

Quality assessment
of ground-based FTIR
O₃ profiles

M. Schneider et al.

Quality assessment of O₃ profiles measured by a state-of-the-art ground-based FTIR observing system

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Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Abstract

Ground-based FTIR measurements are an important component of the global atmospheric monitoring system. Their essential role in validating satellite measurements requires a precise documentation of their quality. Here we present an extensive quality documentation of ground-based FTIR O₃ profiles. This is done in form of theoretical and empirical error estimations. The latter is achieved by intercomparison to ECC-sonde O₃ profiles. The FTIR O₃ amounts are obtained by applying the currently most advanced instrumentation and retrieval strategies. It consequently presents the current potential of this remote sensing technique.

1 Introduction

Ground-based measurements of highly-resolved infrared solar absorption spectra allow ongoing detection of the composition of the atmosphere in a cost-effective manner. They are essential for long-term monitoring and for validating satellite measurements and, thus, they are a vital component of the global atmospheric monitoring system. However, their application as reference measurement requires a precise documentation of their quality. This is often done exclusively by theoretical studies. The errors are then calculated by a method suggested by C. D. Rodgers (Rodgers, 2000). These calculations give a good overview of the achievable data quality, however, they depend on the assumed error sources. Therefore, every assessment of data quality should be completed by a comparison to independent measurements of similar or better quality. Ozone is very suited for such an empirical quality assessment. It is an important atmospheric constituent and is monitored since many years by a great variety of measurement techniques. In this work we use ECC-sondes, launched weekly very close to the FTIR measurement site, for an empirical validation of the FTIR O₃ profiles. The FTIR O₃ profiles are obtained by a optimised retrieval approach (Schneider and Hase, 2008). While the total column amounts obtained from this approach have already been

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures



Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



validated in great detail by an intercomparison to Brewer measurements (Schneider et al., 2008), in this work we concentrate on the profiles.

Similar validation studies of ground-based FTIR O₃ profiles have already been performed by different authors (Pougatchev et al., 1996; Nakajima et al., 1997; Barret et al., 2002; Schneider et al., 2005a; Kagawa et al., 2007). In some of these works the empirical validation is performed for a very reduced number of sonde-FTIR coincidences, which are furthermore measured within a short time range during specific campaigns. Consequently they poorly represent the actual atmospheric variability. In this work we present an extensive empirical validation consisting of 53 coinciding operational ECC sonde and FTIR measurements performed between January 2005 and December 2006 on Tenerife Island. Furthermore, we apply state-of-the-art retrieval strategies and instrumentation. The quality of the FTIR O₃ profiles applied in this paper reflects the current potential of ground-based FTIR systems in monitoring the vertical distribution of all trace gases with absorption signatures similar to those of O₃.

In the following Section we briefly inform about the applied FTIR instrumentation and retrieval strategy. In Sect. 3 we present the results of our theoretical error estimation. In Sect. 4 we compare the ECC and FTIR O₃ profiles.

2 FTIR measurements and retrieval strategies

The FTIR measurements are performed at the Izaña Observatory, which is located on the Canary Island of Tenerife, 300 km from the African west coast at 28°18' N, 16°29' W at 2370 m.a.s.l. From January 1999 to April 2005 a Bruker IFS 120M spectrometer was used (Schneider et al., 2005b). Since January 2005 we operate a Bruker IFS 125HR spectrometer. In this work we only evaluate spectra measured by this new IFS 125HR, which offers a better performance than the IFS 120M. We use the retrieval code PROFFIT 9.4 (Hase et al., 2004) with the option to retrieve isotopologue ratio profiles (Schneider et al., 2006b). It applies the Karlsruhe Optimised and Precise Radiative Transfer Algorithm (KOPRA, Höpfner et al., 1998; Kuntz et al., 1998; Stiller et al., 1998)

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



as the forward model, which was developed for the analysis of MIPAS-Envisat limb sounder spectra. For the atmospheric O₃ retrieval we analyse a combination of small and broad spectral windows between 780–1015 cm⁻¹.

The retrieval strategy is essentially the one described in [Schneider and Hase \(2008\)](#) and consists in a simultaneous retrieval of O₃ and temperature profiles. A-priori knowledge of O₃ (mean profile and covariances) is taken from an ECC sonde climatology calculated from measurements between 1996 and 2006 as depicted in Fig. 1. It is important to mention that we use the same set of a-priori data for all retrievals. We do not vary our a-priori depending on season, a strategy often applied in other studies (e.g. [Barret et al., 2002](#)). This assures that all variability seen in our profile comes from the measurement and can be easily interpreted. The O₃ amounts around the tropopause are highly variable. Under these conditions an inversion performed on a logarithmic scale is superior to a inversion performed on a linear scale ([Hase et al., 2004](#); [Schneider et al., 2006a](#); [Deeter et al., 2007](#)). Furthermore, the inversion on a logarithmic scale allows to constrain against isotopologue ratio profiles ([Schneider et al., 2006b](#)). As a-priori for the typical ozone isotopologue ratio profiles and their covariances we use data reported by [Johnson et al. \(2000\)](#). The applied temperature a-priori profile is a combination of the data from the local ptu-sondes (up to 30 km) and data supplied by the automailer system of the Goddard Space Flight Center. The spectroscopic line parameters are taken from the HITRAN 2004 database ([Rothman et al., 2005](#)). For H₂O we apply the 2006 updates.

