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Comparison of ground-based FTIR and Brewer O_3 total column with data from two different IASI algorithms and from OMI and GOME-2 satellite instruments

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Abstract

An intercomparison of ozone total column measurements derived from various platforms is presented in this work. Satellite data from Infrared Atmospheric Sounding Interferometer (IASI), Ozone Monitoring Instrument (OMI) and Global Ozone Monitoring

- ⁵ Experiment (GOME-2) are compared with data from two ground-based spectrometers (Fourier Transform Infrared spectrometer FTIR and Brewer), located at the Network for Detection of Atmospheric Composition Change (NDACC) super-site of Izaña (Tenerife), measured during a campaign from March to June 2009. These ground-based observing systems have already been demonstrated to perform consistent, precise and
- accurate ozone total column measurements. An excellent agreement between groundbased and OMI/GOME-2 data is observed. Results from two different algorithms for deriving IASI ozone total column are also compared: the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT/ESA) operational algorithm and the LISA (Laboratoire Interuniversitaire des Systèmes Atmosphériques) algorithm.
- A better agreement was found with LISA's analytical approach based on an altitudedependent Tikhonov-Philips regularization: correlations are 0.94 and 0.89 compared to FTIR and Brewer, respectively; while the operational IASI ozone columns (based on neural network analysis) show correlations of 0.90 and 0.85, respectively, compared to the O₃ columns obtained from FTIR and Brewer.

20 **1** Introduction

25

Monitoring of atmospheric ozone concentrations is today an essential activity because it is a key species involved in the troposphere's oxidative capacity as well as in the atmospheric radiative budget and in the chemical cycles relevant to air quality (Finlayson-Pitts et al., 1999). It also absorbs ultraviolet solar radiation in the stratosphere thereby allowing life on Earth. On average, about 90% of the total ozone is present in the stratosphere and only 10% in the troposphere. However, important vertical ozone transport





events occur frequently and need to be quantified accurately to better understand radiative forcing and tropospheric chemistry. For this purpose, data from satellites and ground-based instruments are indispensable, in particular in combination with numerical models of atmospheric transport and chemistry.

- This work presents an intercomparison of various independent O₃ data derived from satellites (IASI, GOME-2 and OMI) with data from ground-based measurements (Fourier-Transform Infra-Red, FTIR, and Brewer) performed at the Izaña Atmospheric Observatory on the Canary Island of Tenerife. This high-altitude observatory is a multi-instrument "super site" which is part of the NDACC (Network for the Detection of Atmospheric Composition Change) and of the WMO/GAW (World Meteorological Organization/Global Atmosphere Watch) networks. Also it is especially well suited for satellite
- tion/Global Atmosphere Watch) networks. Also it is especially well suited for satellite data validation because of its particular meteorological conditions.

This intercomparison leads to the first validation of the IASI O_3 total columns over Izaña by matching them with reference FTIR and Brewer data, and by comparing them with two other UV-visible satellite ozone data (GOME-2 and OMI). Also two different retrieval algorithms for deriving the O_3 total amount from IASI are compared.

In the following chapters, we first present the ground-based instruments and the related O_3 analyses; then we briefly outline the UV-visible satellite measurements and O_3 analysis procedure. Afterwards, the O_3 total columns from the different satellite instruments are compared with the results from ground-based instruments. Finally, the

Instruments are compared with the results from ground-based instruments. Fir results are summarized and perspectives for future studies are discussed.

2 FTIR and Brewer observations of ozone at Izaña

2.1 Presentation of the Izaña super site

15

Izaña Atmospheric Observatory is operated by the Meteorological Sate Agency of Spain Service (Agencia Estatal de Meteorología). It is located on the Canary Island of Tenerife (28°18' N, 16°29' W) at 2370 m a.s.l. (above sea level). Tenerife is about





300 km away from the African west coast, surrounded by the Atlantic Ocean, so it is located far away from industrial activities, leading to clean air conditions. In addition, it is placed in the subtropical region where the descending branch of the Hadley cell offers stable meteorological conditions and clear sky most of the time. Therefore, it is

a site which is well suited for continuously monitoring atmospheric key species such as ozone, and for validating satellite data such as IASI. Both FTIR and Brewer measurements are performed at this site; concerning the Brewer instrument, Izaña is the Regional Brewer Calibration Centre for Europe (http://www.rbcc-e.org/) which guarantees highest quality standards.

