke, B., Walker, K., Bernath, P., Schneider, M., Bony, S., Lee, J., Brown, D., and Sturm, C.: Process-evaluation of tropospheric humidity simulated by general circulation models using water vapor isotopic observations: 2. Using isotopic diagnostics to understand the mid and upper tropospheric moist bias in the tropics and subtropics, *J. Geophys. Res.*, 117, D05304, doi:10.1029/2011JD016623, 2012a. 11089

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**Cross-validation of  
IASI/MetOp  $\delta$ D  
retrievals**

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



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## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



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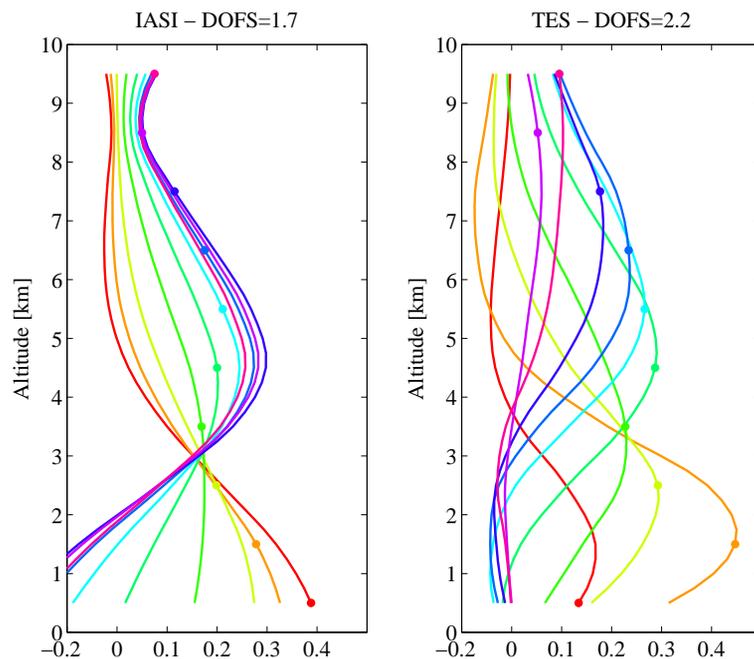






**Cross-validation of  
IASI/MetOp  $\delta D$   
retrievals**

J.-L. Lacour et al.

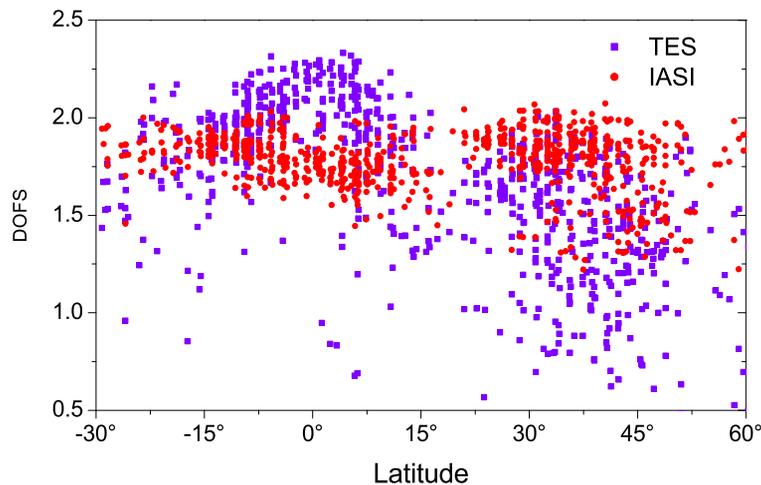


**Figure 2.** Typical averaging kernels in  $\{\delta D\}$  proxy space for IASI (left panel) and for TES (right panel) for a tropical scene ( $2.5^\circ$  N). The nominal heights of the kernels are marked by filled circles.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

**Cross-validation of  
IASI/MetOp  $\delta D$   
retrievals**

J.-L. Lacour et al.