3 Theoretical quality assessment

When contemplating remotely-sensed vertical distribution profiles it is important to remember the inherent vertical resolution of these data. Figure 2 shows typical averaging kernels for the retrieved ⁴⁸O₃ profiles and demonstrates that the FTIR measurements contain information about the vertical distribution from the surface up to 40 km. The best vertical resolution is achieved between altitudes of 10 and 20 km, where the

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



FWHM (full width half maximum) of the kernels is around 5 km. The trace (sum of diagonal entries) of the averaging kernel matrix is a measure of the degree of freedom in the measurement. It indicates the number of independent layers present in the retrieved profile. Summing up the diagonal entries of the averaging kernel matrix gives a good overview of the layers that are independently presented in the retrieved profile. We identify as independent layer the altitude ranges where the sum of the corresponding diagonal entries reaches unity. The right panel of Fig. 2 gives an overview of these layers. It plots the altitude ranges for which the sum of the kernel matrix's diagonal elements reaches unity (x-axis) versus the altitude where this layer is centred (y-axis). The centre of the layer is the weighted mean (weighted by kernel matrix's diagonal elements) of the altitudes contributing to the layer. It shows that up to 20 km the FTIR observing system is able to distinguish layers with a vertical extension of smaller than 8 km and in the middle stratosphere of around 10 km. The best resolution is achieved at the tropopause, where layers with a extension of 5 km can be distinguished. The uppermost layer that can be resolved extends from 26 km to the top of the atmosphere.

Our theoretical error estimation bases on the analytic method suggested by Rodgers (2000), which identifies three error classes: (a) smoothing error, (b) error due to uncertainties in input parameters (instrumental characteristics, spectroscopic data, ...), and (c) errors due to measurement noise:

$$\hat{\mathbf{x}} - \mathbf{x} = (\hat{\mathbf{A}} - \mathbf{I})(\mathbf{x} - \mathbf{x}_a) + \hat{\mathbf{G}}\hat{\mathbf{K}}_p(\mathbf{p} - \hat{\mathbf{p}}) + \hat{\mathbf{G}}(\mathbf{y} - \hat{\mathbf{y}}) \quad (1)$$

We consider the nonlinearities of the forward model within the variability range of the state vector, therefore, we individually apply Eq. (1) to all members of an ensemble of 500 simulated real states which obeys the a-priori statistics: we calculate 500 individual matrices $\hat{\mathbf{A}}$ (averaging kernel matrix), $\hat{\mathbf{G}}$ (gain matrix), and $\hat{\mathbf{K}}_p$ (model parameter sensitivity matrix). In Eq. (1) $\hat{\mathbf{x}}$, \mathbf{x} , and \mathbf{x}_a is the retrieved, real (i.e. $\hat{\mathbf{x}} - \mathbf{x}$ is the error),

and a-priori state, $\hat{\boldsymbol{p}}$ and \boldsymbol{p} the estimated and real model parameters, $\hat{\boldsymbol{y}}$ and \boldsymbol{y} the measured and simulated spectrum, and \mathbf{I} the identity matrix. This procedure assures a very accurate error analysis. The assumed error sources are listed in Table 1.

Figure 3 shows the standard deviation of the errors calculated for the 500 simulations according to Eq. (1). When considering vertically fine structured profiles, the smoothing error is the leading error since the FTIR system only provides sufficient information about rough vertical structures. It reaches 25% in the tropopause region, where the actual profile is highly-structured. The most important parameter errors are remaining ILS distortions (uncertainties in modulation efficiency and phase error), uncertainties in the temperature profile, and errors in the applied pressure broadening parameter. Even though a systematic error source, the pressure broadening coefficient produces random errors since $\hat{\mathbf{G}}$ and $\hat{\mathbf{K}}_p$ of Eq. (1) depend on the actual atmospheric state. Figure 4 depicts the systematic errors of the retrieved profiles (mean value of the errors calculated from the 500 simulations). We find that the uncertainty in the pressure broadening coefficient is the most important systematic error source.

If we only consider rough vertical structures (layers with extension of 5–10 km the smoothing error becomes less important. The right panel of Fig. 2 gives an idea about a reasonable choice for the extension of these layers: e.g. a first layer representing the troposphere (surface – 10 km, subsequently called the TR layer), a second layer the tropopause region (12.5–17 km, subsequently called the TP layer), and a third layer the middle stratosphere (20–30.5 km, subsequently called the MS layer). Tables 2 and 3 present the error estimations for these layers. We additionally include the estimations for the layer ranging from the surface to 30.5 km which corresponds to the altitudes covered by nearly all ECC sondes. The partial column amount errors of these layers are investigated in great detail. While for the VMR profile errors (Figs. 3 and 4) we restricted the discussion to an estimation of the mean and standard deviation, for we separate these partial column amount errors in random error, systematic sensitivity error, and systematic bias error component. Figure 5 illustrates how these different error components are obtained. It depicts the dependence of the error on the actual

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

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

O₃ amount of the MS layer taking the smoothing error as example. The slope of the linear regression line gives the systematic sensitivity error (in our example -7.2%), the offset at the climatological value the systematic bias error (-0.2 DU or -0.1% if referred to the climatological amount of the MS layer), and the scattering around the regression line the random error (2.0 DU or 1.3%). This error treatment is described in Schneider and Hase (2008), which should be consulted for more details.

For the layers as depicted in the right panel of Fig. 2 the sensitivity error does not significantly exceed -10% (i.e. the FTIR system has a sensitivity of around 90%). This is a very satisfactory value, and demonstrates that the high quality measurements together with an advanced retrieval strategy allow an adequate monitoring of these rough atmospheric structures. An artificial increase of this sensitivity by applying seasonally dependent a-priori data is not necessary and would only difficult the interpretation of the FTIR data. Table 3 as well as Fig. 4 show that the systematic errors are dominated by the smoothing error and uncertainties in the spectroscopic line parameters.

