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Authors	E. Botek, S. Chabrillat, Y. Christophe, Q. Errera (BIRA-IASB)
Editor	H. Eskes (KNMI)
Contact	info@gmes-atmosphere.eu

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Summary

BASCOE, operated by BIRA-IASB, is used for the MACC-III project to assimilate the offline observations of stratospheric composition by Aura-MLS. The system performance and operational implementation are described in the companion deliverable D20.2 and D21.1. Its results and usage are reported in the deliverables D19.2, D21.6 and D23.3. Here the quality of the BASCOE analyses of O_3, H_2O, HCl, HNO3, N_2O and ClO are verified by comparison with the assimilated observations and validated through the comparison of a preliminary run with independent observations by ACE-FTS, for the year 2011.

For ozone, the biases between the analyses and assimilated observations are less than 3% in the lower stratosphere and less than 5% at the middle stratosphere. The time series and vertical profiles are also compared with independent satellite observations (ACE-FTS, OMPS, OSIRIS), and maps of total columns are compared with other MACC-III products.

For water vapor, the relative biases between the analyses and the assimilated Aura-MLS observations is smaller than 5% between 3hPa and 150hPa. For nitric acid (HNO_3) the performance is not as good, especially in the upper-middle stratosphere (3-10hPa) where the analyses underestimate the observations by 10% in the Tropics and up to 40% in the polar regions. For HCl the system performs well except in South Pole ozone hole conditions, where the analyses can underestimate the observations by up to 50%. For the short-lived species ClO, the assimilation delivers large relative biases in many regions. Finally for N_2O the performance is good except in the upper-middle (3-10Pa) stratospheric polar night where the analyses underestimate the observations by up to 40%.

It is noted that for all assimilated species, relative biases are larger than 10% only in those regions and seasons where the abundance is small: absolute biases remain quite small in all cases, and the comparison with ACE-FTS shows that the BASCOE analyses have a very good quality.

Contents

1 Introduction

BASCOE (Belgian Assimilation System for Chemical ObsErvations) (Errera et al., 2008; Viscardy et al., 2010; Errera and Ménard, 2012) is a Data Assimilation System primarily designed to deliver analyses of the chemical composition in the stratospheric layer. As explained in detail by Lefever et al. (2015), BASCOE has been contributing since 2009 to the MACC projects through comparison with models based on the Integrated Forecasting System (IFS) as well as SACADA (Elbern et al.,2010) and TM3DAM (Eskes et al.,2003; van der A et al.,2010).

The MACC stratospheric ozone service (http://www.copernicus-stratosphere.eu) is one of the preparatory activities for the future Copernicus Atmosphere Monitoring Service (CAMS). During these pre-operational phases BASCOE has been contributing to the Near Real Time (NRT) production with global analyses of stratospheric O_3, H_2O, HCl, HNO3, N_2O and ClO obtained by assimilation of Aura-MLS observations. These analyses are used in the WMO Antarctic Ozone Bulletins for Global Atmospheric Watch (GAW) research (see MACC-III deliverables D19.2 and D23.3).

During MACC-III, BASCOE 4.3 was run in Near Real-Time (NRT). This version, more advanced than version q2.5 described in Lefever et al (2015), is described in section 2 of the companion deliverable D21.6. The operational configuration is provided in the deliverable D20.2.

2 Validation of a preliminary BASCOE experiment with ACE-FTS observations in 2011

In this section we evaluate the output of a preparatory BASCOE assimilation of Aura-MLS (experiment sc0134A), using a version (v3.11) which was used operationally in 2013 and is still very close to the current operational run (v4.3). The main improvement in v4.3 is the use of a full Background Error Covariance Matrix (Errera and Ménard, 2012) while v3.11 used only a diagonal matrix as in the previous version validated by Lefever et al. (2015). The evaluation of this preliminary experiment relies on comparisons with independent observations by ACE-FTS v3 (Waymark et al., 2014).

2.1 Arctic ozone hole event of 2011

Figures 1 and 2 show the bias of BASCOE during the Arctic ozone hole event of 2011 (Manney et al., 2011). At ozone hole heights, i.e. between 15 and 20 Km of altitude, the biases do not reach more than 5% for ozone and 10% for the other species.

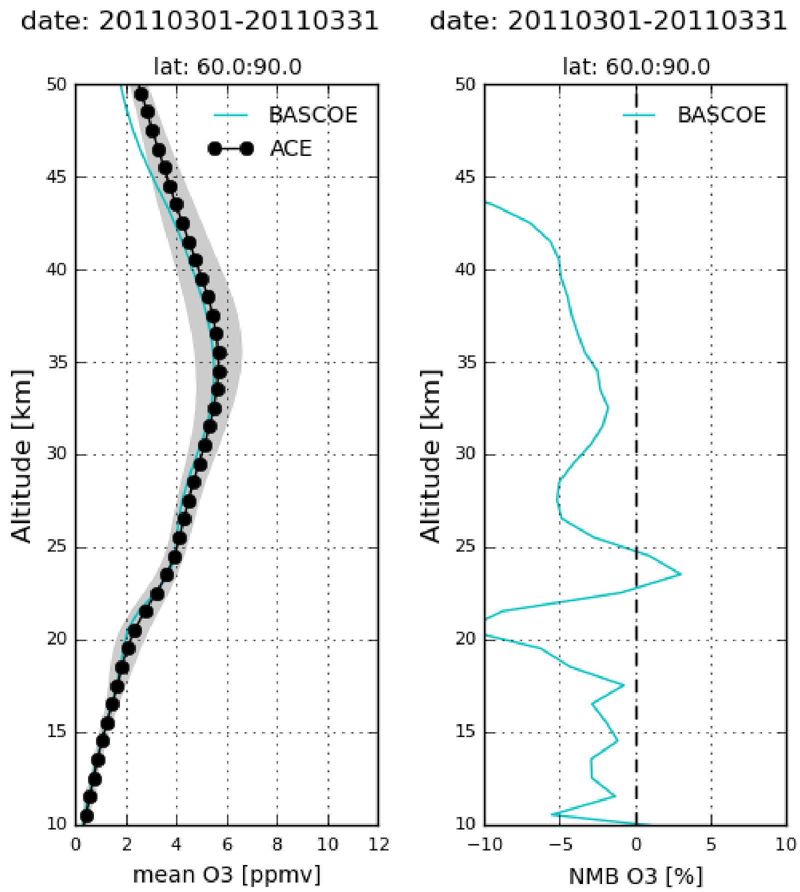

Figure 1: Profiles of ozone mean values (left) and Normalized Mean Bias (right; normalization by the observations) above the Arctic, by BASCOE and ACE-FTS in March 2011. The grey area around the mean values represent the variability of ACE-FTS observations during the considered period.

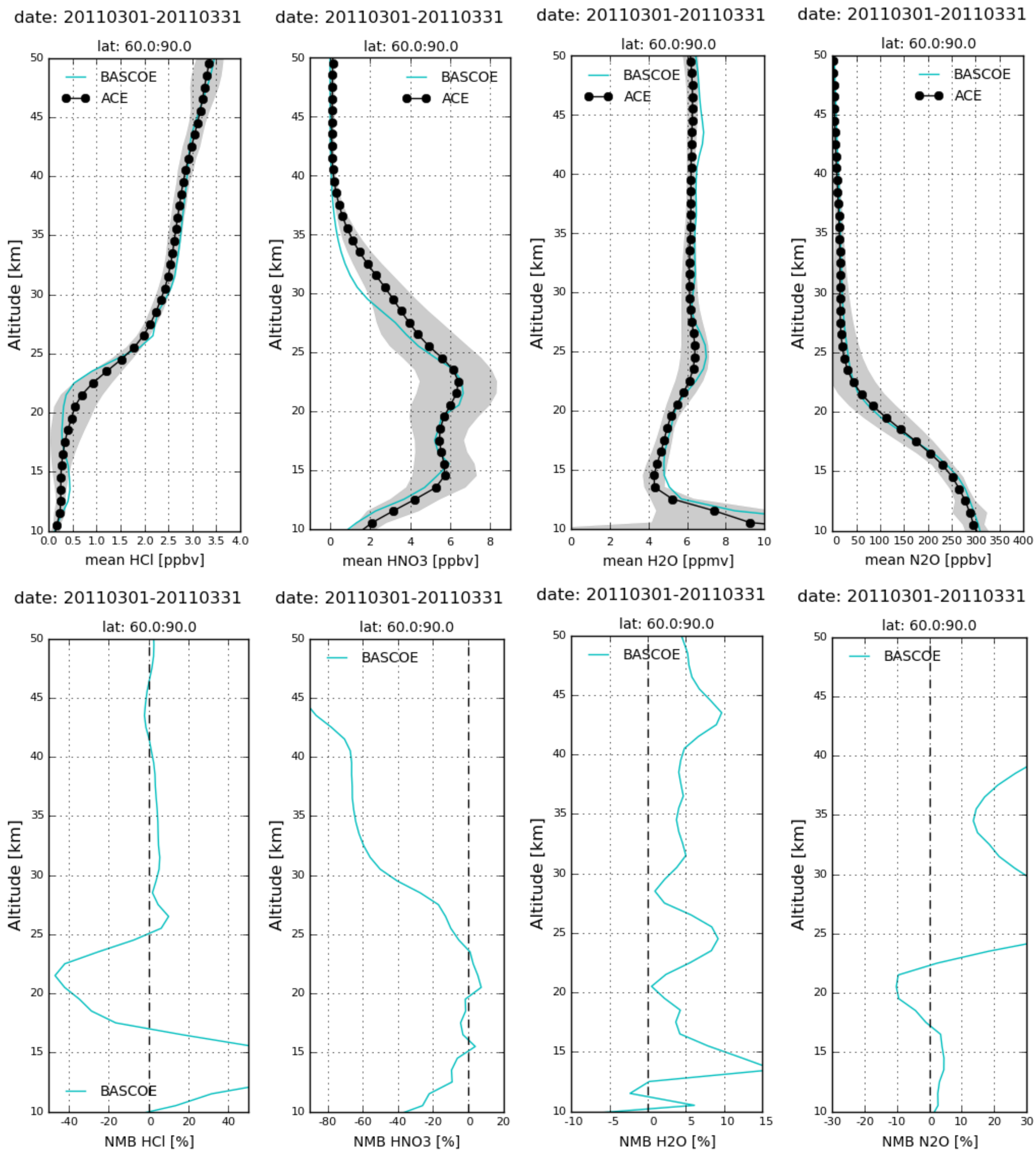

Figure 2: same as figure 1 but for HCl (1st column), HNO3 (2d column), H2O (3rd column) and N2O (4th column).

2.2 Polar and tropical latitude bands in July 2011

The largest relative biases in Fig. 3 are encountered in the lowermost stratosphere above the Tropics and in the polar night vortex, i.e. in regions where the ozone abundance is smaller than 1 ppmv.

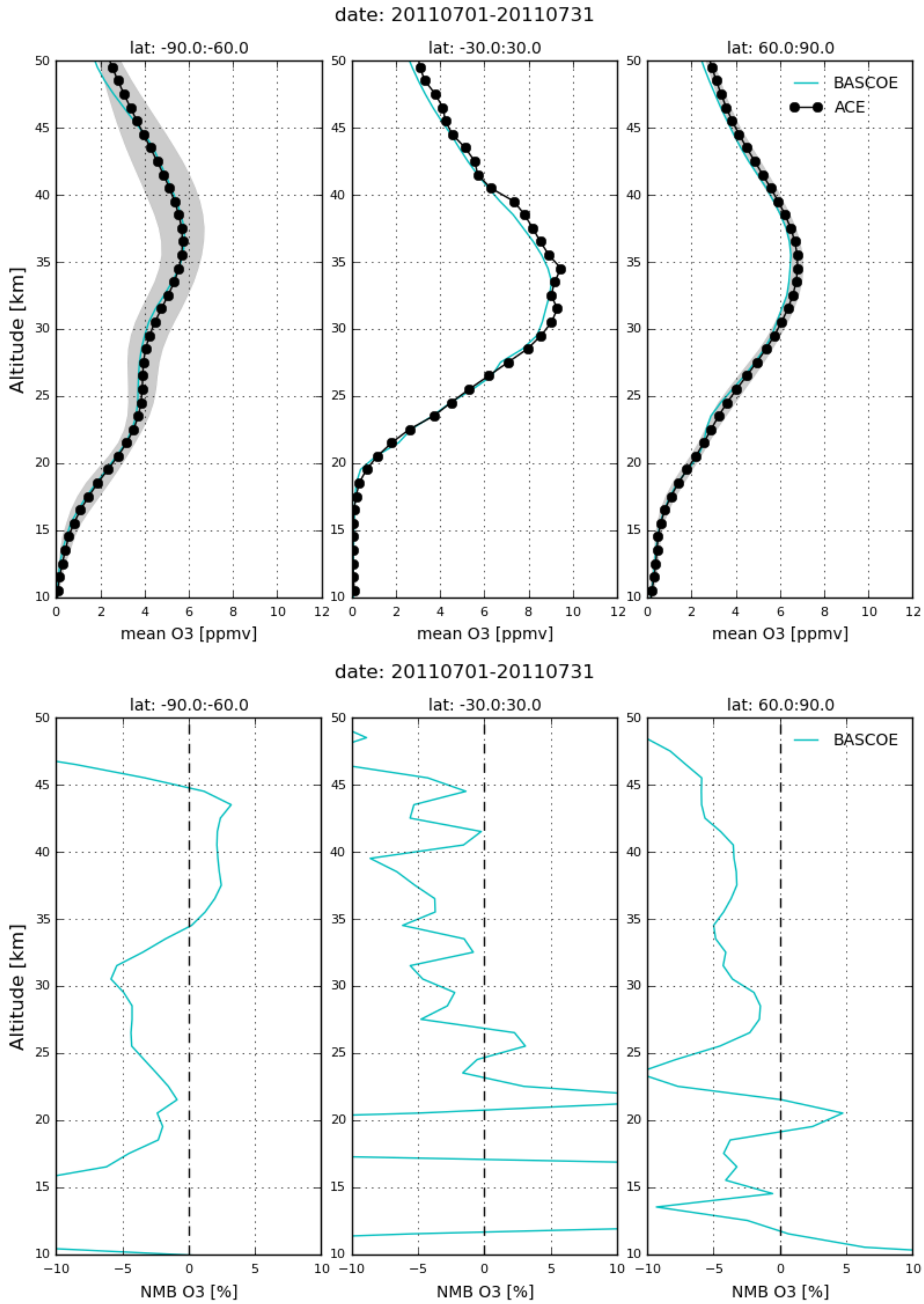

Figure 3: Profiles of ozone mean values (top) and Normalized Mean Bias (bottom; normalization by the observations) above the Antarctic (90°S-60°S; left column), Tropics (30°S-30°N, middle column) and Arctic (60°N-90°N, right column) by BASCOE and ACE-FTS in July 2011. The grey area around the mean values represent the variability of ACE-FTS observations during the considered period.

