4D-VAR chemical data assimilation of ENVISAT chemical products (BASCOE): validation support issues

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ABSTRACT/RESUME

A 4D-VAR chemical data assimilation system, BASCOE, is used to assimilate the chemical observations taken by the three dedicated instruments onboard Envisat. For the first time data assimilation takes active part in the validation of chemical atmospheric observations.
Here we present the results of the assimilation of MIPAS NLE products and NRT products. It is shown that the MIPAS constrained analyses are representative of the MIPAS observed state. The comparison with HALOE show that MIPAS O_3, H_2O, CH_4, NO_x are in very good agreement with HALOE and these results are inline with the current understanding of both instruments.

1. INTRODUCTION

The use of data assimilation in the framework of instrument validation is a new methodology. Data assimilation by a deterministic model aims at representing the actual evolution of the state of a system. Here, the system of interest is the geophysical state of the atmosphere.
The use of data assimilation is best illustrated by numerical weather prediction: the better the representation of the actual state of the atmosphere, the better the prediction. Therefore weather prediction has been and still is a driving force advancing data assimilation. Assimilation of chemical observations has emerged second half of the last decade. In the field of chemical data assimilation, a differentiation can be made by the model of time evolution, ranging from a simple tracer transport model to a full chemistry transport model, depending on the objectives of the assimilation system and availability of observations .
Data assimilation produces here the best estimate of the actual state of the atmosphere, including the composition, based on observations. The results of data assimilation, analyses, offer the potential of comparing all observations with the analyses. Hereby a statistical relevant number of comparisons is easily obtained. It must be highlighted that in the conclusions from these comparisons the errors related to the analyses must be taken into account. The validation support can be accomplished in two modes: the passive and the active mode. In the passive mode the data assimilation system is constrained by independent data and comparing with the to validate observations. In the active mode, the observations to be validated are used to constrain the assimilation system. Thus the analyses represent the composition as observed and can be compared with other independent observations. Here, we present the results using data assimilation with the full chemical couplings in the active mode and focussing on all chemical observations.

2. ASSIMILATION SYSTEM

BASCOE (Belgian Assimilation System for Chemical Observations from Envisat) is an assimilation system based on the 4D variational method. The core is a 3D chemical transport model. BASCOE is a further evolution the assimilation system described in [1]. The standard resolution is 5°× 5°, with 37 vertical levels from the surface up to 0.1 hPa. The chemical scheme now consists of 200 chemical reactions for 57 species. Heterogeneous reactions rate are interactively calculated with online modelling of the microphysical properties of Polar Stratospheric Clouds [2]. Figures 1 and 2 illustrate for the Southern Hemispheric winter 2002 and the Northern Hemisphere winter, the temperature and the modelled nitric acid trihydrate particle surface area density.
The assimilation time window is 24 hours and the constraining observations are the level-2 constituent profiles.