4 Empirical quality assessment

For this assessment we compare the FTIR O₃ profiles to regularly performed ECC-sonde measurements. The ozone sonde program started in November 1992 applying ECC-sondes (type: Scientific Pump 6A). The sondes are launched weekly from Santa Cruz de Tenerife (35 km northeast of the Observatory) and since October 2006 from Güimar (15 km south of the Observatory). In March 2001 Izaña's ECC-sonde together with the Brewer, DOAS, and FTIR activities have been accepted by the NDACC (Network for Detection of Atmospheric Composition Change (<http://www.ndacc.org/>), formerly called NDSC: Network for Detection of Stratospheric Change (Kurylo, 1991, 2000)).

The ECC-sondes generally burst between 30 and 34 km. To use as many sondes as possible and to homogenize the study we use only ECC data measured up to 30.5 km. This altitude is reached by around 90% of all sondes. These criteria provide 53 coin-

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



cing ECC and FTIR measurements (for 33 different ECC measurements).

4.1 Quality check for ECC-sondes

[Schneider et al. \(2008\)](#) demonstrates the high quality of the FTIR total column amounts by an extensive intercomparison to Brewer data. A correlation coefficient of 0.992 and an agreement within 0.6% between coinciding measurements made between 2005 and 2007 allows to conclude that both techniques have a precision of better than 0.5%. However, [Schneider et al. \(2008\)](#) also observes a systematic difference of 4–5%, which is consistent to laboratory studies of [Picquet-Varrault et al. \(2005\)](#). Therefore, we mainly attribute it to inconsistencies between the spectroscopic data in the UV (Brewer), on the one hand, and the infrared (FTIR), on the other hand.

Here we make an analogous brief study for the ECC amounts. As aforementioned we only apply ECC data for altitudes below 30.5 km. However the residual O₃ partial column above this altitude is still around 20% of the total O₃ amount. From the HALOE climatology ([Groß and Russell III, 2005](#)) we deduce a 1σ value for the O₃ variability above 30.5 km of typically 10–15%. Assuming a vertical correlation length of 2.5 km (which corresponds to the length derived from the ECC data around 30 km), we estimate a 1σ variability for the O₃ residual of 4 DU. The left panel of Fig. 6 shows the correlation between Brewer total O₃ amounts and ECC partial O₃ amounts below 30.5 km for all 80 Brewer/ECC coincidences during 2005 and 2006. We calculate a difference of 60.6 ± 6.8 DU. Approximately 4 DU of the scatter between the Brewer and ECC data is caused by the ignorance of the ECC O₃ residual. Since the Brewer total column amounts are very precise (around 1.5 DU), there is a remaining scatter of around $\sqrt{6.8^2 - 4^2} \approx 5.3$ DU (or around 2.0% if referred to the typical amount), which can be attributed to errors in the ECC data or to the observation of different air-masses by the Brewer, on the one hand, and by the ECC sonde, on the other hand. However, this 2.0% is already less than estimated by the laboratory study of [Smit and Sträter \(2004\)](#), which determines an uncertainty of 6% for the Scientific Pump 6A ECC-

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



sonde type. Furthermore, we found no single outlier for all sondes from 2005 and 2006. Consequently we can conclude that the Izaña ECC sonde measurements are of very high quality.

Instead of ignoring the O_3 residual it is often estimated by extending the mixing ratio measured at the balloon's burst altitude until the top of the atmosphere (e.g. Minutes of the NDACC ozonesonde PI meeting in Potsdam, July 1998, available at the NDACC web site: www.ndacc.org). It is argued that this approach accounts for part of the real variabilities present in the O_3 residual. The right panel of Fig. 6 depicts the Brewer total O_3 versus the ECC total O_3 calculated for the so-estimated O_3 residual. Naturally the systematic difference is smaller if compared to the left panel. However, we observe a slightly poorer correlation, indicating that, at least at the subtropical site of Izaña, such a simplified estimation of the O_3 residual introduces more noise than real information.

4.2 FTIR versus ECC-sonde

When validating remotely-sensed vertical distribution profiles it is important to remember the inherent vertical resolution of these data. There are two possibilities to adequately validate remotely-sensed profiles: (a) degrade the vertical resolution of the vertically highly-resolved data towards the vertically poorly-resolved data. By this means we exclude the smoothing error from the comparison. In our case the ECC in-situ measurements are vertically highly resolved. (b) Another possibility is to compare only the rough structures that are supposed to be resolvable by the remote sensing measurements. We estimated these structures in Sect. 3 and depict them in the right panel of Fig. 2. In the following we compare FTIR and ECC profiles applying both method (a) and method (b).