Fig. 4 shows that contrarily to ACE-FTS observations, the analysis of HCl by BASCOE has almost no vertical gradient in the polar vortex below 26 km, leading to significant underestimation between 30 and 20 km and overestimation below 20 km. BASCOE is much less biased in the two other latitude bands.

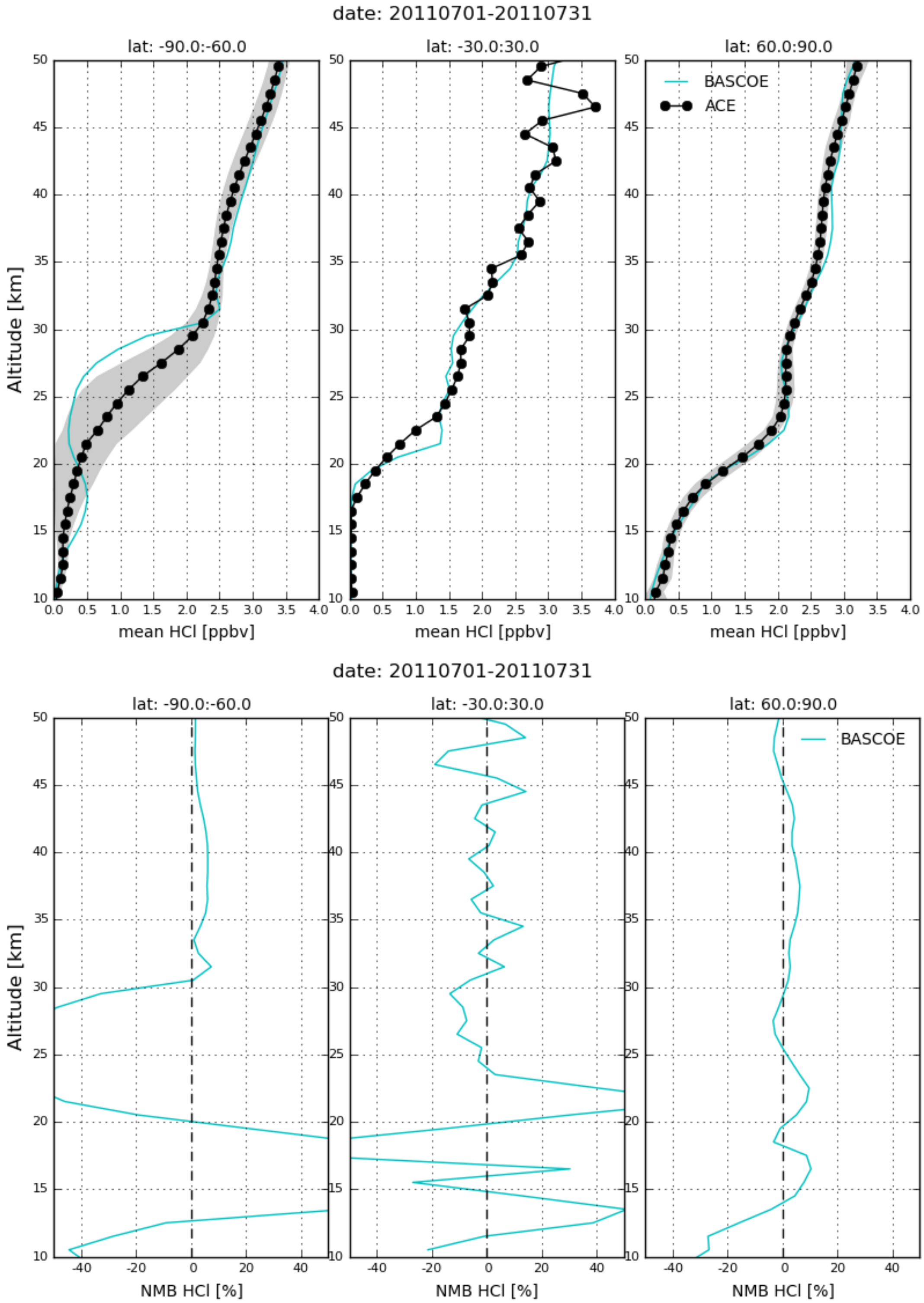

Figure 4: Same as Figure 3 but for HCl.

In the middle stratosphere, the analyses of HNO3 have only very small biases. A serious underestimation is noted in the lower stratosphere and in the Arctic upper stratosphere. In this latter case, the observed increase of HNO3 with altitude may be due to NOx production due to energetic particle precipitation (EPP; see Robichaud et al., 2010): BASCOE cannot assimilate successfully HNO3 in these conditions because this process is not modelled and contrarily to MIPAS, Aura-MLS does not deliver any observations of NO2.

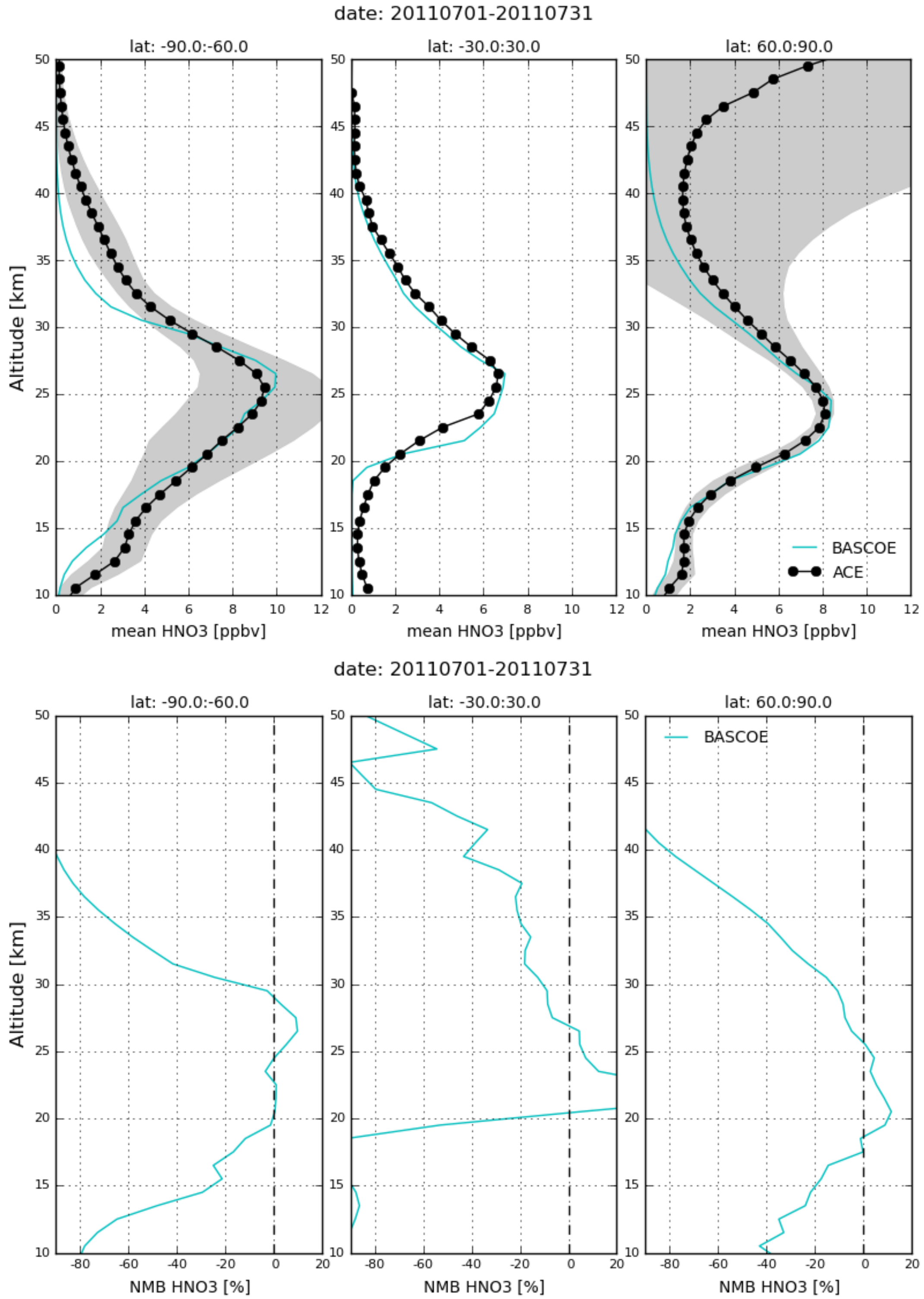

Figure 5: Same as Figure 3 but for HNO3.

As seen on fig. 6, the BASCOE analyses of water vapour have remarkably small biases (< 10%). The only exception is in the lowermost stratosphere where water vapour is difficult to model and the Aura-MLS observations have larger errors.

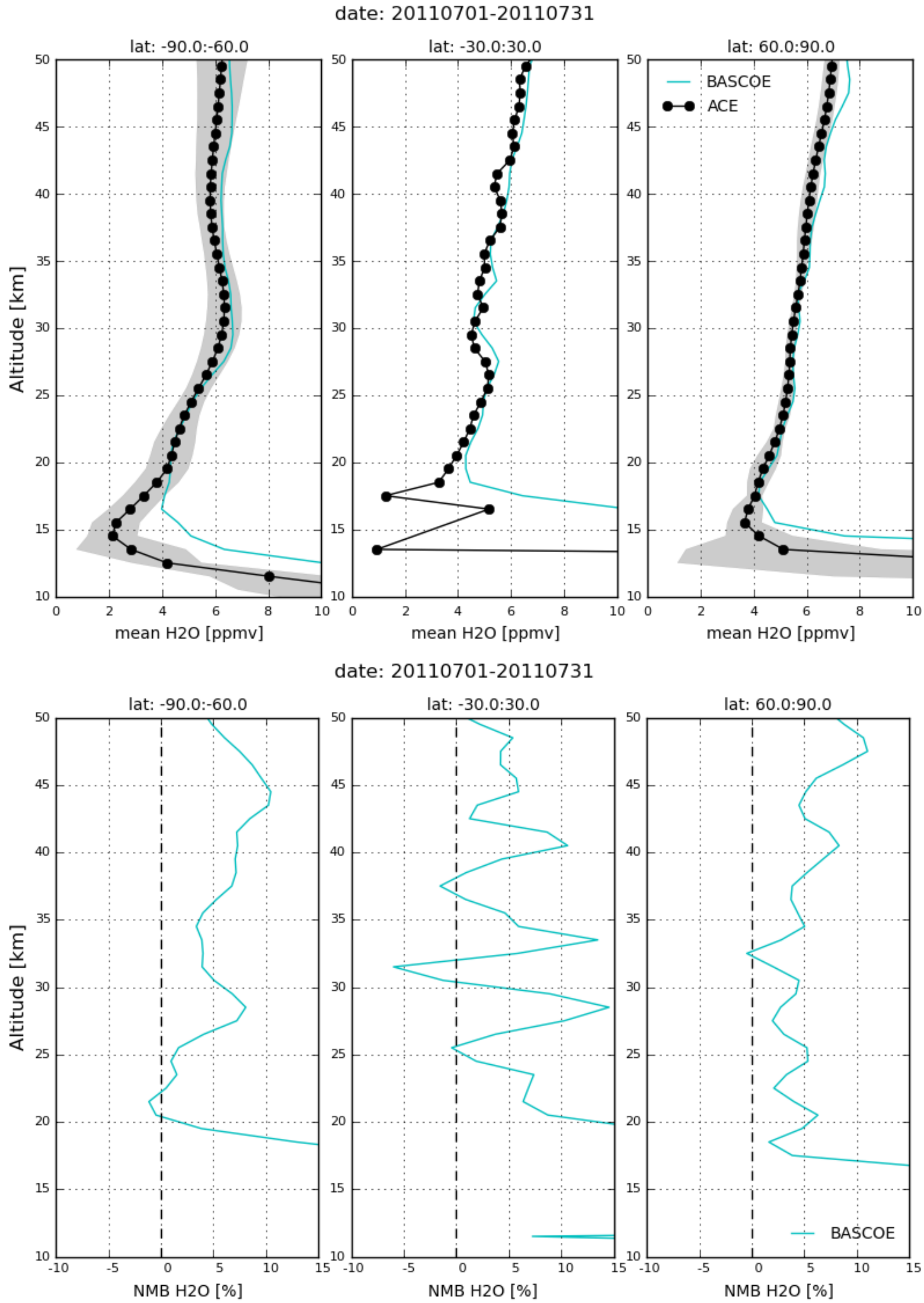

Figure 6: Same as Figure 3 but for H2O.