**Figure 3.** TES (purple) and IASI (red) degrees of freedom for  $\delta D$  along the meridional gradient.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

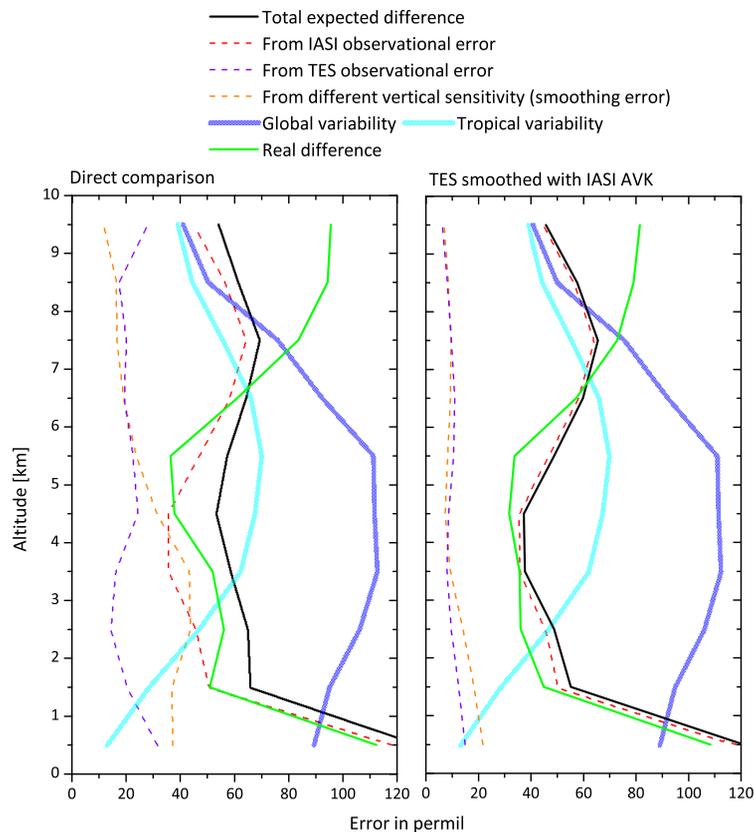
Printer-friendly Version

Interactive Discussion



## Cross-validation of IASI/MetOp $\delta D$ retrievals

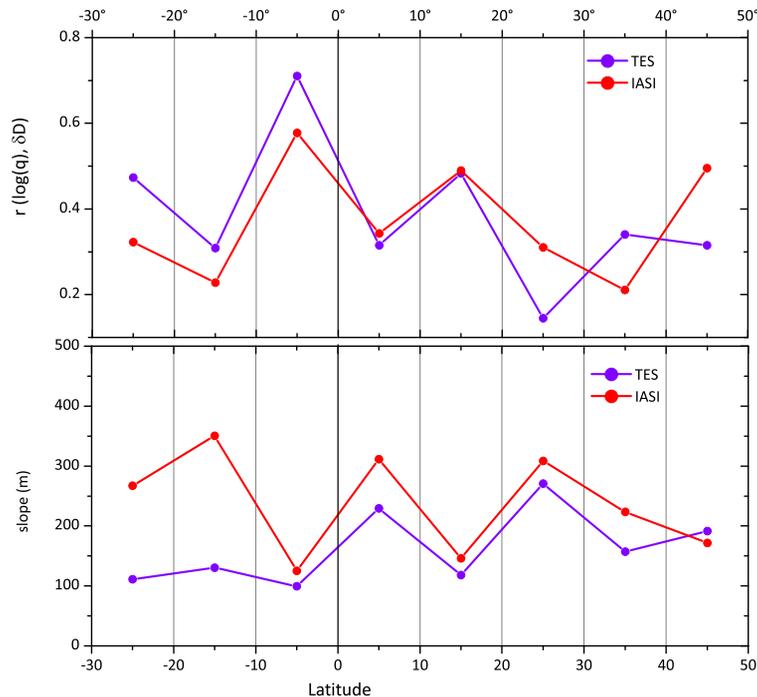
J.-L. Lacour et al.