Quality assessment of ground-based FTIR O_3 profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



4.2.1 Comparison of FTIR and smoothed ECC profiles

The smoothing (or degradation) of the vertically highly-resolved ECC profile x_{ECC} is done by convolving it with the FTIR averaging kernels $\hat{\mathbf{A}}$:

$$\hat{x}_{\text{ECC}} = \hat{\mathbf{A}}(x_{\text{ECC}} - x_a) + x_a \quad (2)$$

5 The result is an ECC profile (\hat{x}_{ECC}) with the same smoothing error as the FTIR profile. Consequently the difference between FTIR and smoothed ECC profile eliminates the smoothing error component, which is the leading error component. Equation (2) requires ECC profile data beyond 30.5 km. However, this data is not available and we extend the ECC profile with the zonally averaged HALOE climatological profile used as
10 a-priori in the FTIR retrieval. Consequently the smoothed ECC profile is a combination of two experiments: the ECC and HALOE experiments. Furthermore, applying a climatological profile above 30.5 km introduces additional random errors in the smoothed ECC profile close to 30.5 km. Figure 7 depicts the mean and standard deviation for the difference between FTIR and smoothed ECC profile. These calculations are comparable to the error estimations presented in Figs. 3 and 4. The grey shaded area indicates the total random error of the FTIR profiles (excluding the smoothing error, thick black line in Fig. 3). The light grey shaded area indicated the sum of the FTIR and ECC random errors. As ECC random error we assumed 6% suggested in Smit and Sträter (2004). From the surface up to 26 km we found systematic differences between the
20 FTIR and smoothed ECC data of -9 to $+9\%$. These differences become significant around 12 and 18 km and are probably due to incorrect line parameterisations (error in the pressure broadening coefficient (compare to Fig. 3)). Above 30 km we observe a clear significant systematic difference of up to 16%. Since we compare a combination of ECC sonde and HALOE with FTIR it is difficult to interpret this observation. The
25 reason may be a systematic underestimation of the ECC sondes above 25 km, systematic FTIR errors (due to line parameterisation), or systematic differences between the applied HALOE climatology and the actual climatology above Tenerife.

The observed standard deviation of the difference between FTIR and ECC is as
4986

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



a mean 5% (between the surface and 30.5 km). It is highest between 10 and 15 km where it reaches 10%. It is in a satisfactory agreement to the expected errors of around 7% (light grey shaded area of Fig. 7). The slightly higher standard deviation may be due to the observation of different airmasses by FTIR and ECC or due to a weak over-estimation of the theoretical vertical resolution of the FTIR. It is important to mention that Fig. 7 provides no comprehensive documentation of the quality of the FTIR profile. This is only possible together with the averaging kernels: Schneider et al. (2005a) also reports an agreement within 5–10% to ECC sondes but for FTIR profiles inverted by applying spectra of poorer quality and non-optimised retrieval strategies. This leads to broader averaging kernels and provides a stronger smoothing of the ECC profile. The agreement is similar, but the compared vertical structures are much rougher.

4.2.2 Comparison of partial column amounts

A straight forward comparison of partial columns has the advantage that the results are easy to interpret. Figure 8 depicts the correlation of the TR, TP, MS and surface – 30.5 km partial columns calculated from the FTIR and original ECC sonde data. The corresponding estimated FTIR errors are collected in Tables 2 and 3. We found good consistency between these estimations and the FTIR/ECC intercomparison. The scatter between the FTIR and ECC amounts is close to the estimated FTIR random errors. For the TR and TP layers we get correlation coefficients of at least 0.96. For the MS layer we still get a coefficient of 0.92 and for the layer from the surface up to 30.5 km a coefficient of 0.96. The scattering around the regression line is 1.5 DU (or 6.8% if related to the climatological amounts) for the TR layer, 1.6 DU (12.1%) for the TP layer, 3.0 DU (1.8%) for the MS layer, and 5.2 DU (2.4%) for the layer from the surface to 30.5 km. Concerning the systematic differences we expect a sensitivity error for the FTIR data of –5.4 and –7.2% for the TR and MS layer, respectively, and a larger error of around –11% for the TP layer (see Table 3). This estimated FTIR sensitivities are confirmed by the comparison to the ECC amounts. Figure 8 shows higher slopes for the TR and MS layers (0.94 and 0.88, respectively) than for the TP layer (0.81). A

**Quality assessment
of ground-based FTIR
O₃ profiles**

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



bias in the FTIR data is mainly produced by errors in the spectroscopic parameters. We estimate that it is more important for the TR and TP layer than for the MS layer (see Table 3). This is quantitatively confirmed by the intercomparison. If related to the climatological amounts there is a systematic bias between FTIR and ECC amounts of $\frac{-0.75 \text{ DU}}{21.61 \text{ DU}} = -3.5\%$ and $\frac{0.54 \text{ DU}}{12.61 \text{ DU}} = +4.0\%$ for the TR and TP layer, respectively, and a smaller bias of $\frac{2.62 \text{ DU}}{161.01 \text{ DU}} = +1.6\%$ for the MS layer. For the layer between the surface and 30.5 km it is $\frac{4.00 \text{ DU}}{218.62 \text{ DU}} = +1.8\%$. This is a relatively low value remembering that between the total column amounts of FTIR and Brewer a bias of up to 5% was observed (Schneider et al., 2008). FTIR and ECC amounts are in good agreement. The observed differences between both experiments are close to the differences expected due to the FTIR errors. This indicates that the ECC sonde provides very precise O₃ data and/or that the FTIR error estimation is rather conservative.