Figure 7 shows relatively small (<20%) biases of N2O above 20 km altitude. A large overestimation (up to 50%) is noted in the analyses below 20 km, both in the polar vortex and in the tropical band. This difference deserves further investigation.

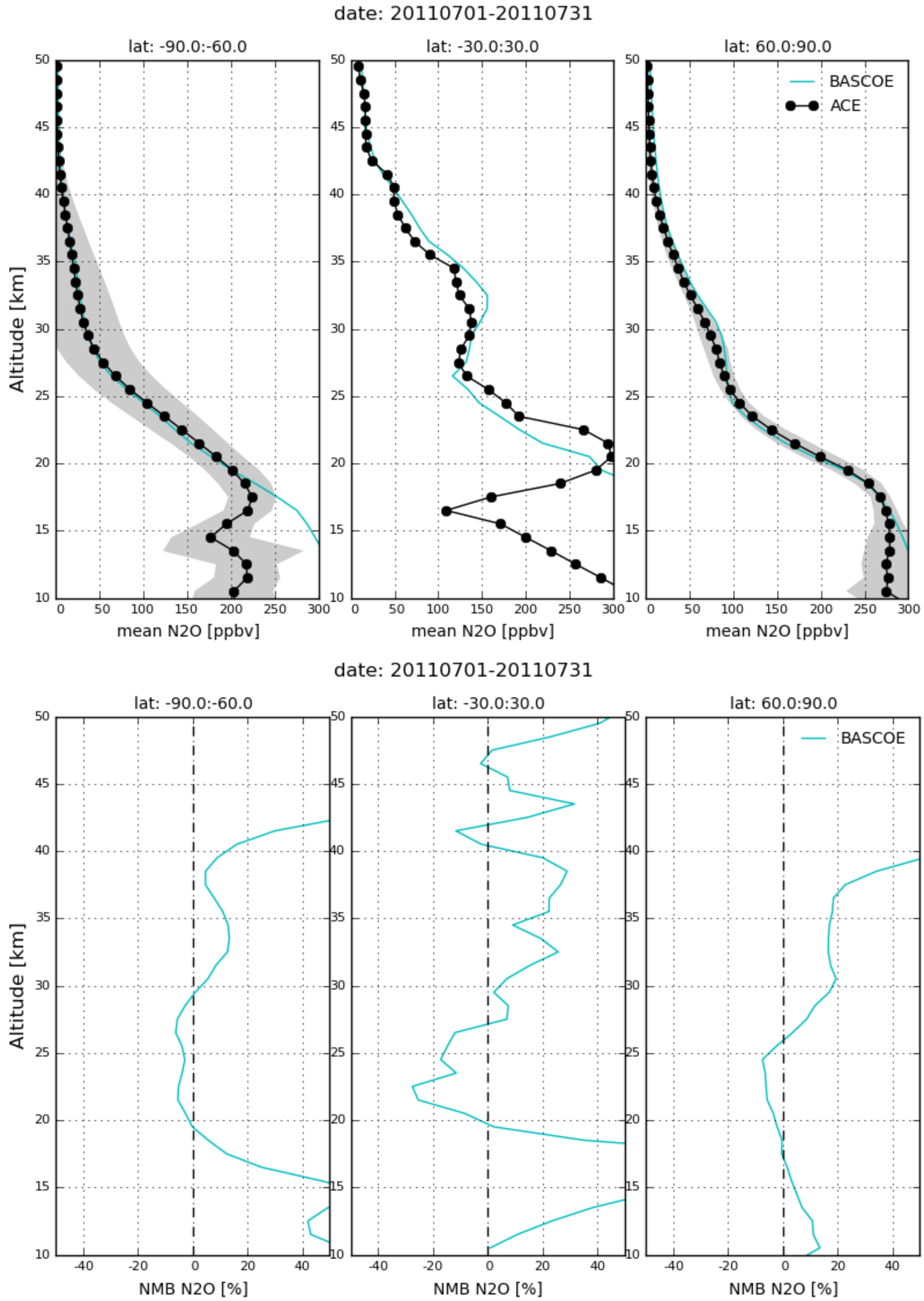

Figure 7: Same as Figure 3 but for N2O.

3 Validation of ozone analyses delivered in NRT by BASCOE in 2014-2015: comparison with Aura-MLS, OSIRIS and OMPS

We now validate the analyses deliver by BASCOE v4.3 in Near Real-Time since 2014-02-01. This version and configuration are described in the companion deliverable D20.2 and D21.6.

In **Figure 8** the time series of relative differences between BASCOE and MLS are plotted for the middle stratosphere (layers 3-10hPa, top) and the low stratosphere (layers 30-70hPa, bottom) at the polar and tropical regions for the year 2014. Everywhere the biases do not exceed 5% showing a global underestimation of satellite values. Indeed, in the middle stratosphere the errors are very small at the poles (generally less than 2%), with the exception of the Antarctic ozone hole season where we obtain a maximum bias peak of -4.5% in September. At the tropics the underestimation increases up to 3%. The biases are still smaller in the low stratosphere of around -0.5% everywhere and again a peak of -3% during the Antarctic ozone hole season. The reason of such slight different biases for such season could perhaps be explained by a deficient abundance evaluation of ozone depletion substances assimilated or not by BASCOE.

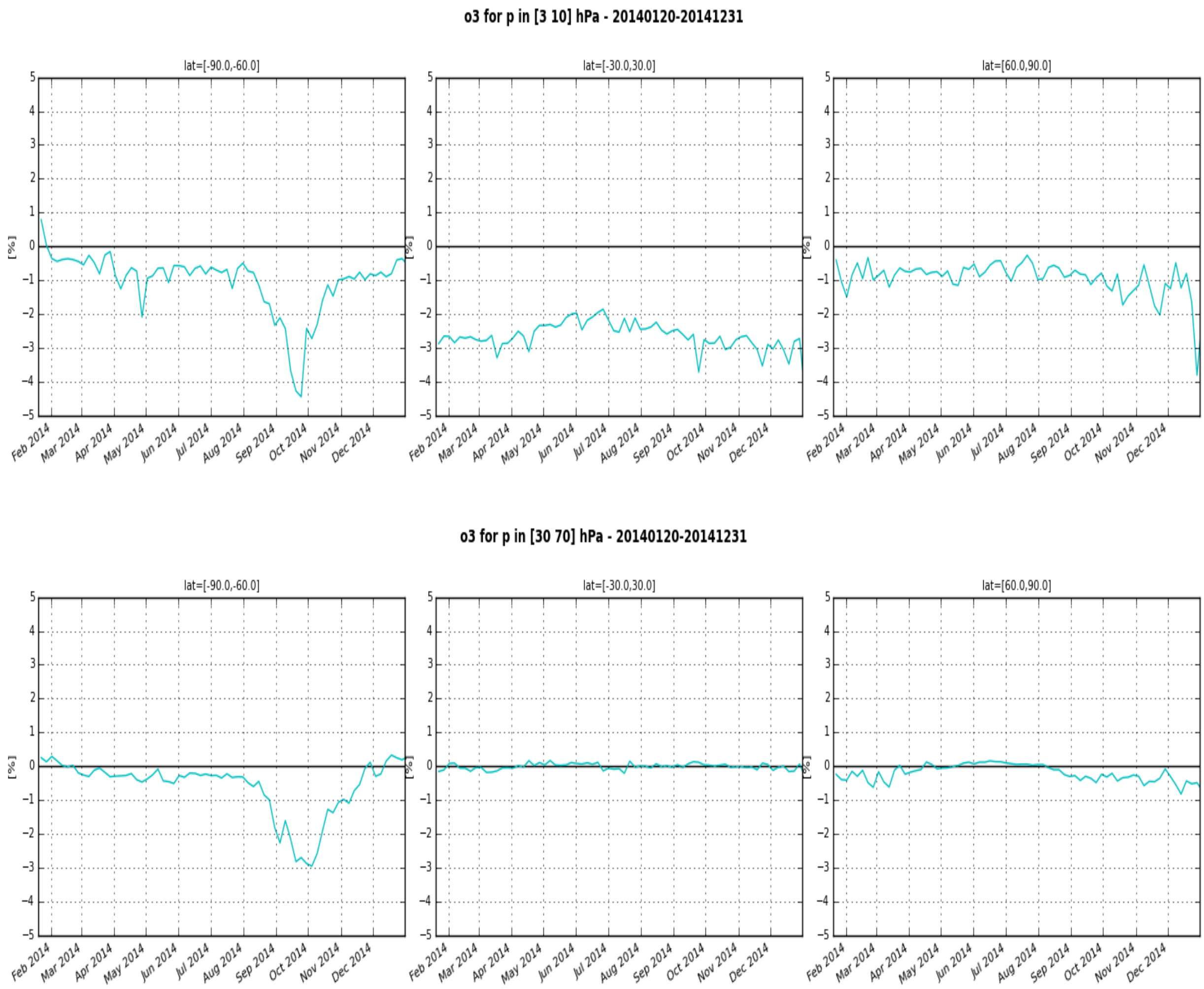

Figure 8: Verification of ozone (O3) analyses by BASCOE: time series of the relative differences between BASCOE and the assimilated data (i.e. MLS) for the layers 3-10hPa (top) and 30-70 hPa (bottom) at the Tropics and the poles for the year 2014.

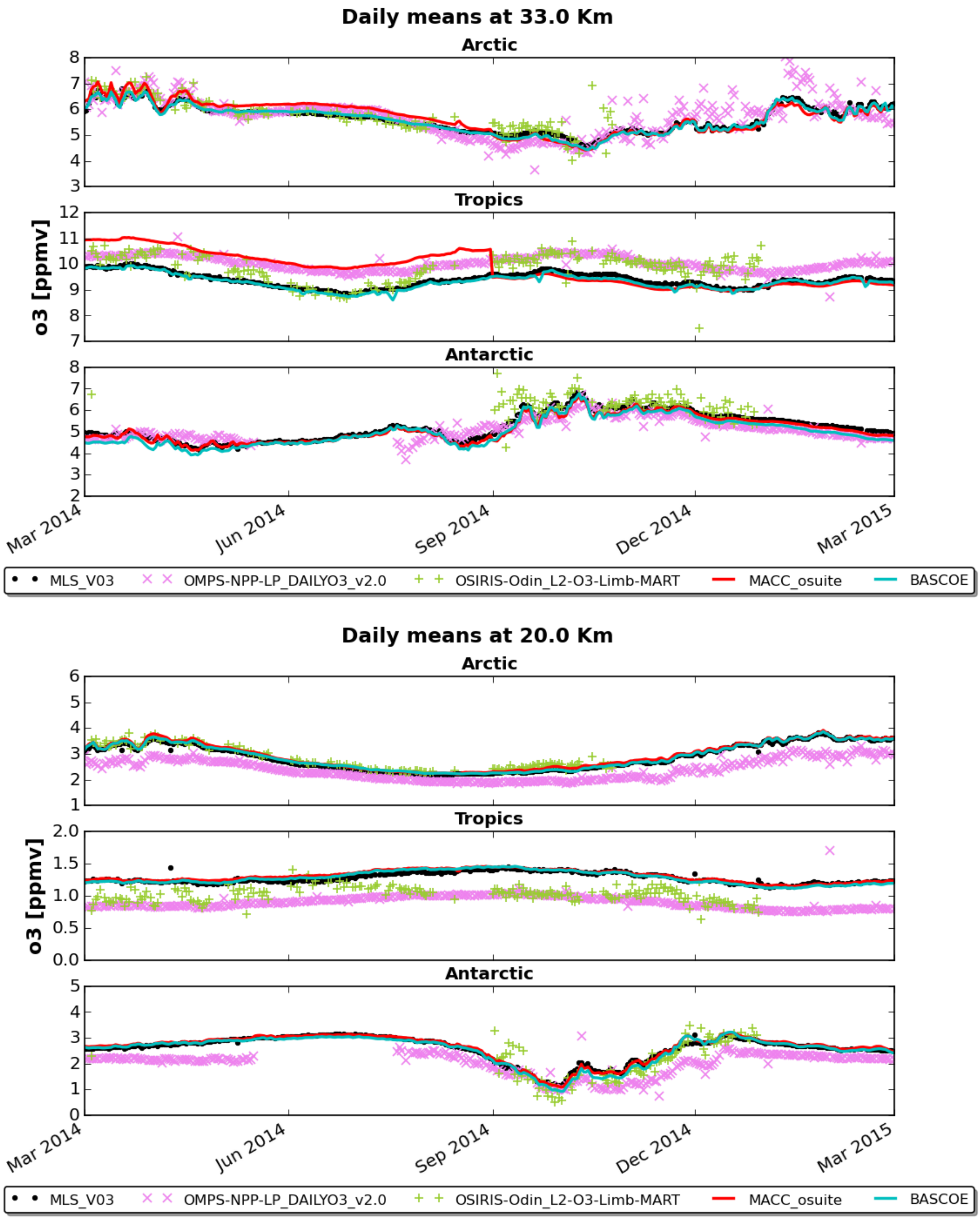

Figure 9: Evaluation of the ozone analyses delivered by BASCOE and te MACC o-suite: daily mean time series of ozone abundances from MACC_osuite (red line) and BASCOE (cyan line) with satellite observations by Aura-MLS (i.e. assimilated dataset), and independent OMPS and OSIRIS observations for the period 2014/03/01-2015/03/01 interpolated at altitudes 20 Km (bottom) and 33 Km (top).