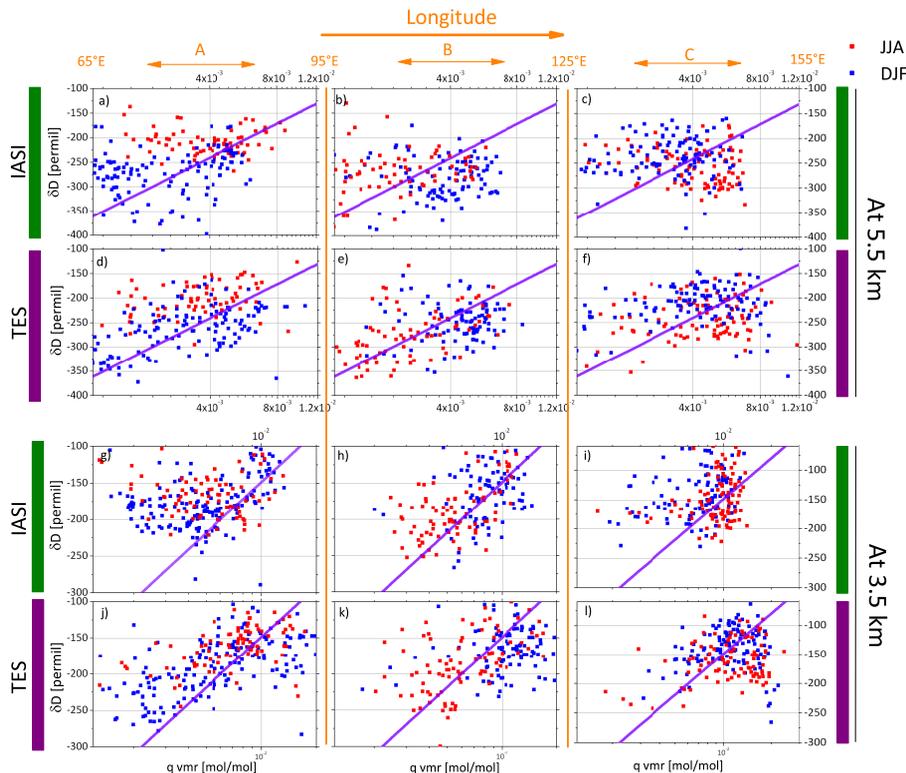
**Figure 4.** Expected difference of the IASI and TES retrieval at tropical latitudes and its different contribution sources according to Eq. (8) for the direct comparison (left) and to Eq. (10) for the smoothed comparison (right). The squareroot of the diagonal elements of the  $\mathbf{S}_\delta$  matrix as well as the different contribution matrices are plotted. Real differences are also shown in green.

**Cross-validation of  
IASI/MetOp  $\delta D$   
retrievals**

J.-L. Lacour et al.



**Figure 5.** Top panel: variation of the correlation coefficient between  $\log(q)$  and  $\delta D$  at 4.5 km along the meridional gradient for TES (purple) and IASI (red). Bottom panel: variation of the slope of the linear regression between  $\log(q)$  and  $\delta D$  (spatial and temporal variability within the  $10^\circ$  bin) along the meridional gradient for TES (purple) and IASI (red).



**Figure 6.** Spatio temporal variations of the  $\delta D$ – $q$  relation for the PIO dataset. Retrieved  $\delta D$  and  $q$  are separated in 3 longitudinal boxes of  $30^\circ$  (A, B, C) from  $65$  to  $155^\circ$  E to highlight spatial variations. Winter (DJF, blue squares) and summer (JJA, red squares) are also separated to highlight seasonal variations. (a–c) correspond to IASI retrieved values at  $5.5$  km, and (g–i) to IASI retrieved values at  $3.5$  km. (d–f) correspond to TES retrieved values at  $5.5$  km, and (j–l) to TES retrieved values at  $3.5$  km. The purple line represents a Rayleigh distillation curve computed according to Eq. (11) with  $q_0 = 0.03 \text{ mol mol}^{-1}$  and  $\delta D_0 = -70\text{‰}$ .