In Sect. 4.1 we compared the Brewer total O₃ amounts to the ECC O₃ amounts between the surface and 30.5 km. This comparison reveals a remaining scatter of around 2%, which can be contributed to errors in the ECC measurements or to the observation of different airmasses by the two experiments. Brewer and FTIR analyse the same airmass (they have the same observation geometry) and the disagreement between the FTIR and the ECC data is very similar to the disagreement between the Brewer and the ECC data. This is demonstrated in Fig. 9, which depicts the differences between the ECC partial column amounts ($\text{PC}_{\text{ECC}} = \int_{2.37 \text{ km}}^{30.5 \text{ km}} x_{\text{ECC}} dz$) and the Brewer total column amounts ($\text{TC}_{\text{Brewer}}$) versus the differences between the ECC and FTIR partial column amounts ($\text{PC}_{\text{FTIR}} = \int_{2.37 \text{ km}}^{30.5 \text{ km}} x_{\text{FTIR}} dz$). We can use the Brewer data to account for the observation of different airmasses or for the errors in the ECC data. Therefore we normalise the ECC data to the Brewer total column amounts:

$$x_{\text{ECC},\text{norm}} = \frac{\text{TC}_{\text{Brewer}}}{\text{PC}_{\text{ECC}} + 60.6 \text{ DU}} x_{\text{ECC}} \quad (3)$$

Here 60.6 DU is the mean value of the residual O₃ amount. Figure 10 compares the normalised ECC partial column amounts to the FTIR partial column amounts. This

figure gives a good insight in the real performance of the FTIR system. The normalisation according to Eq. (3) produces changes of about 5% if referred to the typical O₃ amounts (see Fig. 9). In the stratosphere the natural variability is of a similar magnitude (5–10%), and the normalisation to the Brewer data significantly improves the correlation between FTIR and ECC partial columns (compare panel (c) of Fig. 10 and 8). On the other hand, in the troposphere or tropopause the natural variability is very large (between 30 and 70%) and an alteration of the ECC data by only 5% has no significant effect

In 4.1 we analysed the ECC quality by the Brewer total O₃ measurements. The variability of the residual O₃ above the sonde's burst altitude is 4 DU (or 1.4%). The ignorance of this variability together with the error of the Brewer data of around 0.5% limits the validity of this test to $\sqrt{1.4^2+0.5^2}=1.5\%$. This uncertainty range becomes even larger if the balloon bursts already below 30.5 km. As demonstrated in this paper a state-of-the-art FTIR system provides partial column amounts of good quality. At supersites like Izaña the quality of the ECC sondes can be checked by the FTIR partial column amounts. This enables to perform good quality checks even for sondes whose balloon's burst at lower altitudes. For sondes reaching 30.5 km the quality check can be performed with a precision of 0.8% (0.8% is the estimated random error for the FTIR partial column amounts below 30.5 km; see Table 2).

5 Summary and conclusions

We made an extensive theoretical error estimation for O₃ profiles measured by a state-of-the-art ground-based FTIR observing system. The FTIR system provides high quality data with a vertical resolution of 4.5–7 km for O₃ amounts below 20 km and of around 10 km in the middle stratosphere. The altitude range with the best vertical resolution coincides with the tropopause region. The application of a unique a-priori facilitates the interpretation of annual cycles. We do not recommend the usage of seasonally varying a-priori data since the measurement alone contains sufficient information.

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



**Quality assessment
of ground-based FTIR
O₃ profiles**M. Schneider et al.

At the Izaña Observatory ECC sonde, Brewer, and FTIR measurements are performed continuously at high quality. It offers world-wide unique conditions for intercomparing these different O₃ monitoring techniques, and to document their quality. Such quality documentations are essential if the measurements are to be applied for the validation of satellites. The comparison between ECC and FTIR amounts agrees with our theoretical estimations about the FTIR precision. Furthermore, it indicates that the ECC sonde provides data with a precision of better than 5% from the surface up to the middle stratosphere. This demonstrated good performance of the ECC measurements is an in-field confirmation of extensive laboratory studies (Smit and Sträter, 2004). We found no significant systematic difference between the ECC and FTIR O₃ partial column amounts between the surface and 30.5 km ($\frac{PC_{FTIR} - PC_{ECC}}{PC_{ECC}} = (1.8 \pm 2.4)\%$).

We made the quality assessment for ground-based FTIR O₃ profiles, since O₃ offers a unique opportunity of comparison to other measurement techniques. The good confirmation of our theoretical error estimation by the empirical comparisons strengthens the validity of future FTIR profile error estimations of other absorbers like N₂O, HF, HCl, CO₂, ... which, due to the absence of other co-located measurement techniques, are difficult to be confirmed empirically.

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

References

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ACPD

8, 4977–5006, 2008

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



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ACPD

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Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



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15

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Table 1. Assumed uncertainties.

error source		random	systematic
phase error		0.01 rad	+0.01 rad
modulation eff.		1%	+1%
z. bl. offset		0.1%	+0.1%
T profile ¹	at surface	1.7 K	–3.5 K
	rest of troposphere	0.7 K	–
	at 30 km	1 K	up to +4 K
	above 50 km	6 K	up to –12 K
solar angle		0.1 °	–
line intensity		–	–2%
pres. broad. coef.		–	–5%

¹ for more details please refer to [Schneider and Hase \(2008\)](#).

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

I◀

▶I

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Table 2. Estimated random errors relative to climatological amounts (in %) for the 3 layers representing the troposphere, the tropopause region, and the middle stratosphere, and for the layer covering the measurement range of the ECC sonde (surface – 30.5 km)

error source	surface – 10 km (TR)	12.5–17 km (TP)	20–30.5 km (MS)	surface – 30.5 km
smoothing	4.3	13.2	1.3	0.7
phase error	0.2	1.2	0.2	0.2
modulation eff.	<0.1	0.4	0.3	0.1
zero baseline offset	<0.1	0.5	0.5	0.3
temperature	<0.1	1.0	0.2	0.1
solar angle	0.4	0.4	0.3	0.3
line intensity	<0.1	<0.1	<0.1	<0.1
pres. broad. coef.	1.6	2.4	0.4	0.1
meas. noise	0.3	0.6	0.1	0.1
total	4.0	13.4	1.6	0.8

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

Table 3. Estimated systematic sensitivity errors and bias errors relative to climatological amounts for the same layers as in Table 2.