10 2.2 FTIR ozone measurements: description and analysis

Since 1999, solar atmospheric spectra have been recorded in Izaña with high resolution FTIR spectrometers using solar occultation. Until 2004, a Bruker IFS 120M, and since 2005, a Bruker IFS 125HR spectrometer have been used. For "operational" measurements, the spectral resolution is $0.005 \,\mathrm{cm}^{-1}$ in the mid-infrared region (750–

- ¹⁵ 4300 cm⁻¹), which is covered by six individual measurements applying different filters in order to achieve an optimal signal to noise ratio. Solar absorption spectra are recorded via a solar tracker controlled by both astronomical calculations and a quadrant photodiode detector. A KBr beamsplitter and a liquid-nitrogen cooled MCT detector are used for the 750–1350 cm⁻¹ spectral region. The entire instrumental set-up is very similar for all NDACO stations. The analytical for the 20 stations are activated by a solar tracker by a situated by a solar tracker by a solar by a situated by a solar by a so
- for all NDACC stations. The spectral windows applied for the O₃ retrieval are situated between 962 and 1044 cm⁻¹ and contain more than 100 individual O₃ rotation-vibration lines with different intensities and widths that provide information on O₃ in different altitude layers. Figure 1 shows an example of a measured spectrum, the corresponding simulated spectrum and the difference between simulation and observation for a selected micro-window.

For the O_3 retrievals, the PROFFIT 9.6 code (Hase et al., 2004) is used based on PROFFWD (PROFile ForWarD) as forward model. The inversion procedure and the radiative transfer calculation require a discretised model of the atmosphere (41 levels





from ground to the top) and a priori knowledge of concentration profiles of O₃ and interfering species as well as proper meteorological conditions. All O₃ retrievals were made on a logarithmic scale in order to well reproduce the high variability of ozone around the tropopause (Hase et al., 2004; Deeter et al., 2007). Since major O_3 isotopologues have distinct absorption lines, retrievals were performed for several individual O_3 isotopologues, i.e. ${}^{48}O_3$, asymmetric and symmetric ${}^{50}O_3$ and ${}^{49}O_3$. In addition, temperature profiles have been retrieved simultaneously, which significantly improves the quality of the retrieved ozone data (Schneider and Hase, 2008).

To obtain column integrated atmospheric O_3 abundances from a given spectrum, the radiative transfer has to be calculated in order to retrieve the O₃-profile. The in-10 version procedure is an ill-posed problem and requires the use of constraints (usually provided by the a priori information) to stabilize the solution. Here the Optimal Estimation Method is used (Rodgers, 2000). The a priori O_3 mean profile and covariances are calculated from ECC-sonde measurements on Tenerife between 1996 and 2006.

- together with the extended HALOE profile climatology for 30° N (Schneider et al., 2005, 15 2008b). The a priori temperature profiles are obtained from the Goddard Space Flight Center (NCEP). The calculated spectrum derived from the forward calculation is iteratively compared to the measured spectrum in order to minimize the root-mean-square (rms) of the difference between the two spectra. The relevant spectroscopic line parameters are taken from the HITRAN 2004 database (Rothman et al., 2005) except
- 20 for H_2O lines the spectral parameters of which are from HITRAN 2006 (Gordon et al., 2007).

PROFFIT 9.6 also allows performing an error estimation analysis based on the analytical method suggested by Rodgers (Rodgers, 2000):

5

²⁵ $\hat{x} - x = (\mathbf{A} - I)(x - x_a) + \mathbf{GK}_p(p - \hat{p}) + \mathbf{G}(y - \hat{y})$

 \hat{x} , x and x_a are the estimated, real and a priori state of the atmosphere, \hat{p} , p are the estimated and real model parameters, respectively, and \hat{y} , y represent the measured and modeled spectra. A is the averaging kernel matrix providing information on the



(1)

vertical resolution that is characteristic for the retrieval. Its trace represents the degrees of freedom in the measurement, indicating the number of independent pieces of information in the retrieved profile. G is the gain matrix and K_p is the model parameter sensitivity matrix.