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

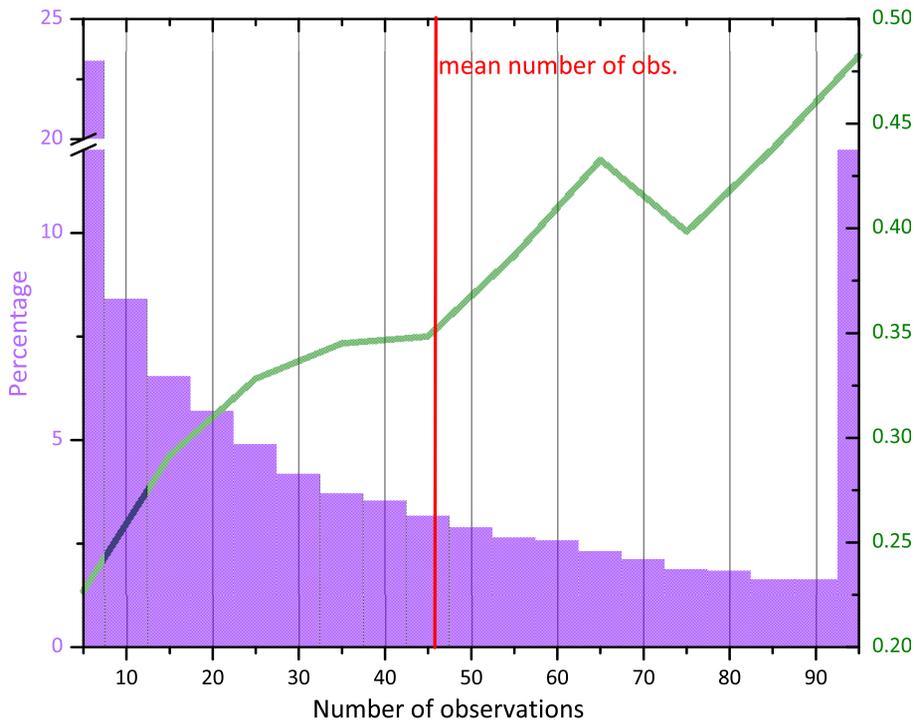
Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion





**Figure 7.** On the background (purple): histogram in percent of the number of IASI observations available per model cell for the LMDZ-IASI comparison (daily values) above the Pacific and Indian oceans dataset. In green, correlation coefficient between  $\delta D$  simulated by LMDZ and averaged  $\delta D$  from all observations available in the cell in function of the number of observations available.

**Cross-validation of IASI/MetOp  $\delta D$  retrievals**

J.-L. Lacour et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

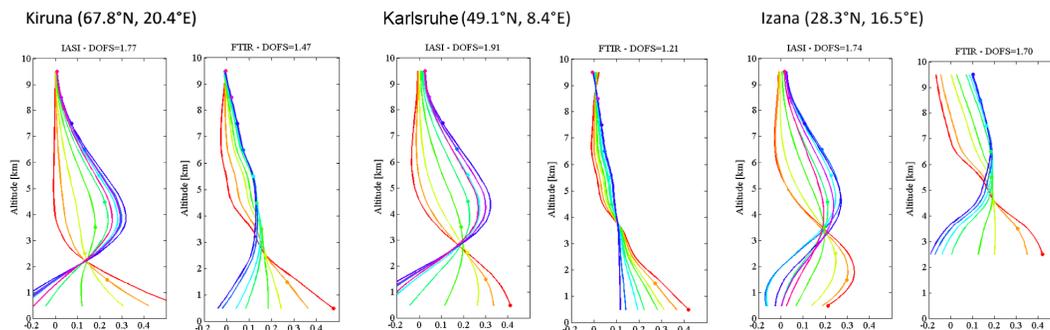
Printer-friendly Version

Interactive Discussion



## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.



**Figure 8.** Averaging kernels in  $\{\delta D\}$  proxy space for the three different sites of the comparison: (a) and (b) for Kiruna, (c) and (d) for Karlsruhe and (e) and (f) for Izana. (a), (c) and (e) corresponding to IASI and (b), (d) and (f) to the ground-based FTIR.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