error source	surface – 10 km (TR)		12.5–17 km (TP)		20–30.5 km (MS)		surface – 30.5 km	
	sensitivity [%]	bias [%]	sensitivity [%]	bias [%]	sensitivity [%]	bias [%]	sensitivity [%]	bias [%]
smoothing	–5.4	+0.5	–10.7	–0.3	–7.2	–0.1	–1.0	–0.3
phase error	–0.1	+0.2	+0.3	+0.7	+0.3	+0.1	+0.2	+0.2
modulation eff.	–	–	+0.2	–	+0.6	+0.3	+0.1	+0.1
z. bl. offset	–0.2	–	–0.3	–	–1.0	–0.5	–0.8	–0.3
temperature	+0.1	–	+1.0	+1.4	–1.2	–0.7	–0.2	–0.3
line intensity	+2.1	+2.0	+1.9	+2.0	+1.9	+1.9	+2.0	+2.0
pres. broad. coef.	+4.7	+4.3	–0.8	+2.3	–2.0	+0.8	–	+1.6
meas. noise	–0.1	–	–	–	+0.1	–	–	–

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

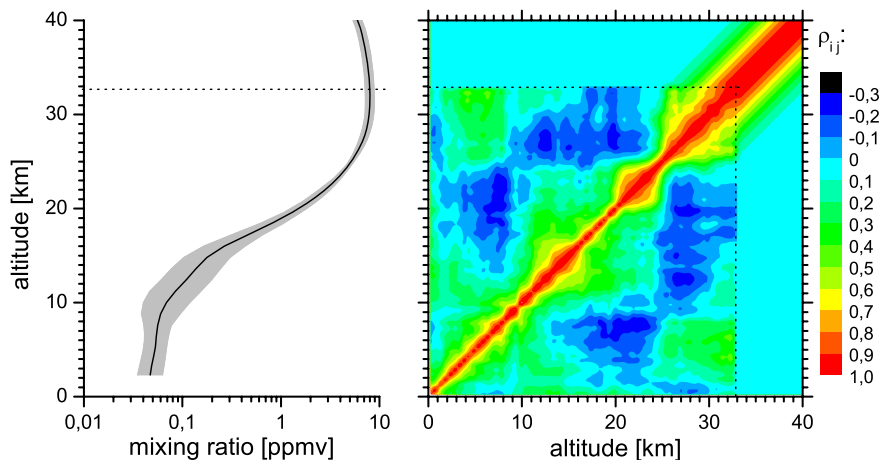


Fig. 1. Left panel: Black line: a-priori mean O₃ profile and its typical variability (shaded area around line) for Tenerife. Right panel: a-priori correlation matrix of ozone mixing ratios. Up to 32.8 km profiles and interlevel correlations are from sonde data measured between 1997 and 2006. Above 32.8 km the values are estimated.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



**Quality assessment
of ground-based FTIR
 O_3 profiles**

M. Schneider et al.

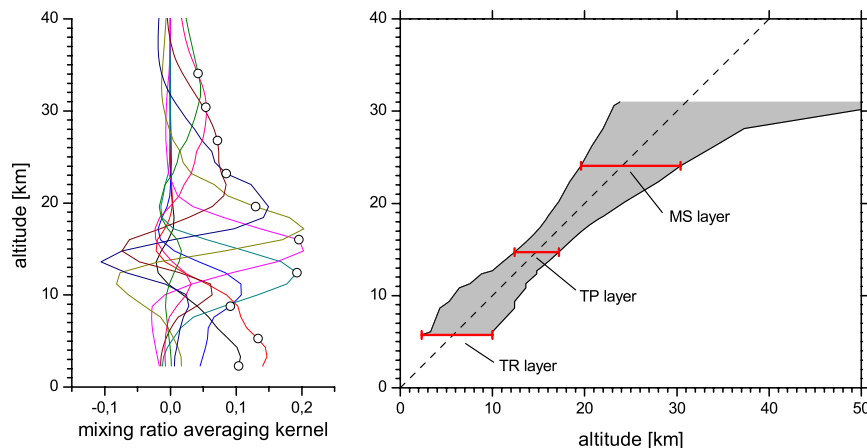


Fig. 2. Left panel: Colored lines: some typical mixing ratio averaging kernels for the main isotopologue $^{48}O_3$ normalized to 1 km thick layers; open circles: diagonal elements of the kernel matrix. Right panel: altitude ranges for which the sum of the diagonal elements of the kernel matrix reaches 1. The TR, TP, and MS layers are indicated by red bars.

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

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

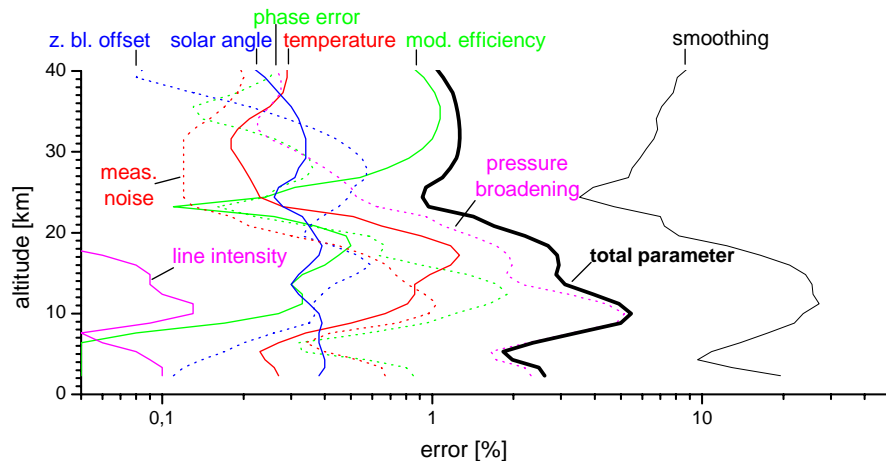


Fig. 3. VMR random errors relative to actual VMRs. Solid black: smoothing; solid green: modulation efficiency; dashed blue: zero baseline offset; solid red: temperature profile; solid blue: solar elevation angle; solid magenta: line intensity; dashed magenta: pressure broadening coefficient; dashed red: measurement noise; thick solid black: total parameter errors (sum of all errors except of smoothing).