- The first term in Eq. (1) represents the smoothing error that is the main source of 5 error for vertical concentration profiles. Since in this study the main focus is on the total O₃ amount (columns), this error is considered separately. The second term stands for the estimated error due to uncertainties in input parameters, such as instrumental parameters or spectroscopic data. In addition, the third term represents the error due to the measurements noise. This error analysis, based on the separation of the 10 type of error sources (systematic and statistic), was performed with an ensemble of 200 retrievals. Figure 2 shows the statistical and systematic estimated error profiles for a typical O₃ retrieval and for different error sources (such as temperature, noise, instrumental line shape ...). In this figure, one can note that the main systematic
- error source is the uncertainty of spectroscopic parameters, whereas the major sta-15 tistical error source is the uncertainty of the parameterization of the Instrumental Line Shape (ILS). By adding up systematic and statistical error sources for a given altitude and then integrating it along the error patterns (Rodgers, 2000), we estimate the total systematic and random error on FTIR O₃ total columns to 2.0% and 0.5%, respectively.
- In addition, the smoothing error is estimated to be less than 0.2% on O_3 total columns. 20 Table 1 shows random and systematic total column errors due to various error sources showed in Fig. 2. Smoothing error is also given for total column. These error analysis results are in good agreement with those found in (Schneider and Hase, 2008; Schneider et al., 2008b).

Brewer ozone measurements: description and analysis 2.3 25

The Brewer instrument is a spectroradiometer measuring in the UV region between 290-365 nm. It detects spectral irradiance in six channels in the UV (303.2, 306.3, 310.1, 313.5, 316.8, and 320.1 nm) by using a holographic grating in combination with



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a slit mask that selects the channel to be analyzed by a photomultiplier. Each channel covers a bandwidth of 0.5 nm with a resolution power of about 600. The first channel at 303.2 nm is only used for spectral wavelength checks by means of internal Hg-lamps, the second channel is used for measuring SO₂, and the remaining four channels at longer wavelength for determination of the O₃ total column. This double monochromator instrument (MK-III), known to widely reduce the impact of straylight on the measurements, works in a completely automatic way, and usually measures continuously during the whole day. The total column of O₃ is calculated on the basis of relative intensities at these different wavelengths using the Bass and Paur (Bass and Paur, 1985) ozone absorption cross-sections at fixed temperature of -45 °C (Kerr, 2002) The retrieval precision is approximately ±1%. More information about the Brewer instrument

3 Satellite observations of ozone over Izaña

3.1 IASI measurements: description and analysis

is given in (Fioletov et al., 2005) and (Scarnato et al., 2009).

The IASI instrument (Clerbaux et al., 2007, 2009) launched in October 2006 onboard the satellite MetOp-A is a meteorological instrument that started with operational measurements in June 2007. It measures the thermal infrared radiation emitted by the Earth's surface and the atmosphere in Nadir geometry. IASI is a Michelson-type Fourier-transform spectrometer, with a spectral resolution of 0.5 cm⁻¹ after a Gaussian apodization, covering the spectral range from 645 to 2760 cm⁻¹. The MetOp-A satellite flies in a polar sun-synchronous orbit and covers each geographic region at least twice per day (at 09:30 and 21:30 LT – local time). At the Nadir point, the size of one IASI pixel is 50 × 50 km. Each such pixel consists of four sub-pixels with a diameter of 12 km (at the sub-satellite point). IASI covers a swath-width of 2200 km in 14SI is to provide meteorological products (temperature and humidity profiles) but its





accuracy and spectral range allow retrieving also important atmospheric trace gases. In particular, recent studies have demonstrated the capability of IASI to monitor tropospheric ozone, stratosphere-troposphere exchanges, or biomass burning events and tropospheric transport (Eremenko et al., 2008; Keim et al., 2009; Dufour et al., 2010).

 IASI is also well suited to monitor the global distribution of O₃ (Boynard et al., 2009). In this study, O₃ columns derived from two different retrieval algorithms are compared: one from the (operational) neural network approach and the other one from an analytical approach (see Eremenko et al., 2008). The neural network interpolates a training dataset and selects the best matching profile from the training dataset, whereas
 the analytical approach is based on constrained (altitude-dependent Tikhonov-Philips) least-squares fits.