Further comparisons are displayed in **Figure 9** for a year ranging from March 2014 to March 2015. In this case time series from daily means of the MACC models and BASCOE are contrasted with MLS, OMPS and OSIRIS observations at two specific altitudes (20 and 33 Km). It must be noticed that while all observational instruments are also sampled to daily means, the models outputs were not interpolated to the location of the observations, allowing only a crude comparison between models and observations. Some general comments can be established from the present plots concerning the satellite data. Firstly, at the lower stratosphere (20 Km) OMPS yields lower observed ozone abundances than MLS up to about 30% at all latitude bands. We can identify such an underestimation for OSIRIS data in the Tropics. Secondly, at the middle stratosphere (33 Km) where the ozone maximum is observed by MLS, the other instruments seem to be in global agreement at the Poles with MLS data, but a general overestimation of about 1 ppm in average all over the period is obtained at the Tropics. These comparisons show that the analyses may still disagree with independent observations, such as OSIRIS and OMPS. The latter instrument is expected to become of particular importance for the future validation and operation of Copernicus models.

From the vertical profiles of **Figures 10-11**, it can be pointed out a very good performance of BASCOE throughout the stratosphere with the smaller biases of at most 3% between 100 and 10 hPa. With respect to the standard deviation of observations (plotted in grey), it is interesting to note that the dispersion is about half a ppmv nearly all along the whole vertical range during October, which indicates a larger incertitude of measures during the ozone hole episode.

An intercomparison of ozone total column maps between MACC_products MACC_osuite, SACADA, TM3DAM and SACADA is displayed in **Figure 12** for December 2014. BASCOE shows features very similar to the other systems.

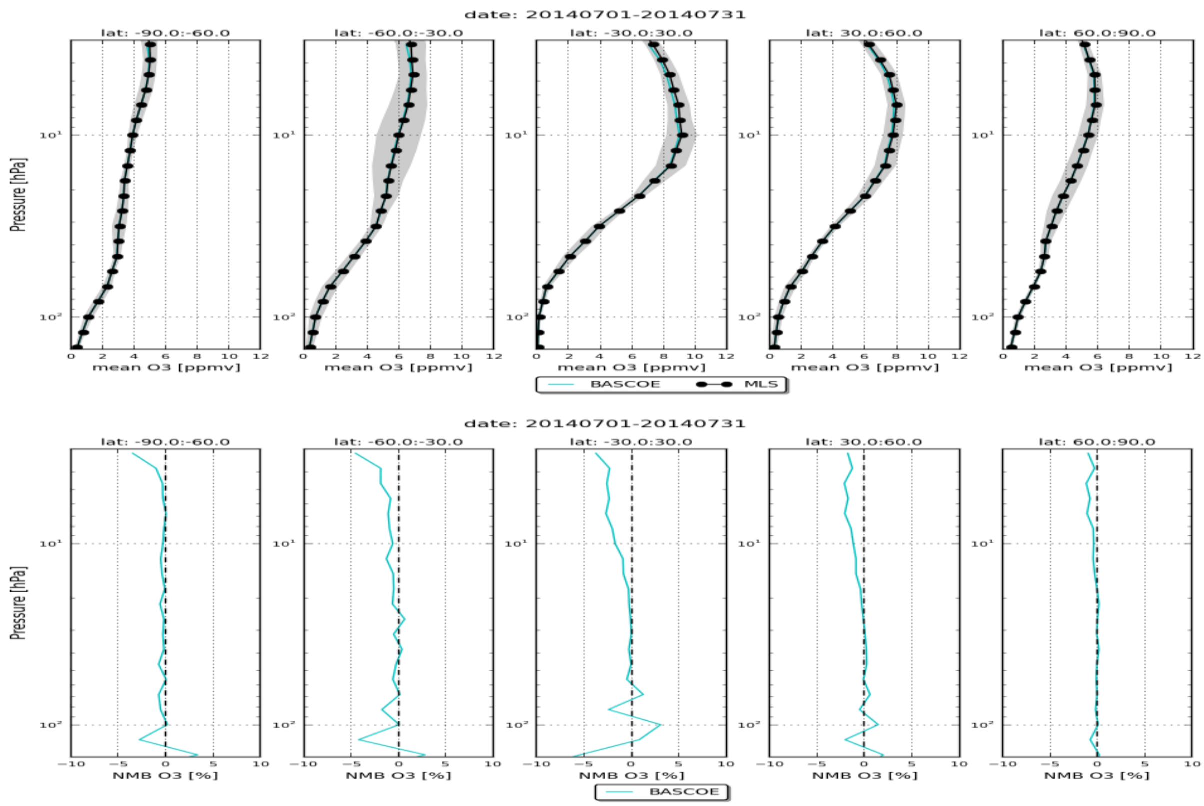

Figure 10: Normalized mean ozone profiles (top) and bias (bottom) of the ozone profile between BASCOE and MLS observations for July 2014.

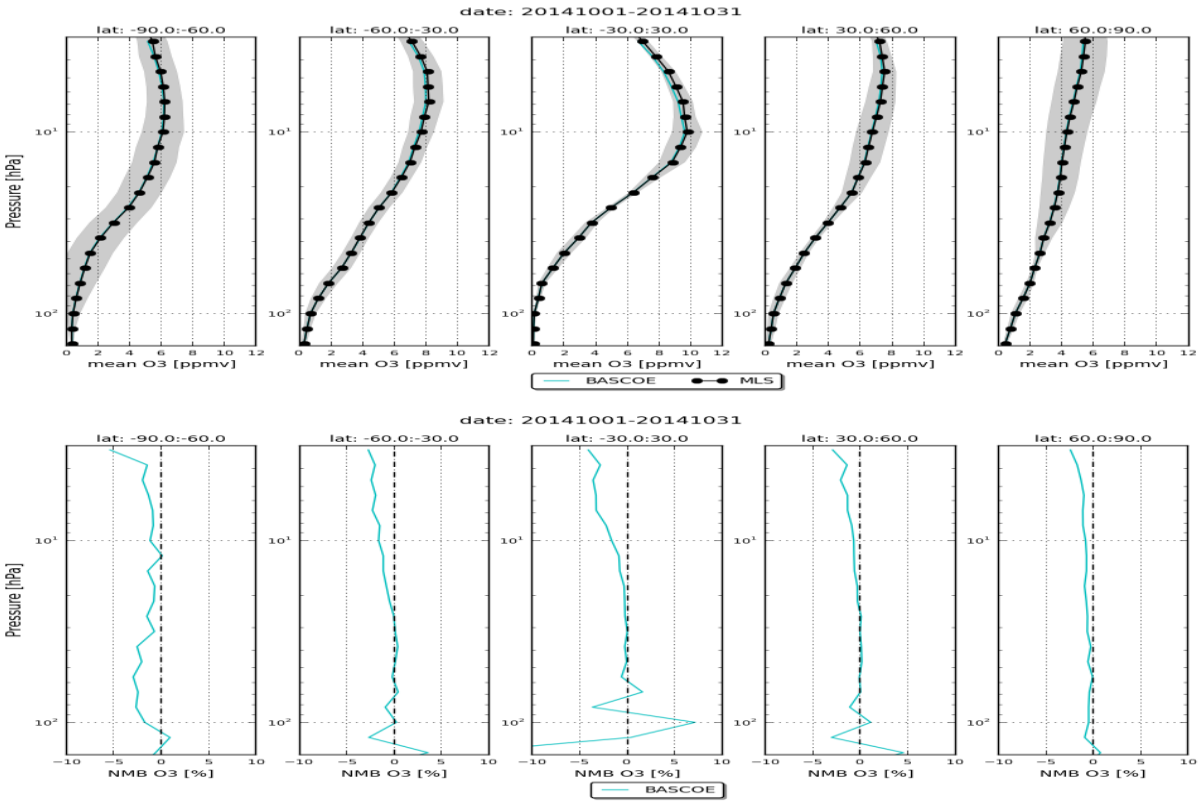

Figure 11: Normalized mean ozone profiles (top) and bias (bottom) of the ozone profile between BASCOE and MLS observations for October 2014.

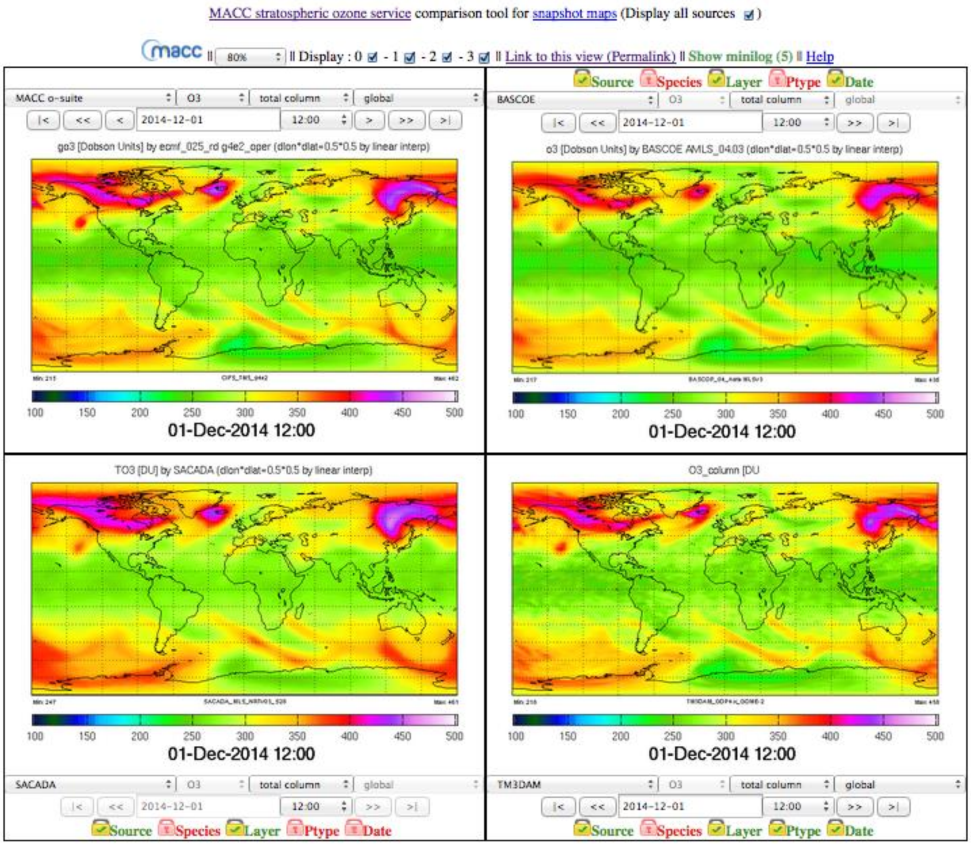

Figure 12: Ozone total columns maps comparison between MACC_osuite, BASCOE, SACADA and TM3DAM from the intercomparison tool of the MACC stratospheric service on December 1st 2014.

4 Verification of the analyses of H2O, HNO3, HCl, ClO and N2O delivered in NRT by BASCOE in 2014-2015: comparison with the assimilated Aura-MLS observations

In order to correlate the biases obtained for ozone in the last section - implying particularly the Antarctic ozone hole season- with BASCOE performance for the other species assimilated, the time series during 2014 and vertical profiles of H2O, HNO3, HCl, ClO and N2O for the low stratosphere (30-70 hPa) and the middle stratosphere (3-10hPa) are examinated below in **Figures 13 to 27**.

Figures 13-**15** demonstrate the very good performance of BASCOE assimilation for water vapor. The biases at the lower stratosphere do not exced 2%, with underestimations at the South pole during the ozone hole event and overestimations at the tropics between March and November. Elsewhere the differences are less than 0.5%.

HNO3 assimilation (**Figures 16-18**) is slightly worse at the lower stratosphere not exceding 6%, overestimating in winter and underestimating in spring. On the other hand, the perfomance is still worse at the polar middle stratosphere, where the differences can attain -30% in the Antarctica and -45% in the Artics. At tropical regions the biases attain -12%. The dispersion of the observational values is particularly substantial at the South pole and the tropics for July and October with deviations of the order of the mean values.

HCl present very small deviations at the middle stratosphere of at most 1%, but it delivers underestimations up to 30% during the Antarctic ozone hole event and 12% at the North pole during winter (see **Figures 19-21**).

ClO exists in low quantities in the stratosphere (see **Figures 22-24**). At the low stratosphere There are sudden marked changes in the biases at the poles that turn around -70% during summer an fall and +/-20% in winter and spring. At the middle stratosphere the biases changes are more gradual passing from 5% in average during summer and fall to a maximum of -30% in winter. A regular underestimation of about 60% is observed at the tropical low stratosphere, whereas a slight overestimation of about 5% is obtained for the middle stratosphere.

N2O BASCOE assimilation performance is rather deficient in the middle and upper stratosperic layers of the polar night region, as can be observed in **Figures 25-27**. An increasing negative deviation begins in autumn; it passes through a maximum of 40% in winter and decreases to negligible values at the end of the season. At the lower stratosphere an overestimation of about 4% occurs during October and November. Elsewhere the biases are at most of 1%.