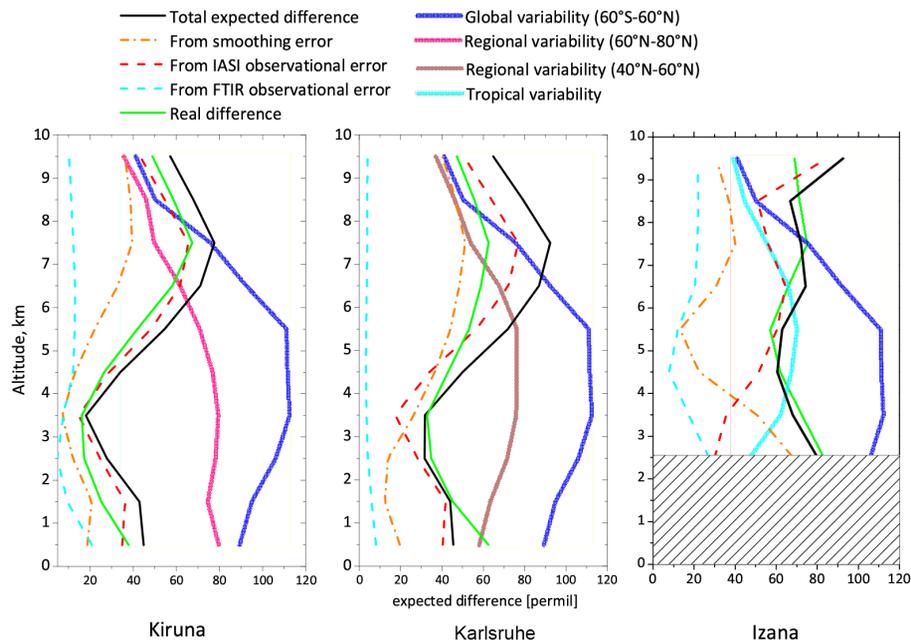
Printer-friendly Version

Interactive Discussion



## Cross-validation of IASI/MetOp $\delta D$ retrievals

J.-L. Lacour et al.



**Figure 9.** Same as Fig. 5 but for the comparison between IASI and the ground-based FTIR of Kiruna (left) and Karlsruhe (right).

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

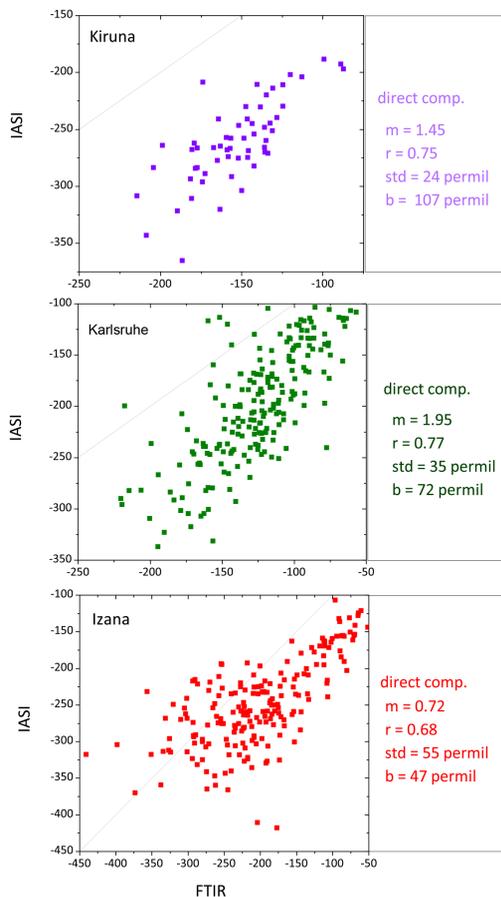
Printer-friendly Version

Interactive Discussion



**Cross-validation of IASI/MetOp  $\delta D$  retrievals**

J.-L. Lacour et al.