3.1.1 Neural network retrieval

The neural network used for ozone at EUMETSAT is of feedforward type with two hidden layers. The training dataset consisted of a collection of atmospheric state vectors and their associated synthetic spectra computed with the forward model RTIASI (Matricardi and Saunders, 1999). Vertical atmospheric profiles came from a global chemistry transport model, MOZART (Model of Ozone And Related Tracers) (Brasseur et al., 1998; Hauglustaine et al., 1998) connected with UGAMP climatology (Li and Shine, internal report, 1995) above the tropopause. Temperature profiles arise from ECMWF (European Centre for Medium-Range Weather Forecasts) analysis. Simulations were

performed with a constant surface emissivity, clear atmospheric conditions (no clouds and aerosols) and without taken relief into account (Turquety, 2003). The spectroscopic parameters are taken from HITRAN 1996 (Rothman et al., 1998). We refer to (Turquety et al., 2004) for more details. The target accuracy of the total column was set to 2.5%.





3.1.2 Analytic retrieval approach

The O_3 retrievals are performed between 975 and 1100 cm⁻¹ using an analytical altitude-dependent regularisation method with the regularization matrix containing first and second order Tikhonov constraints (Tikhonov, 1963), together with altitude dependent coefficients optimized to maximize the degree of freedom of the retrievals. More details about the IASI inversions are given in (Eremenko et al., 2008). The spectroscopic parameters of different atmospheric species are taken from HITRAN 2004 (Rothman et al., 2005). The uncertainty of the O_3 total column is estimated to be ~2.5%.

3.2 Other ozone independent data sets

3.2.1 GOME-2 satellite data and algorithms for O₃ total columns

The Global Ozone Monitoring Experiment (GOME-2) aboard MetOp-A is a scanning spectrometer that captures light reflected from the Earth's surface and backscattered by aerosols and the atmosphere. The measured spectra are mainly used to derive ozone total columns and vertical profiles, as well as concentrations of nitrogen dioxide, bromine monoxide, water vapour, sulfur dioxide and other trace gases, and also cloud properties and aerosols. It covers the UV/visible and near-infrared region from 240 nm to 793 nm at a resolution of 0.2 nm to 0.4 nm. GOME-2/MetOp has 24 forward-scan pixels with a nominal resolution of 40 km × 80 km, and 8 back-scan pixels with a
nominal resolution of 40 km × 240 km. The default across-track swath width is 1920 km which enables global coverage within 1.5 days.

The O₃ columns used here are from the Level 3 of GOME-2, i.e. geophysical parameters that have been spatially and/or temporally re-sampled from Level 2 data. The O₃ algorithm retrieval, GOME Data Processor (GPD), version 4.2 (see DLR Report 28 January 2009) has been applied in this paper and is based on two methods: the DOAS (Differential Optical Absorption Spectroscopy) method (Platt et al., 1994), and



the iterative AMF/VCD (Air Mass Factor/ Vertical Column Density) computation (Van Roozendael et al., 2006). Total ozone columns derived from this algorithm have been validated using ground-based networks (Balis et al., 2007).

Error analysis indicates an accuracy and precision of O₃ total columns of 3.6–4.3% and 2.4–3.3%, respectively (Van Roozendael et al., 2004). In addition, an initial validation with one full year of ground-based and satellite measurements shows that GOME-2 total ozone products have already reached an excellent quality (Balis et al., 2008; Validation report, can be obtained from: http://wdc.dlr.de/sensors/gome2/).

3.2.2 OMI satellite data and algorithms for O₃ total columns

- ¹⁰ The Ozone Monitoring Instrument, OMI (Levelt, 2002), is one of the four sensors aboard the EOS-Aura satellite (launched in July 2004). With its 2600 km viewing swath width, it provides daily global measurements of different species: O₃, nitrogen dioxide, sulfur dioxide and aerosols from biomass burning and industrial emissions, HCHO, BrO, OCIO and surface UV irradiance. It is a Nadir-viewing imaging spectrograph that
- ¹⁵ measures the solar radiation backscattered by the Earth's atmosphere and surface between 270–500 nm with a spectral resolution of about 0.5 nm. O_3 total column data, measured from ground to approximately 80 km, are retrieved using both the TOMS technique (developed by NASA) (Bhartia, 2002) and a DOAS technique developed at KNMI. The O_3 products used in the present study are from the Level-3 Aura/OMI based
- on the Level-2 OMDOA product that uses DOAS multi-wavelength algorithm (Veefkind et al., 2006; http://disc.gsfc.nasa.gov/Aura/OMI/omdoae_v003.shtml). The O_3 total column uncertainty from OMI is estimated to 3% (Bhartia, 2002). Furthermore, recent validations of OMI O_3 products have been performed (Balis et al., 2007; Liu et al., 2010; Kroon et al., 2008; McPeters et al., 2008).