In summary, for all the five species investigated and closely related to the Antarctic ozone hole season, BASCOE presents some significant deficiencies only to simulate low abundances situations. Both HCl and ClO, for example, display underestimations that rise to 25% during the hole event, but they cannot explain an underestimation of ozone during the hole episode. HNO3, on the other hand, shows an overestimation of around 6% during the time of formation of PSC’s, but later it is underestimated during fall, which could has an indirect influence on the ozone deficit. Indeed, HNO3 is a recervoir of NO2, which regulates the ClO-ozone cycle depletion. At the end, all these differences result to be rather small and other species not assimilated like CFC’s substances could also play a role.

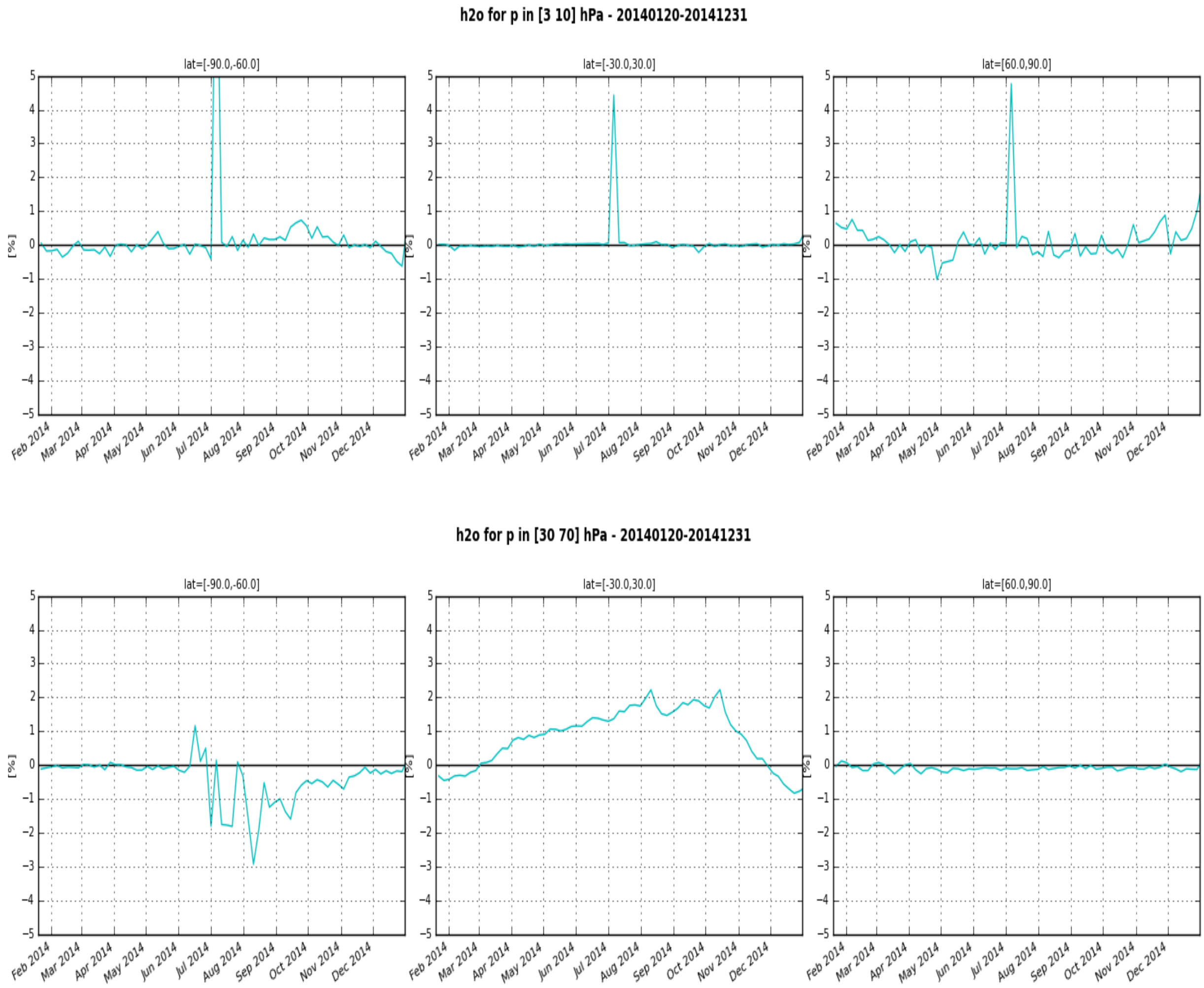

Figure 13: Verification of water vapor (H2O) analyses by BASCOE: time series of the relative differences between BASCOE and the assimilated data (i.e. MLS) for the layers 3-10hPa (top) and 30-70 hPa (bottom) at the Tropics and the poles for the year 2014.

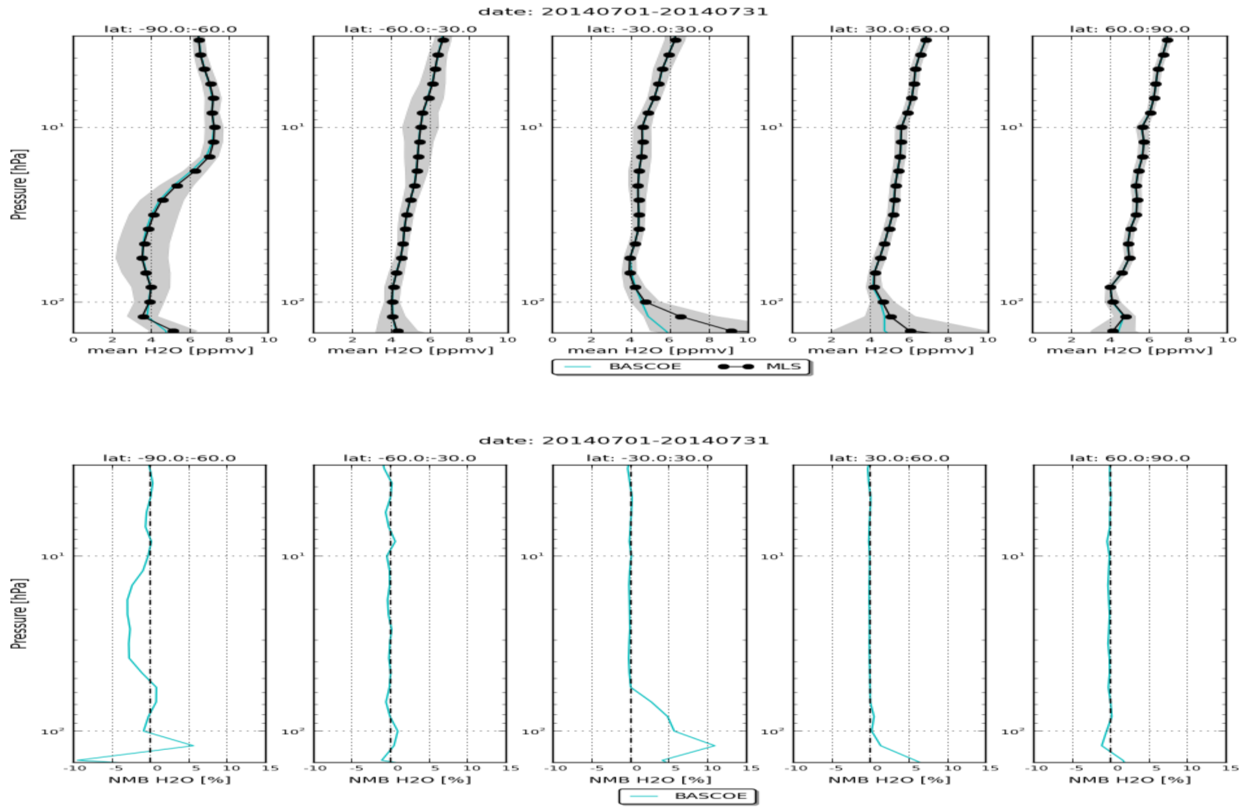

Figure 14: Normalized mean H2O profiles (top) and bias (bottom) between BASCOE and MLS observations for July 2014.

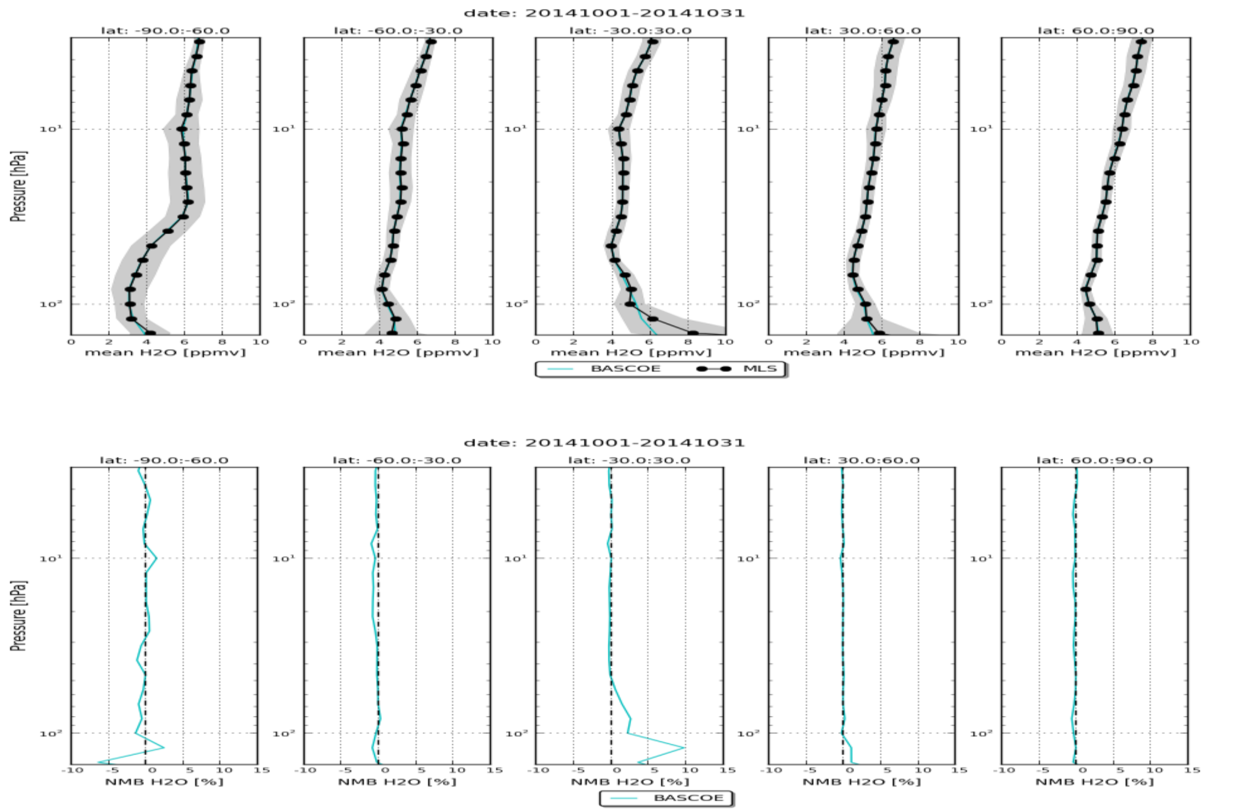

Figure 15: Normalized mean H2O profiles (top) and bias (bottom) between BASCOE and MLS observations for October 2014.