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

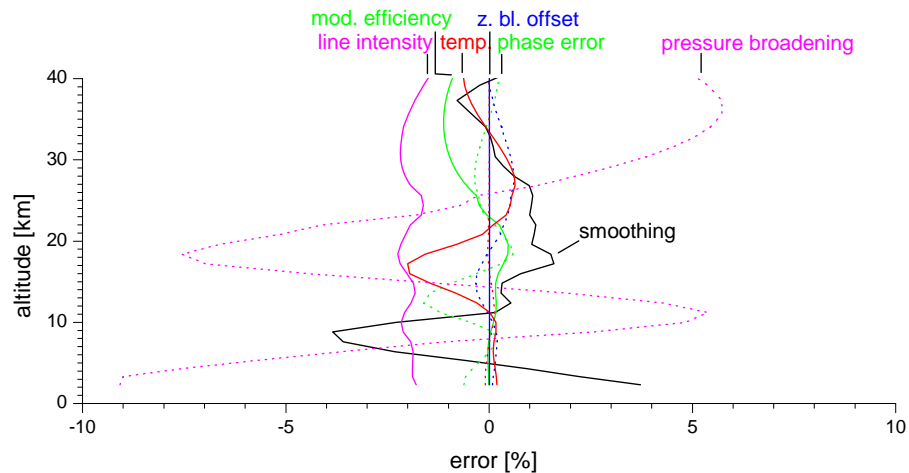


Fig. 4. VMR systematic errors relative to actual VMRs. Line style and color as in Fig. 3.

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

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

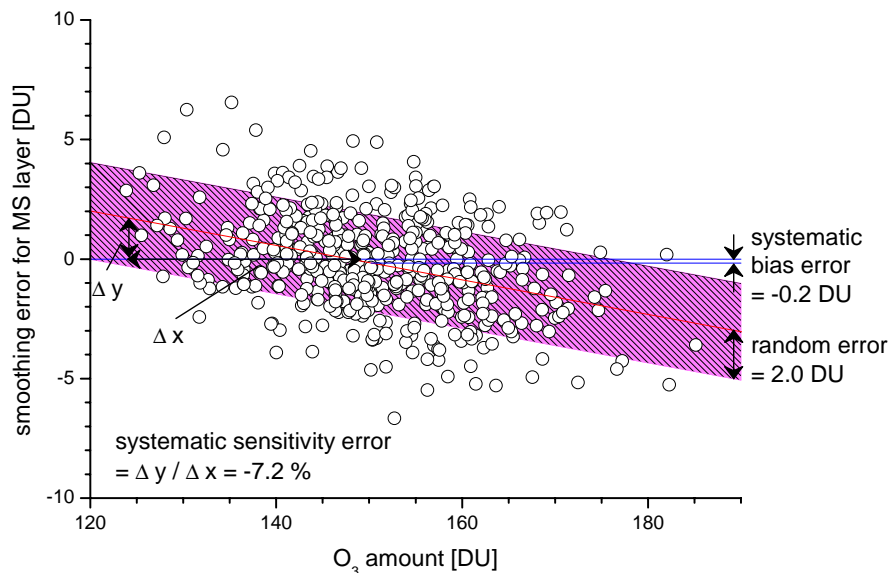


Fig. 5. Dependence of the smoothing error in the MS layer on the actual O₃ amount. Separation into error components (random, systematic sensitivity, and systematic bias error) is done by a linear least squares fit. Circles: individual error simulations; red line: linear regression line. Random error: 1σ scattering around the regression line (indicated by magenta area); systematic sensitivity error: slope of the regression line; systematic bias error: offset of the regression line at the a-priori value.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



**Quality assessment
of ground-based FTIR
O₃ profiles**

M. Schneider et al.

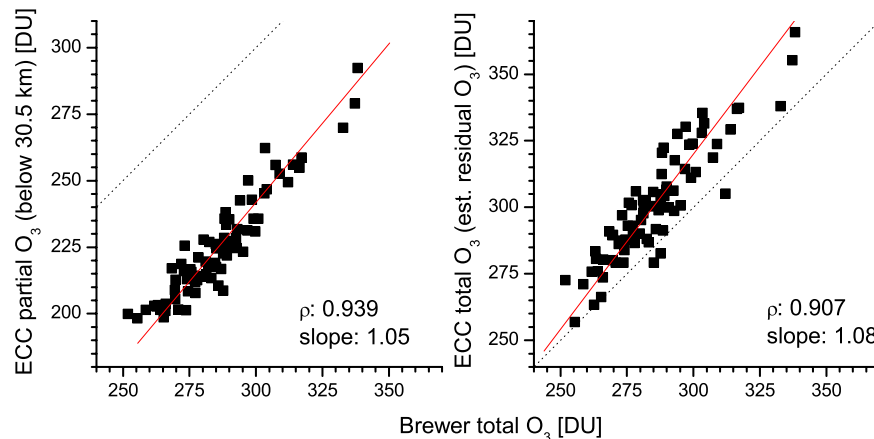


Fig. 6. Comparison between ECC and Brewer O₃ amounts. Solid squares: individual coincidences; red lines: regression lines of linear least squares fits; dotted line: diagonal. Left panel: Ignoring the ECC O₃ residual. Right panel: considering the ECC O₃ residual by assuming a constant mixing ratio from the balloon's burst altitude until the top of the atmosphere.