4 Comparison of O₃ total columns over Izaña from FTIR, Brewer, IASI, GOME-2, and OMI

4.1 Validation strategy

In order to perform relevant comparisons of data from different sources, coincidence
criteria based on space, time, and number of observations, were used. First, all measurements had to pass a quality filter (i.e. signal-to-noise ratio for FTIR, cloud-filter for IASI, ...). Then, they had to be referred to a precise location: Satellite data were selected for a 2° latitude belt, i.e. between 27.5° and 29.5° N, and 27.7° and 29.7° N, and 27.3° N and 29.3° N for GOME-2, OMI and IASI respectively. Finally, to evaluate the threshold value of the temporal criterion, the daily total ozone variability has been calculated from Brewer measurements for each day of the comparison period. The hourly mean total column at noon was taken as a reference of the day, in order to calculate the relative ozone variability at each time step (half an hour) for each day. Figure 3 shows the relative differences (related to noon) of the total ozone variability is observed

- on a daily scale, varying from day to day, because this analysis is performed during ozone high variability season. Note that the total ozone variability can reach $\pm 6\%$ in extreme cases. Since the daily ozone variability cannot be neglected, daily mean total columns derived from ground-based cannot be used for the comparison with satellite
- ²⁰ data. A restrictive temporal criterion of one hour has thus been applied and groundbased measurements have been time-selected in function of the satellite passing hour.

The comparison time period is from 1 March to 22 June 2009, for the FTIR measurements, and from 1 March to 30 June 2009, for the Brewer measurements. Since FTIR measurement campaign was performed during this period, ozone data were provided

in an intensive way (i.e. more than one or two spectra per day) in order to match satellite passing hour. One note that Brewer measurements are completely automatised, thus more ozone data are routinely available.





Despite this quite restrictive approach, due to the suitable climatological conditions over Izaña, a rather large number of clear-sky days were successfully selected for FTIR and Brewer, respectively.

4.2 Comparison of FTIR and Brewer data: two ground-based measurements

- In order to verify the quality of the reference measurements used in the present study, we have compared first the two different types of ground-based measurements in the relevant period (March to June 2009). A detailed comparison of FTIR and Brewer in Izaña has already been published in 2008 by (Schneider et al., 2008a). Since both high quality ground-based instruments perform measurements at the same location, a
- temporal criterion of 20 min is applied here for the comparison (Wunch et al., 2007). Figure 4 shows a time series of O₃ total columns retrieved by both instruments (upper panel) and the correlation between Brewer and FTIR data (lower panel). The agreement between the Brewer and FTIR data is very good in terms of the variations in the difference (standard deviation) but a persistent bias of 4.2 (±0.7)% exists. The most likely explanation for this is a bias in the UV and TIR spectroscopy of ozone as discussed further down. In addition, a correlation coefficient of 0.99 is observed. We note

that the relative difference is calculated as:

[(FTIR O₃ column – Brewer O₃ column)/Brewer O₃ total column] × 100

The mean relative difference (MRD) of 4.2% is in perfect agreement with a previous comparison study (Schneider et al., 2008a) and the small one sigma standard deviation of 0.7% demonstrates the high quality of both the UV and IR data. The FTIR measures systematically higher O₃ total columns than the Brewer instrument, which may be due to inconsistencies in the spectroscopic parameters. Indeed, the FTIR retrieval algorithm uses the HITRAN infrared line intensities (Rothman et al., 2005) whereas the Brewer algorithm is based on the ultraviolet absorption cross-sections of Bass and

Paur (Bass and Paur, 1985). Such a systematic difference has also been observed in laboratory UV/IR intercomparison experiments: systematic differences respectively of



(2)



3.6 (±1.0)% (Guinet et al., 2010) between IR (10 μ m, HITRAN 2008) and UV (254 nm), 5.5% (Picquet-Varrault et al., 2005) and 4.0 (±0.1)% (Gratien et al., 2010) between IR (10 μ m) and UV (300–350 nm).

4.3 Comparison of FTIR and Brewer total ozone columns with the two IASI products

In this section, O_3 total columns derived from the ground-based instruments at Izaña are compared with data from two different IASI retrievals: one from a neural network (so-called operational) approach and one using a physical method with a regularization (analytical) algorithm.