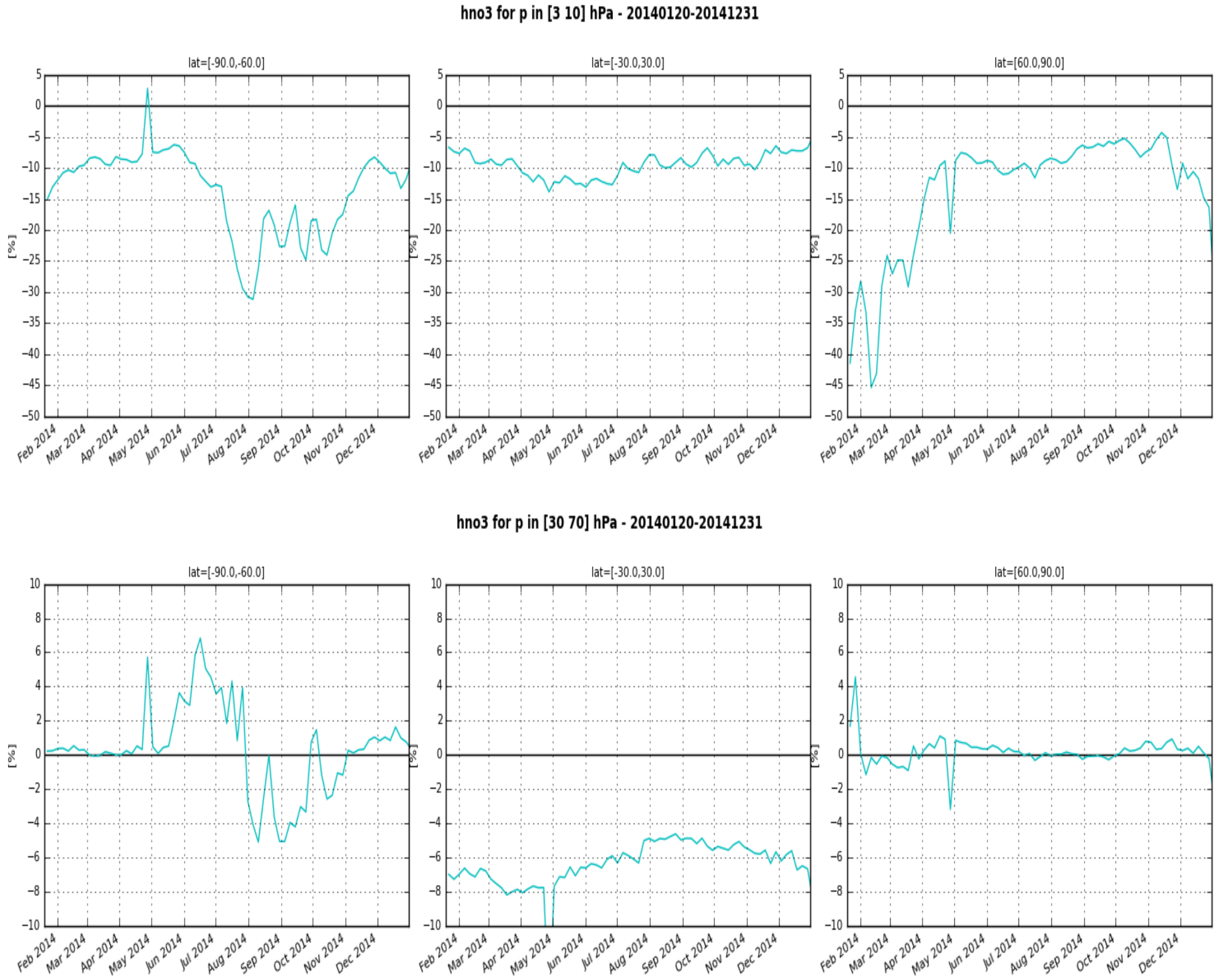

Figure 16: Verification of nitric acid (HNO3) analyses by BASCOE: time series of the relative differences between BASCOE and the assimilated data (i.e. MLS) for the layers 3-10hPa (top) and 30-70 hPa (bottom) at the Tropics and the poles for the year 2014.

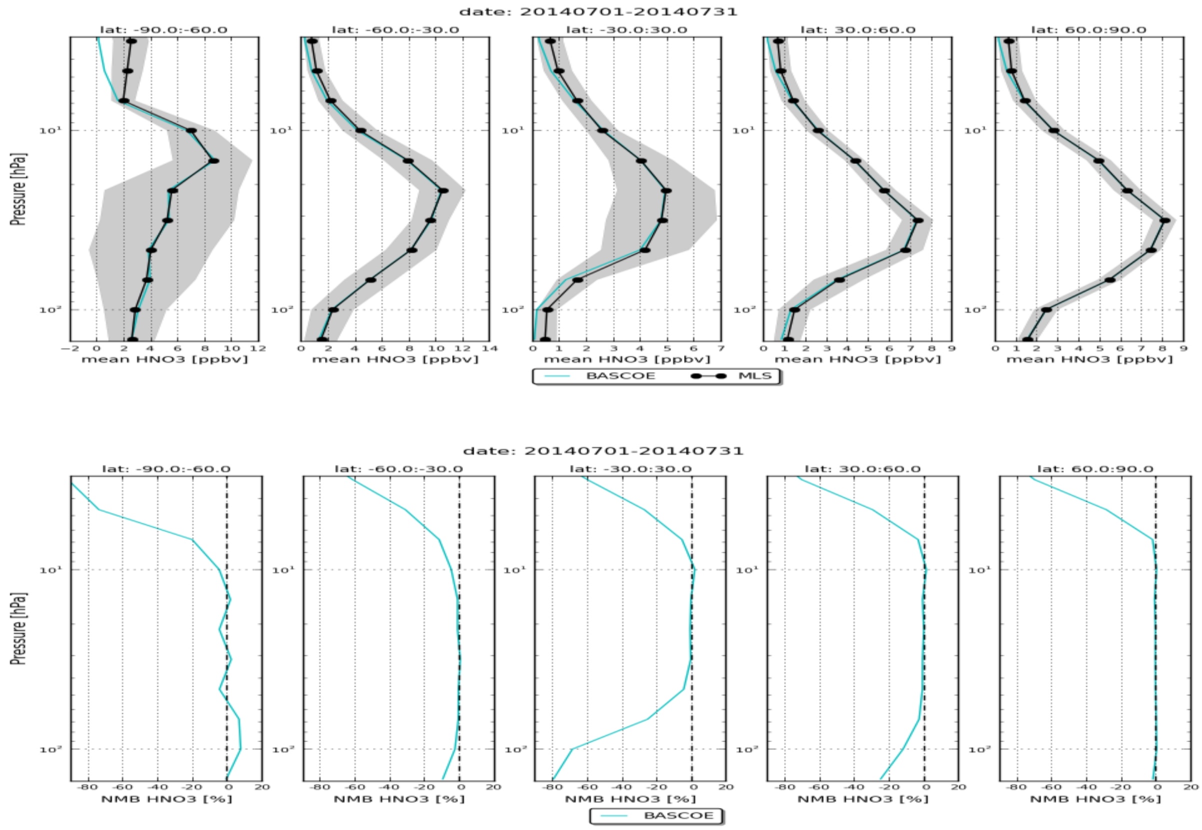

Figure 17: Normalized mean HNO3 profiles (top) and bias (bottom) between BASCOE and MLS observations for July 2014.

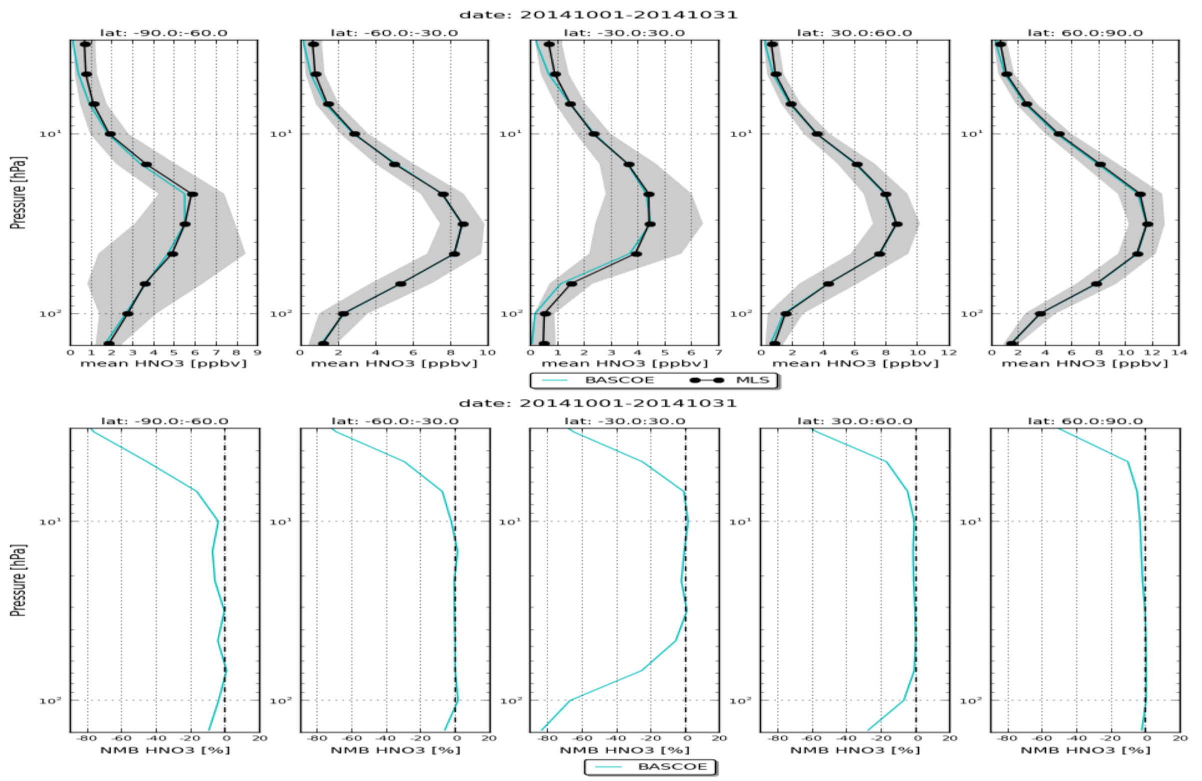

Figure 18: Normalized mean HNO3 profiles (left) and bias (right) of the ozone profile between BASCOE and MLS observations for July (top) and October (bottom) 2014.

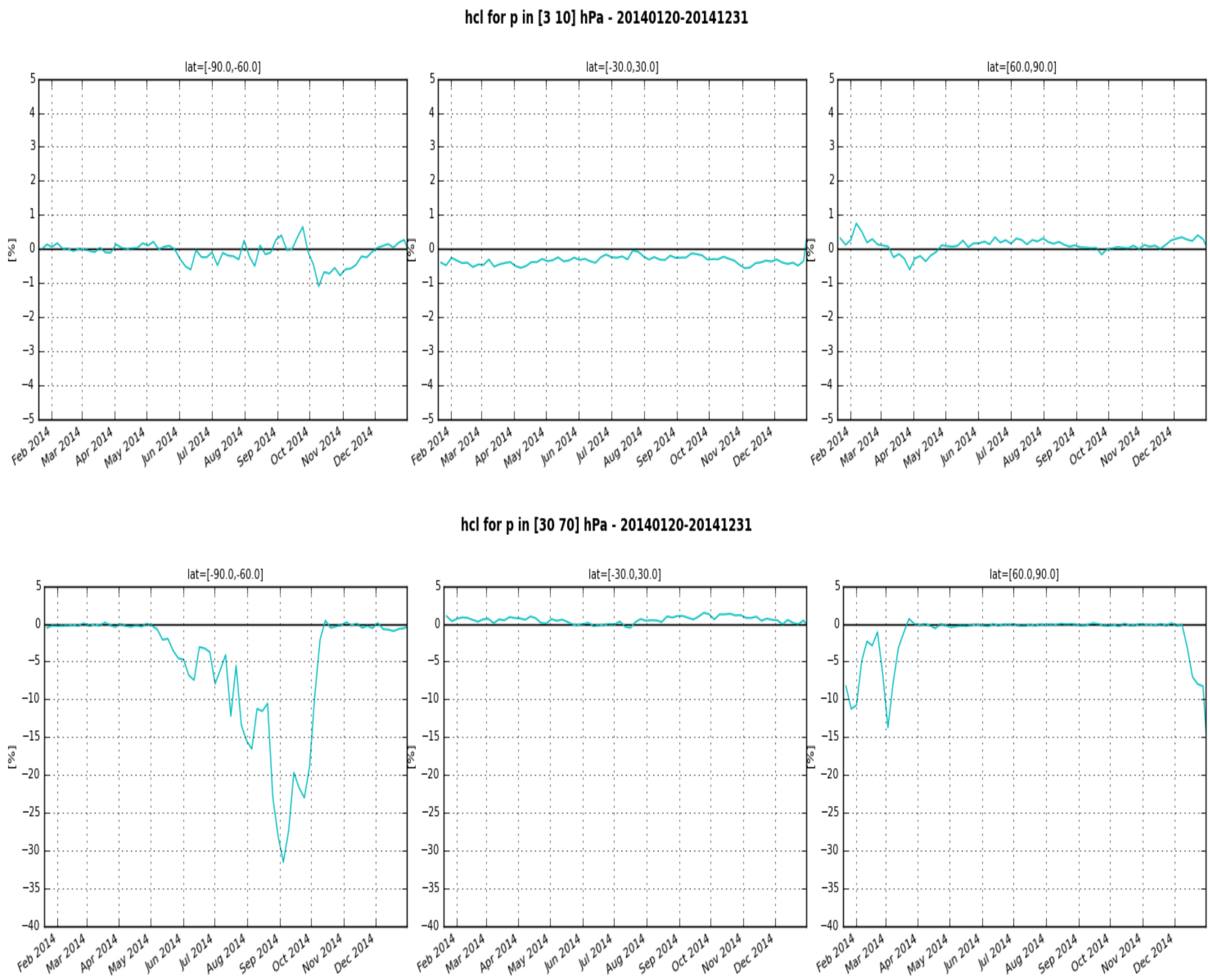

Figure 19: HCl time series of the relative differences between BASCOE and MLS for the layers 3-10hPa (top) and 10-30 hPa (bottom) at the tropics and the poles for the year 2014.