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

**Quality assessment
of ground-based FTIR
O₃ profiles**M. Schneider et al.

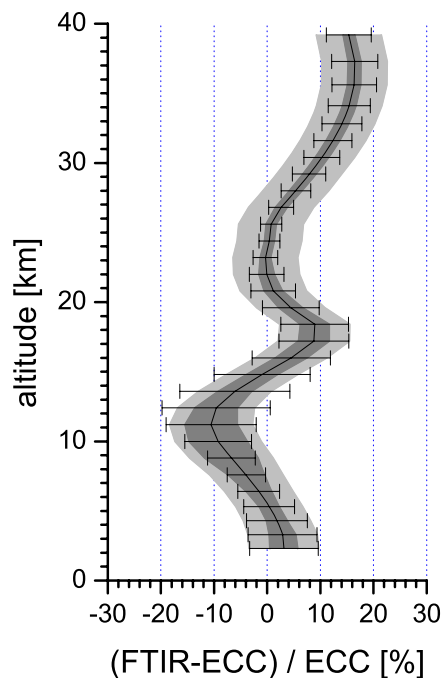


Fig. 7. Difference between FTIR and smoothed ECC sonde profiles. Shown are mean and standard deviation of the difference for the 53 FTIR/ECC coincidences. The grey shaded area indicates the expected FTIR error (excluding the smoothing error); the light grey shaded area indicates the expected random error of $(\text{FTIR-ECC})/\text{ECC}$.

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

Quality assessment
of ground-based FTIR
O₃ profiles

M. Schneider et al.

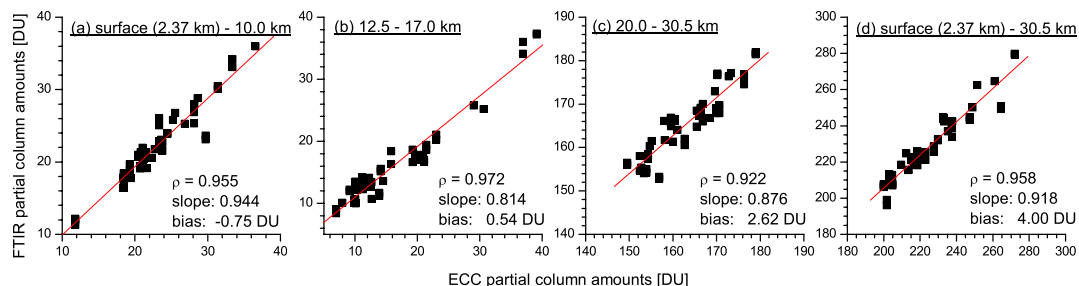
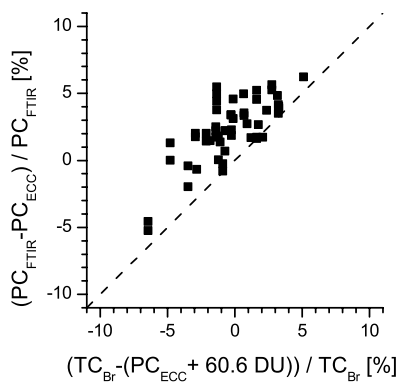


Fig. 8. Correlation between FTIR and ECC measurements. Black squares: individual measurements; red lines: linear regression line of least squares fits. Panel (a): TR layer, panel (b): TP layer, panel (c): MS layer, panel (d): layer from surface – 30.5 km.

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

**Quality assessment
of ground-based FTIR
O₃ profiles**

M. Schneider et al.

**Fig. 9.** Correlation between differences Brewer-ECC and differences FTIR-ECC.[Title Page](#)[Abstract](#)[Introduction](#)[Conclusions](#)[References](#)[Tables](#)[Figures](#)[⏪](#)[⏩](#)[◀](#)[▶](#)[Back](#)[Close](#)[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)

Quality assessment of ground-based FTIR O₃ profiles

M. Schneider et al.

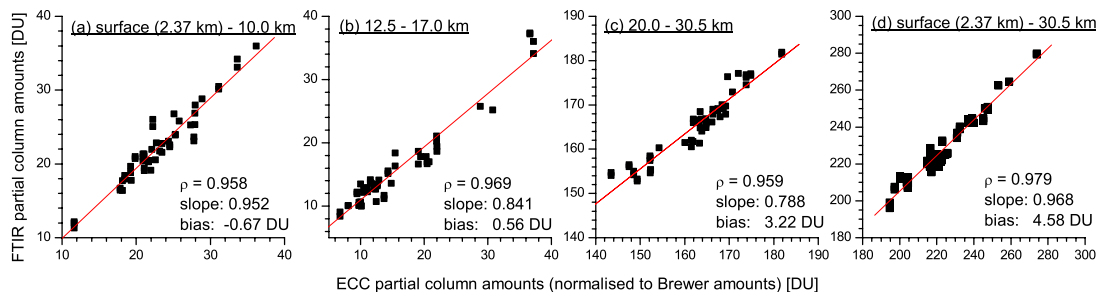


Fig. 10. Same as Fig. 8, but for ECC data normalized to Brewer total column amounts.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