Figure 5 shows the time series of O_3 total columns derived from Izaña FTIR (top) compared with the O_3 total columns obtained using IASI data with analytical (left panel) and operational (right panel) retrievals. The same comparisons are performed with Brewer measurements (lower panels).

One can see that the daily ozone variations are well captured by both IASI retrieval techniques. However, the operational IASI O_3 total columns seem to be lower than the FTIR ones. The mean relative differences (MRD) between IASI analytical and IASI operational total O_3 columns, respectively, are $-2.0 (\pm 1.4)\%$ and $-5.2 (\pm 1.9)\%$ compared with the FTIR data, and 1.5 (± 2.2)% and $-0.9 (\pm 2.5)\%$ compared with the Brewer data. All mean relative differences between Izaña ground-based O_3 total columns and other independent data are summarized in Table 2. The MRD is calculated as:

[(Satellite O₃ column – ground-based O₃ column)/ground-based O₃ total column]

× 100

25

5

(3)

Although less coinciding points are used in the analytical IASI retrieval (13 and 55 for IASI analytical, compared to 22 and 77 for the IASI operational product, the first number related to FTIR and the second to Brewer observations, respectively), there is a slightly better agreement with ground-based results. The difference in the IASI data sets for





these two retrievals is the result of different methods used for the treatment of the IASI measurements: Each method uses indeed its own criteria for the quality check and for the cloud filtering. It is important to note that only for the operational IASI retrieval, the difference exceeds the estimated uncertainty.

Figure 6 shows O₃ total columns retrieved from IASI data using analytical (left) and operational (right) algorithms as a function of the O₃ total columns derived from FTIR at Izaña (top) and from Brewer at Izaña (below). A linear fit passing by the origin is used.

The correlation coefficients are 0.90 and 0.94 in the case of FTIR comparison
 with the operational and analytical IASI retrievals, respectively. Correlation coefficients of 0.85 and 0.89 are obtained when comparing the operational and analytical IASI retrievals, respectively, to Brewer. Note that the comparisons with ground-based data systematically show that the IASI operational data produce smaller correlation coefficients. Furthermore, the slopes of linear fitting of analytical IASI retrieval:
 ground-based measurements are closer to unity than for the IASI operational retrieval:
 0.98 (FTIR) and 1.0 (Brewer) for IASI analytical retrievals, compared to 0.95 (FTIR) and
 0.99 (Brewer) for IASI operational retrievals. Hence, the analytical retrieval method for deriving total atmospheric ozone columns appears more consistent with ground-based reference data.

20 4.4 Comparison of FTIR and Brewer ozone data with GOME-2 and OMI data

In this section, FTIR measurements at Izaña are compared with GOME-2 and OMI satellite data. Figure 7 shows the time series of ozone columns derived from FTIR at Izaña (black/top) and Brewer data (purple/below) and from GOME-2 (cyan) and OMI (green). The mean relative differences of FTIR data are -0.5 (±0.7)% with OMI and ²⁵ -2.4 (±1.1)% with GOME-2, while for Brewer data one obtains 3.5 (±1.2)% difference with OMI and 1.5 (±1.5)% with GOME-2. Here, a very good agreement is observed between ground-based and satellite measurements since the mean differences do not exceed the uncertainties. One can see in Fig. 8 the good correlations between Izaña





FTIR and satellite data for the corresponding measurement period: 0.99 and 0.97 for OMI and GOME-2, respectively, and between Brewer and the satellite data (correlation coefficient of 0.97 for OMI and 0.96 for GOME-2). The slopes of the linear regressions are 0.99 for OMI and 0.98 for GOME-2 concerning the comparisons with FTIR, and 1.0 for both satellite instruments comparing with Brewer data

5 1.0 for both satellite instruments comparing with Brewer data.

5 Discussions and conclusion

In this study, ground-based (FTIR and Brewer) measurements performed at Izaña in the period from March to June 2009, were used to validate total O_3 columns from the IASI sensor aboard the MetOp platform.