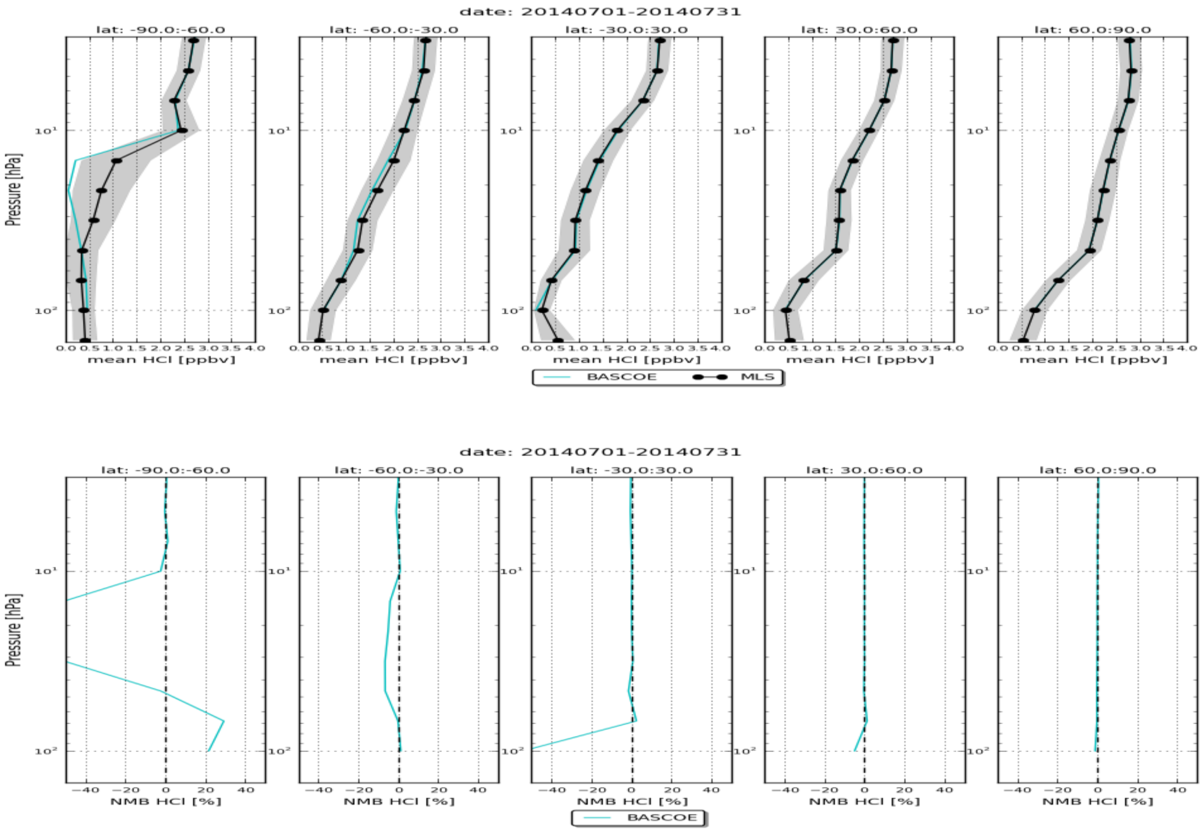

Figure 20: Normalized mean HCl profiles (top) and bias (bottom) between BASCOE and MLS observations for July 2014.

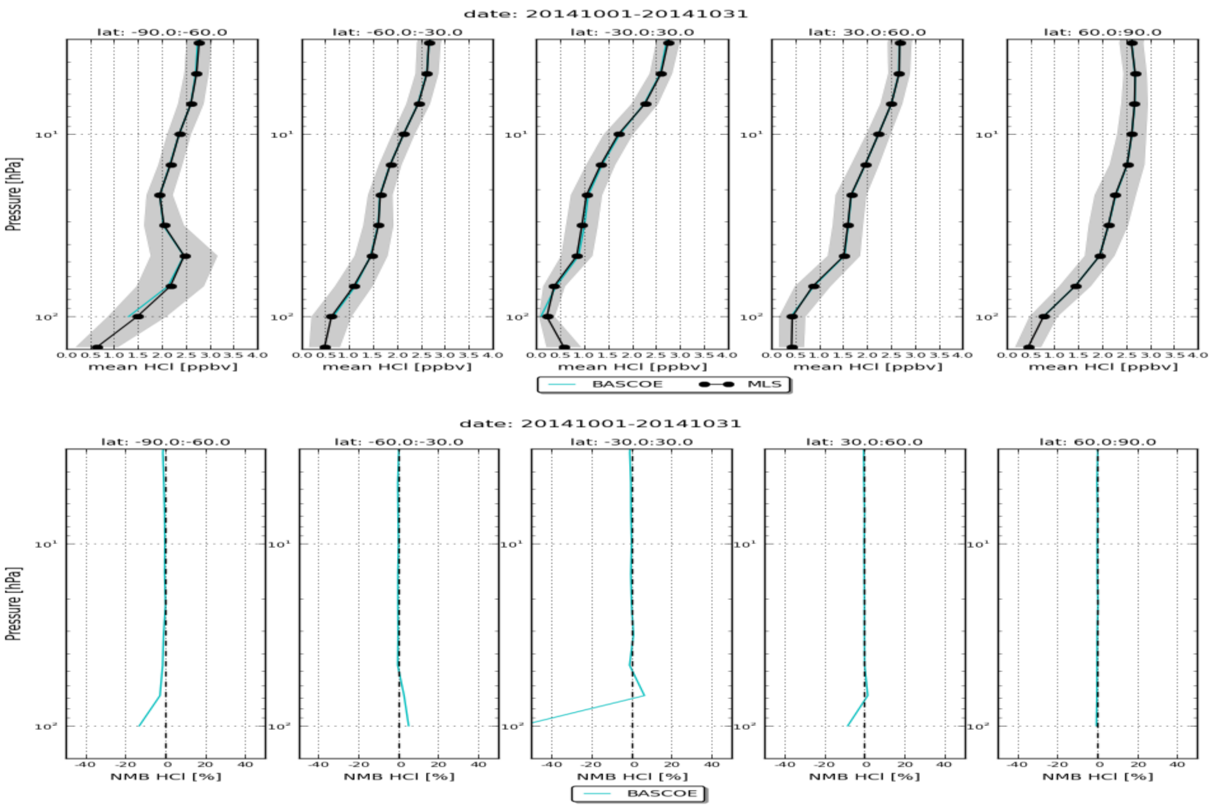

Figure 21: Normalized mean HCl profiles (top) and bias (bottom) of the ozone profile between BASCOE and MLS observations for October 2014.

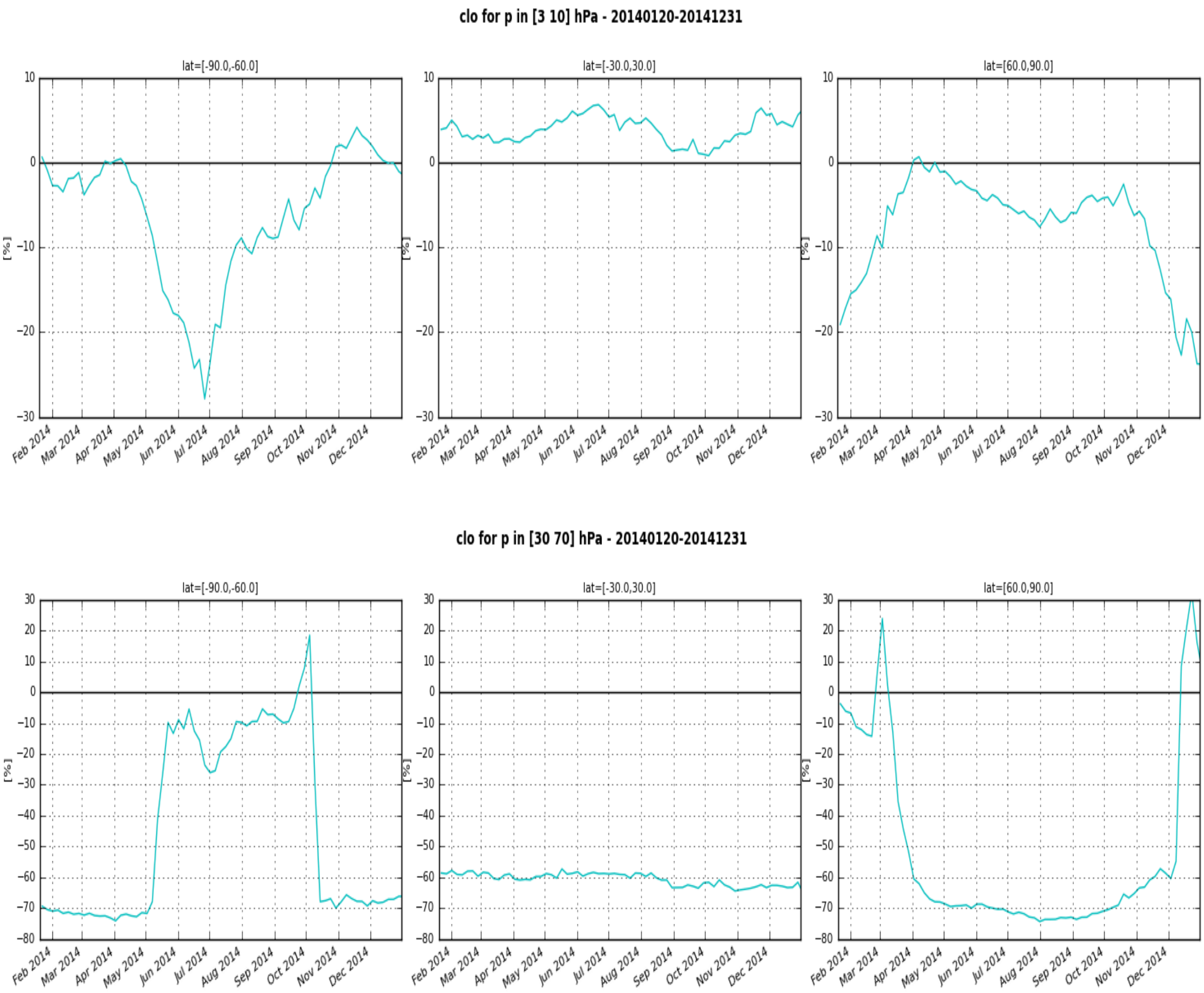

Figure 22: Verification of chlorine monoxide (ClO) analyses by BASCOE: time series of the relative differences between BASCOE and the assimilated data (i.e. MLS) for the layers 3-10hPa (top) and 30-70 hPa (bottom) at the Tropics and the poles for the year 2014.

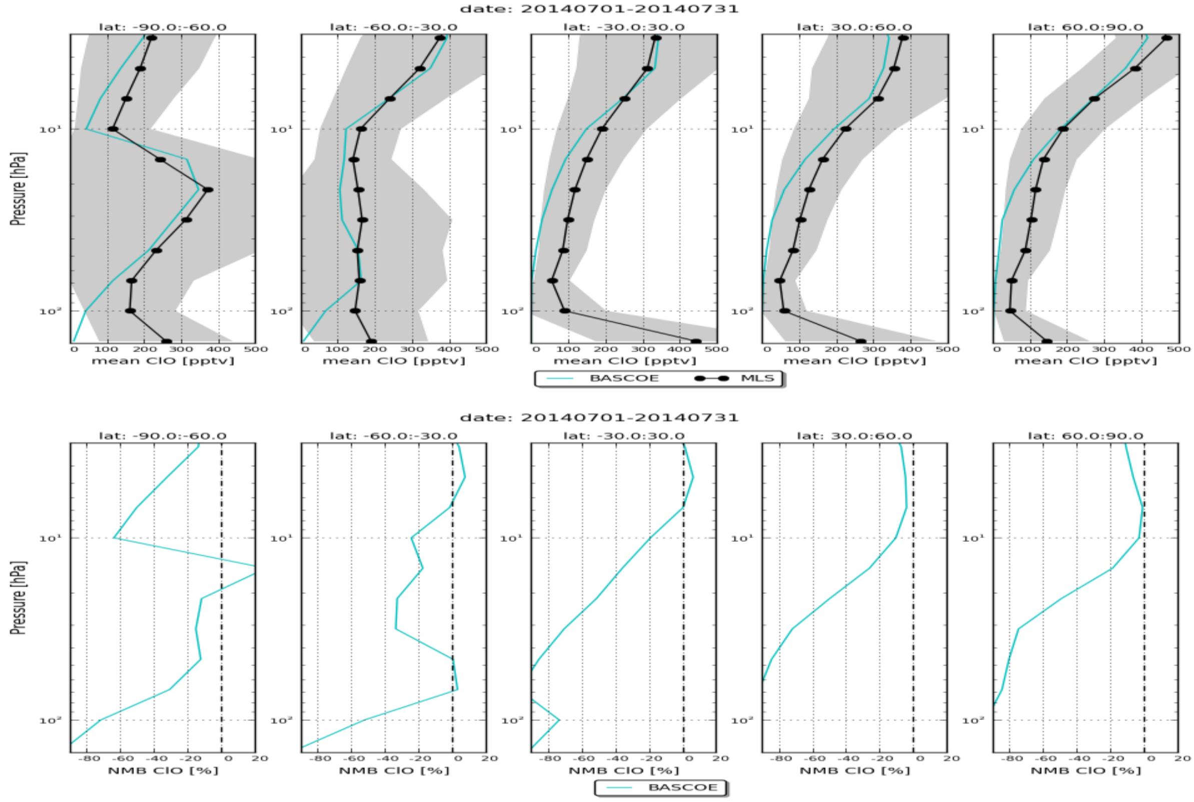

Figure 23: Normalized mean ClO profiles (top) and bias (bottom) between BASCOE and MLS observations for July 2014.