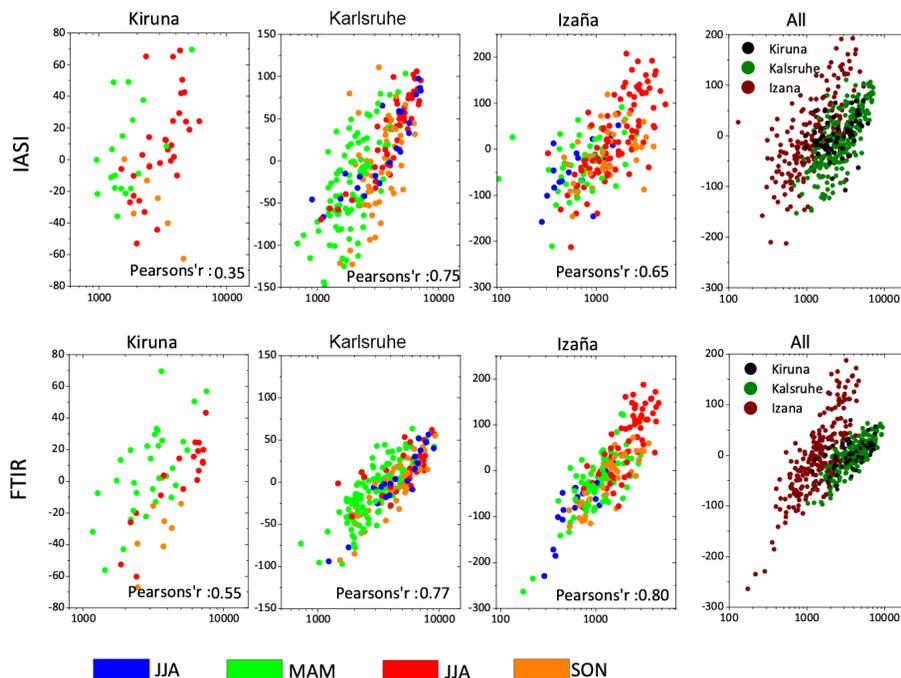


**Figure 10.** Scatter plot of IASI vs. FTIR  $\delta D$  from top to bottom for Kiruna (2.5 km), Karlsruhe (2.5 km) and Izana (5.5 km). We give the slopes of the major axis regression curves ( $m$ ), the Pearson correlation coefficient ( $r$ ), the SD of the difference and the mean bias ( $b$ , FTIR-IASI).

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

## Cross-validation of IASI/MetOp $\delta D$ retrievals

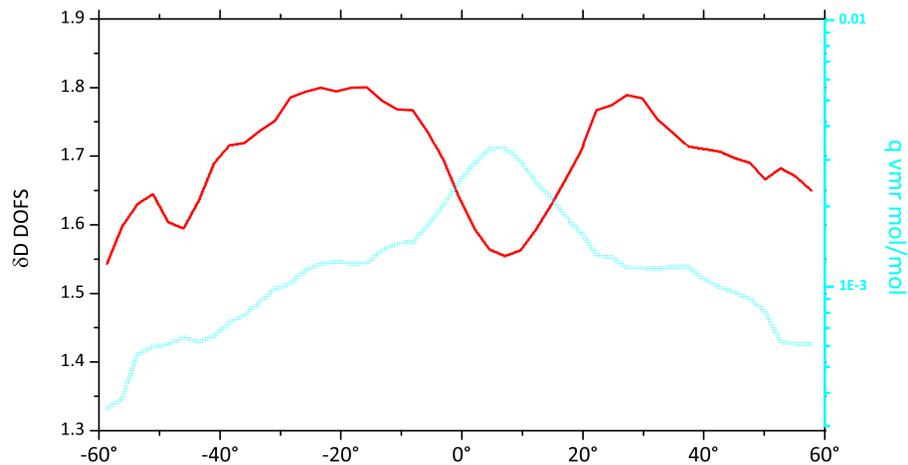
J.-L. Lacour et al.



**Figure 11.** Distributions of IASI (top) and FTIR (bottom) observations in the  $\log(q)$ – $\delta D$  space for the three different sites (from left to right: Kiruna, Karlsruhe and Izaña). The colours refer to seasons. Distributions for the three sites together are given on the right panel, with colours differentiating the sites: brown is for Izaña, green for Karlsruhe and yellow for Kiruna.  $\delta D$  values are presented in relative variations. Pearson correlation coefficient between  $\delta D$  and  $\log(q)$  are also documented in the bottom of the plots.

**Cross-validation of IASI/MetOp  $\delta D$  retrievals**

J.-L. Lacour et al.



**Figure A1.** Variation of the degrees of freedom for IASI  $\delta D$  retrieval along the latitudinal gradient (red) and mixing ratio of water vapour at 4.5 km.

[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[◀](#)[▶](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)