- ¹⁰ First of all, the consistency of the two ground-based measurement methods was evaluated. A scatter of only 0.7% documents the very good quality of the ground-based data. However, we also observe a systematic difference of 4.2% (MRD). These observations confirm the observations of the study published by (Schneider et al., 2008a). This systematic difference may be due to systematic errors in the spectroscopic param-
- eters. Therefore, further investigations have to be carried out to elucidate this issue. Furthermore, the O₃ total columns over Izaña from FTIR and Brewer were compared to results derived from two different IASI retrieval algorithms. An excellent agreement of -2.0 (±1.4)% and 1.5 (±2.2)% was found when comparing FTIR and Brewer with IASI results derived from an analytical algorithm. On the contrary differences of
- $_{20}$ -5.2 (±1.9)% and -0.9 (±2.5)% were found with the operational product of IASI compared to the FTIR and Brewer measurements. This operational approach data may underestimate the O₃ total column since the MDR is negative for both ground-based comparisons. In contrast, it can be concluded that the analytical retrieval algorithm is a consistent method to derive O₃ total columns from IASI since it is in excellent agree-
- ²⁵ ment with both ground-based measurements whereas IASI operational algorithm data match only with Brewer measurements.





Finally, we have also compared the O₃ total columns over Izaña from this study with data derived from other satellite instruments (OMI, GOME-2). Again, excellent agreement is observed: $-0.5 (\pm 0.7)$ % and $3.5 (\pm 1.2)$ % for OMI, and $-2.4 (\pm 1.1)$ % and $1.5 (\pm 1.5)$ % for GOME-2, compared with FTIR and Brewer, respectively. These agreements corroborate recent studies (Kroon et al., 2008; Antón et al., 2009; Boynard et al., 2009). Note that all these comparison were made with adequate temporal and spatial matching criteria.

In conclusion, this study demonstrates that FTIR and Brewer are high quality instruments, perfectly suited for satellite validation of total ozone columns. At the subtropical site of Izaña, O₃ data from these ground-based measurements are in excellent agreement with data from OMI and GOME-2. Therefore, with all these independent comparisons, IASI O₃ total columns derived from the analytical retrieval approach have been validated in the present work. Only the operational IASI O₃ total columns seem to need further improvement.

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Table 1. FTIR/Izaña error analysis: estimated ozone total column errors for statistical and systematic contributions (in %) in function of error source. Smoothing contribution estimated for ozone total column is added in the last column.

Error source	statistical	systematic	smoothing	
Baseline	0.2	0.2		
ILS	0.3	0.2		
LOS	0.2	*		
Solarlines	*	*		
Temperature	0.1	*		
Spectroscopy	*	1.9		
Noise	0.2	*		
Total	0.5	2.0	0.2	

* Value lower than 0.1%.



Table 2. Summary of the comparison between O_3 total columns derived from Izana FTIR and Brewer and from various satellites data ("IASI-an" is the data produced by the analytical retrievals, "IASI-op]] is the operational product). "*N*" is the number of daily averaged total ozone columns for the coincidences, "MRD" is the Mean Relative Difference (in %) with the relative rms at 1 σ , "*R*" is the correlation coefficient of the linear regression and the relative slope of the linear regression is given in the last columns.

FTIR				_	Brewer				
	Ν	MRD in % (rms 1 σ)	R	slope		Ν	MRD in % (rms 1 σ)	R	slope
IASI-an	13	-2.0 (1.4)	0.94	0.98		55 77	1.5 (2.2)	0.89	1.00
GOME-2	22 20 10	-5.2(1.9) -2.4(1.1) -0.5(0.7)	0.90 0.97 0.99	0.95 0.98 0.99		90 74	-0.9 (2.5) 1.5 (1.5) 3.5 (1.2)	0.85 0.96 0.97	0.99 1.00 1.00



















Fig. 3. Daily total ozone variability calculated from Brewer measurements. Hourly mean total columns at noon are taken as reference and relative differences of total ozone column has been calculated for each half an hour (from 08:00 a.m. to 18:30 p.m.) and for each day of the comparison period.



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Fig. 4. Ground-based comparison of O_3 total columns. Left panel: time series of O_3 total column derived from FTIR at Izaña (black) and from Brewer (purple) measurements. Right panel: O_3 total column derived from Brewer measurement as a function of the FTIR O_3 measurements. Red line is a linear fit with zero y-intercept.



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Fig. 6. O_3 total columns derived from IASI analytical (left panel) and IASI operational (right panel) as a function of O_3 total columns from FTIR at Izaña (top) and as a function of Brewer (below). Red line is a linear fit with zero y-intercept.











Fig. 8. O_3 total columns derived from GOME-2 (left panel) and OMI (right panel) as a function of O_3 total columns from FTIR at Izaña (top) and as a function of Brewer data (below). Red line is a linear fit with zero y-intercept.



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