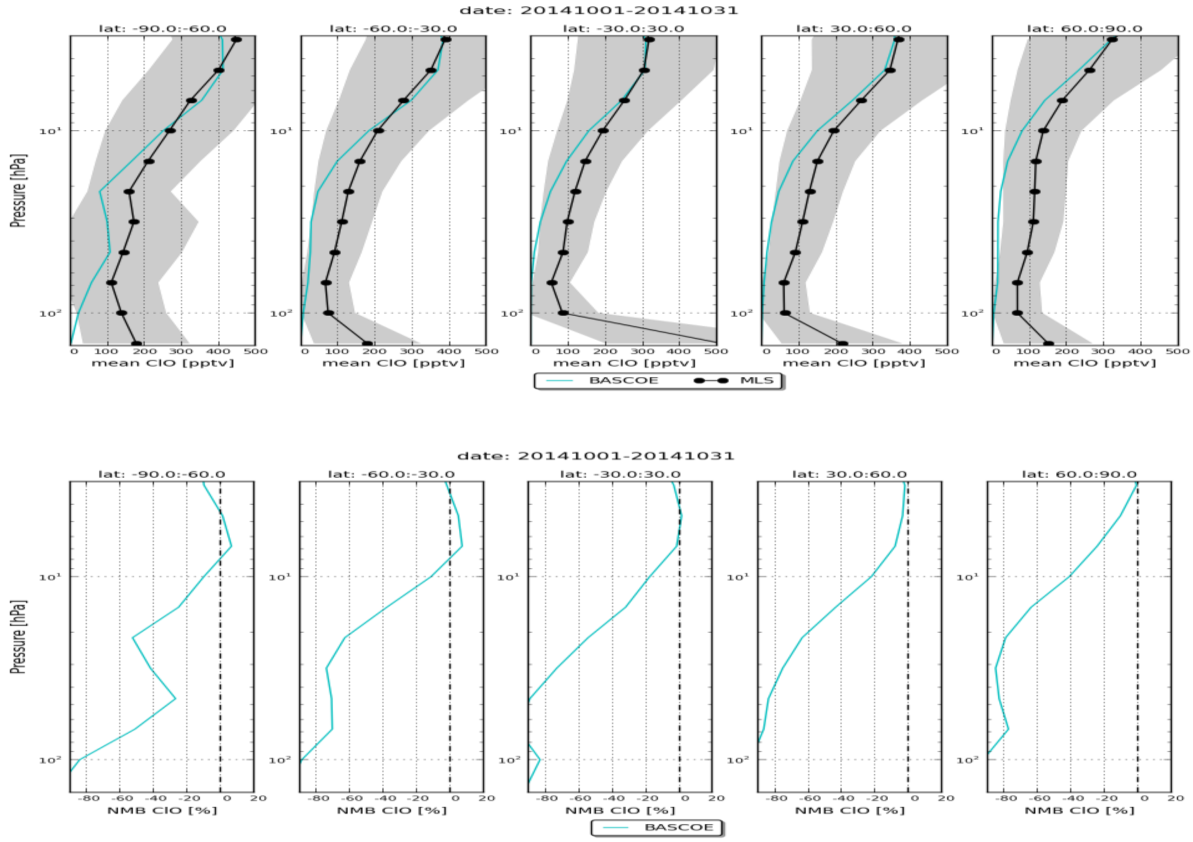

Figure 24: Normalized mean ClO profiles (top) and bias (bottom) between BASCOE and MLS observations for October 2014.

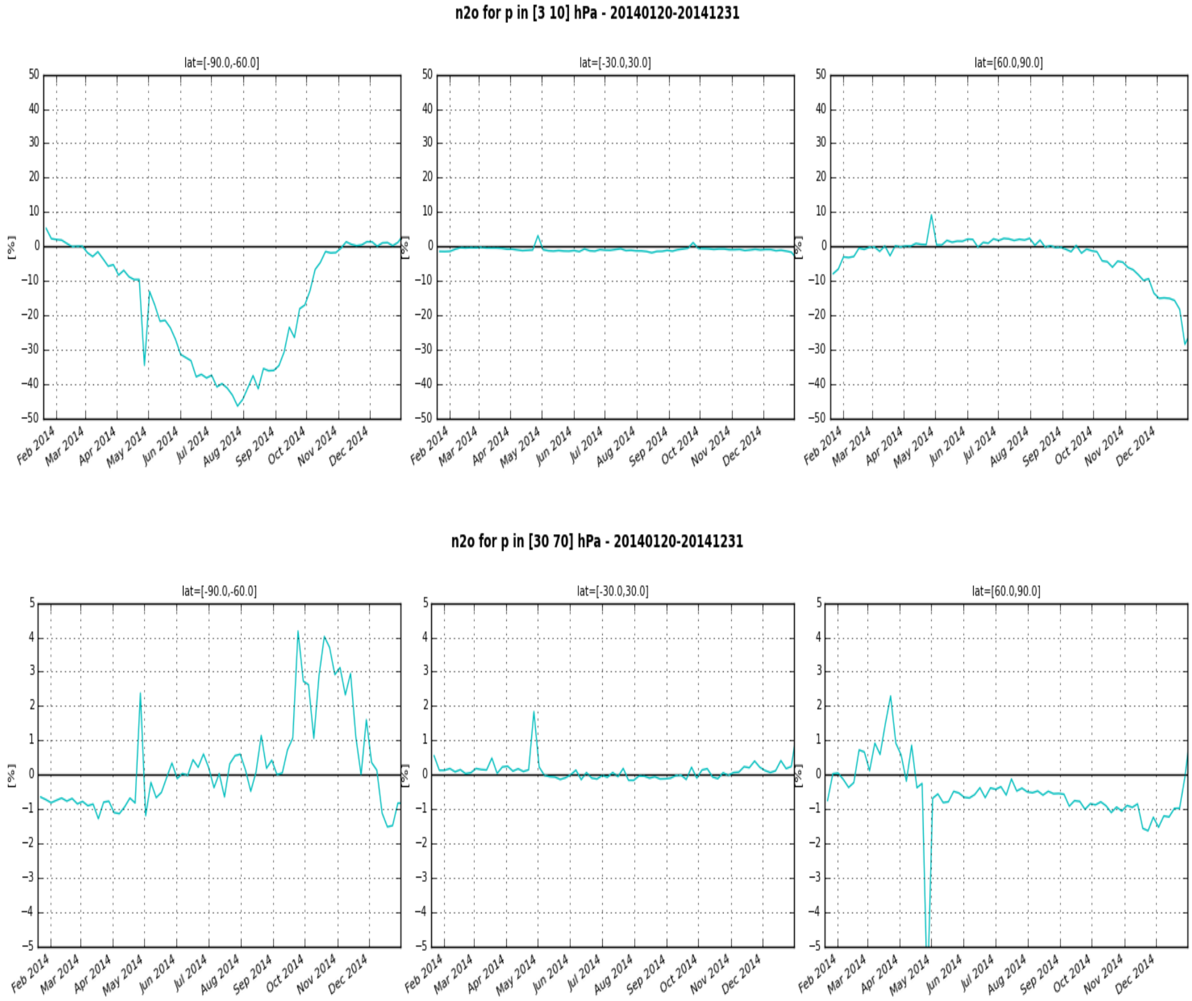

Figure 25: Verification of N2O analyses by BASCOE: time series of the relative differences between BASCOE and the assimilated data (i.e. MLS) for the layers 3-10hPa (top) and 30-70 hPa (bottom) at the Tropics and the poles for the year 2014.

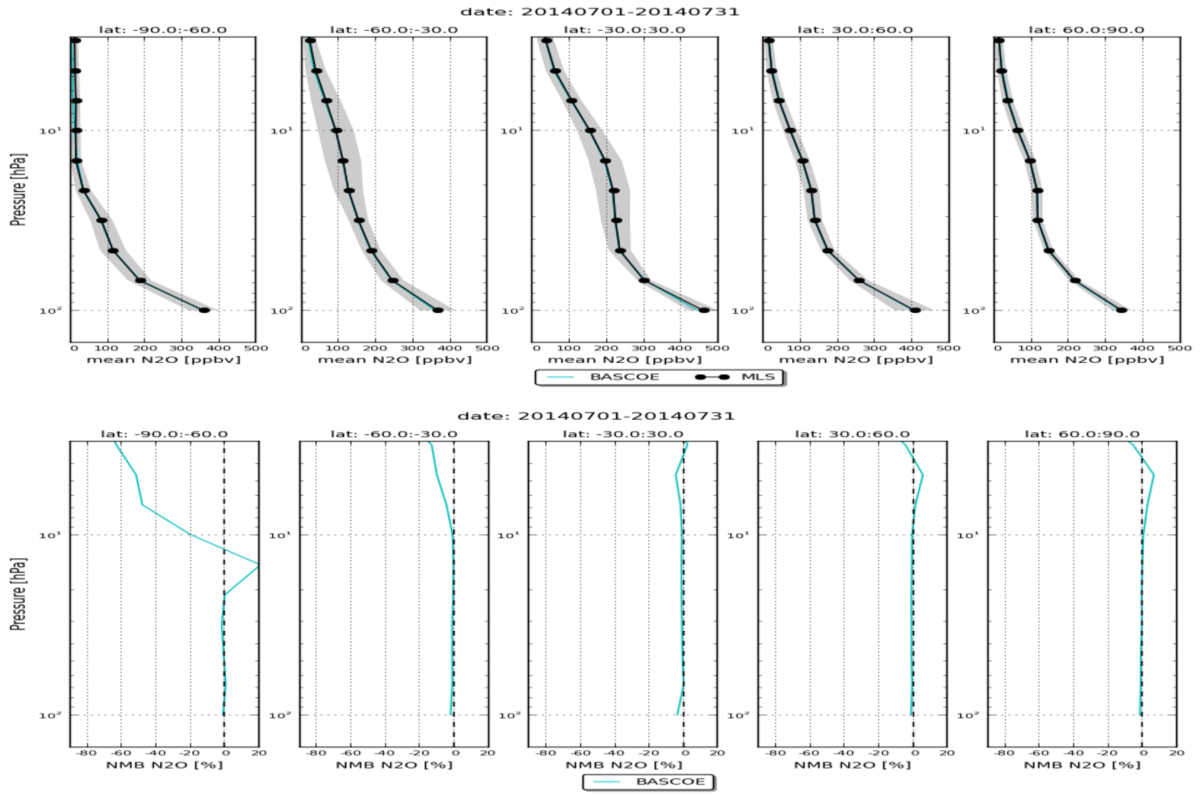

Figure 26: Normalized mean N2O profiles (top) and bias (bottom) between BASCOE and MLS observations for July 2014.

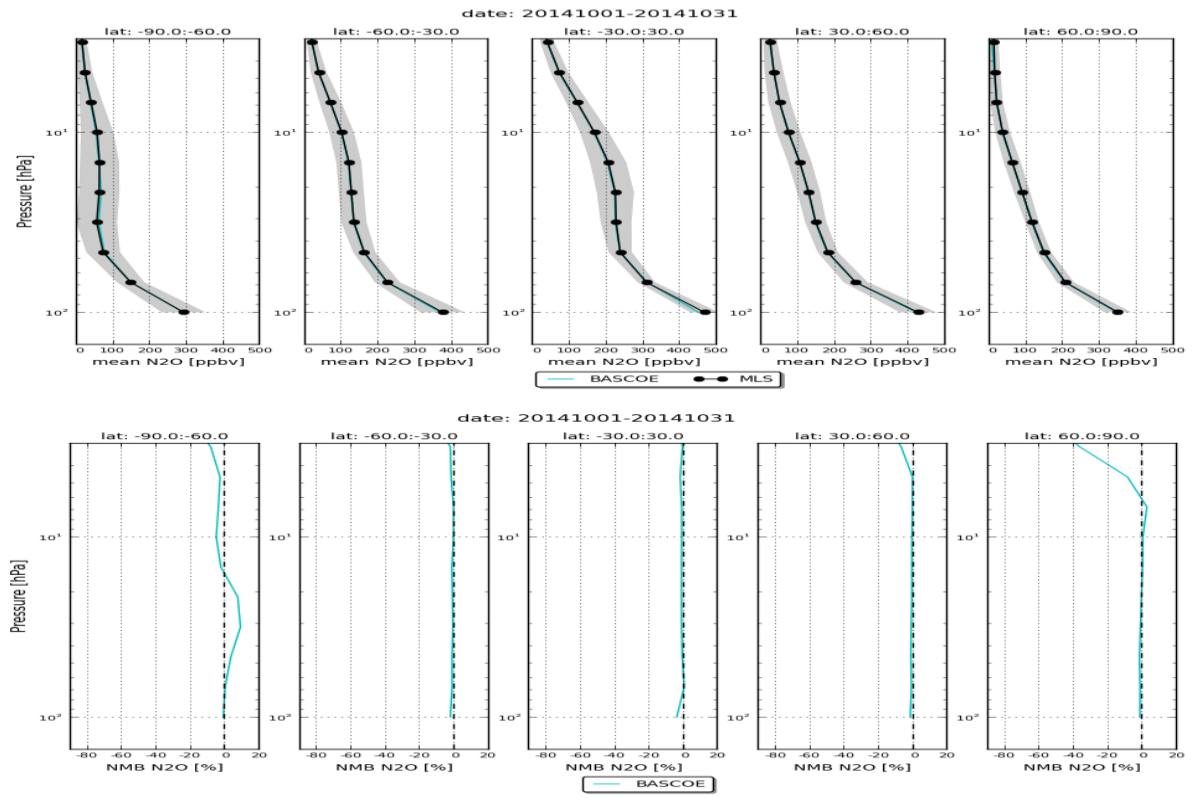

Figure 27: Normalized mean N2O profiles (top) and bias (bottom) between BASCOE and MLS observations for October 2014.

5 References

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Aura-MLS data quality document : http://mls.jpl.nasa.gov/data/v3_data_quality_document.pdf

Copernicus stratospheric ozone service : http://www.copernicus-stratosphere.eu/

WMO Antarctic Ozone bulletins: http://www.wmo.int/pages/prog/arep/gaw/ozone/.

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