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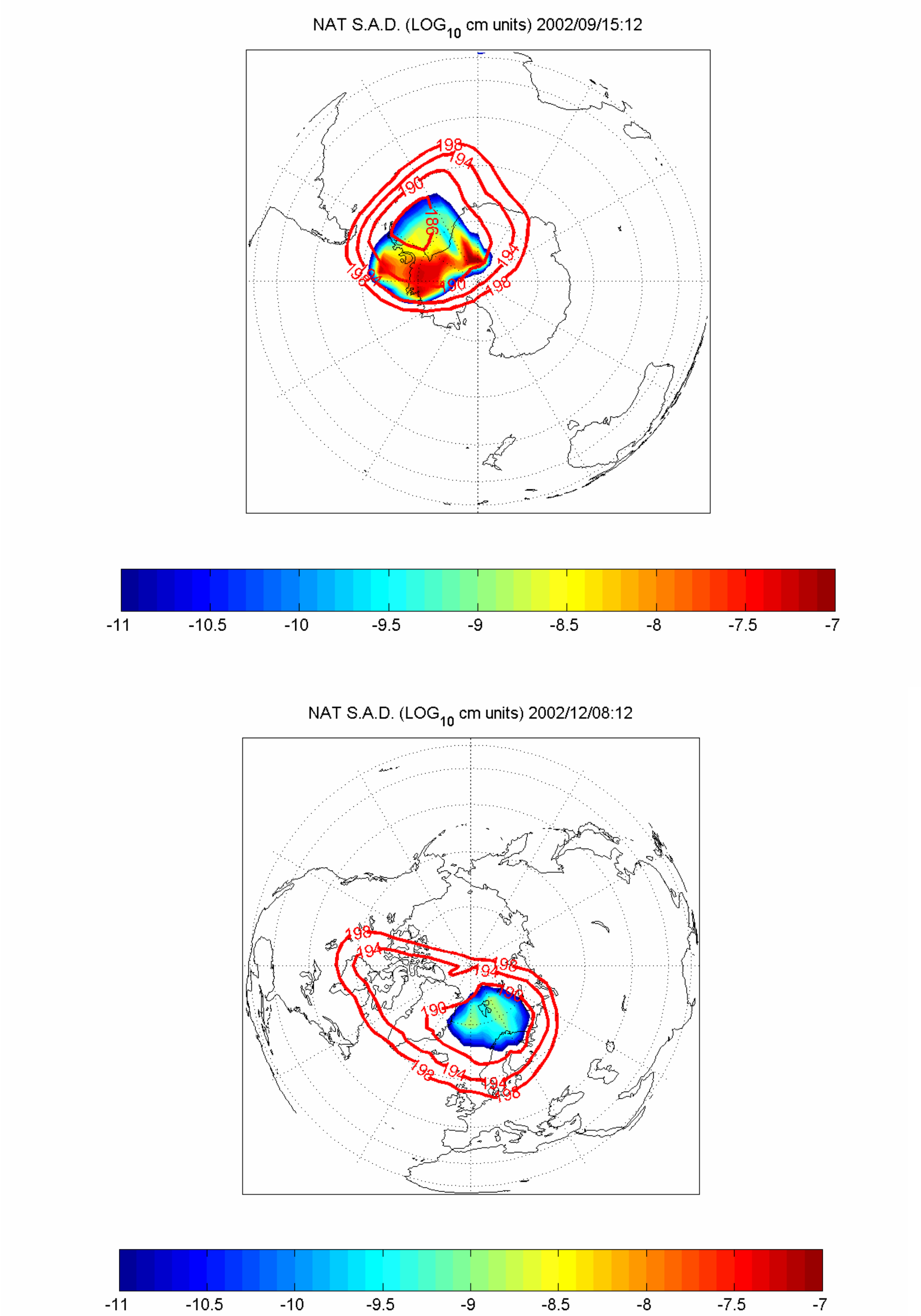


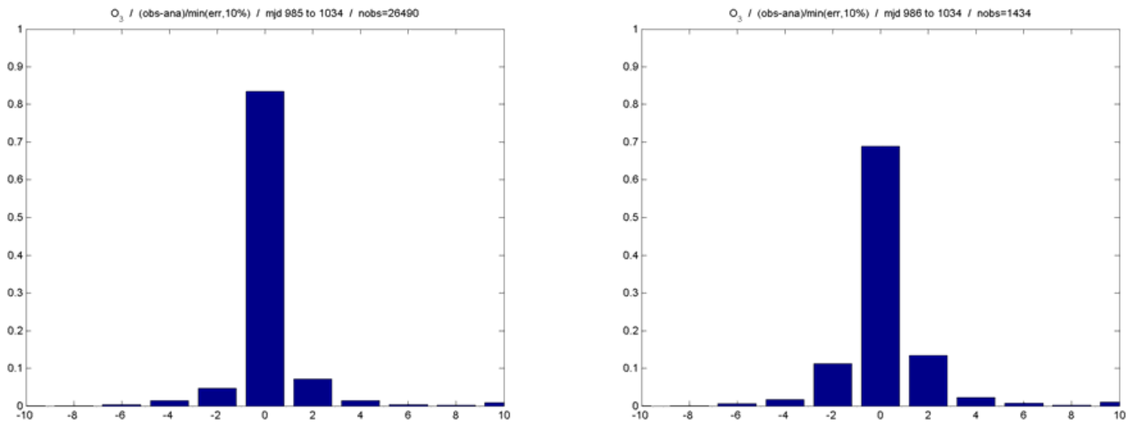
Figuur 1-2: Polar view of NAT surface area density in LOG10 (cm units), (color shaded) and temperature (contour lines) at model level 28 hPa for 15 September (top) and 8 December (bottom) at 12 UT.

3. MIPAS ASSIMILATION

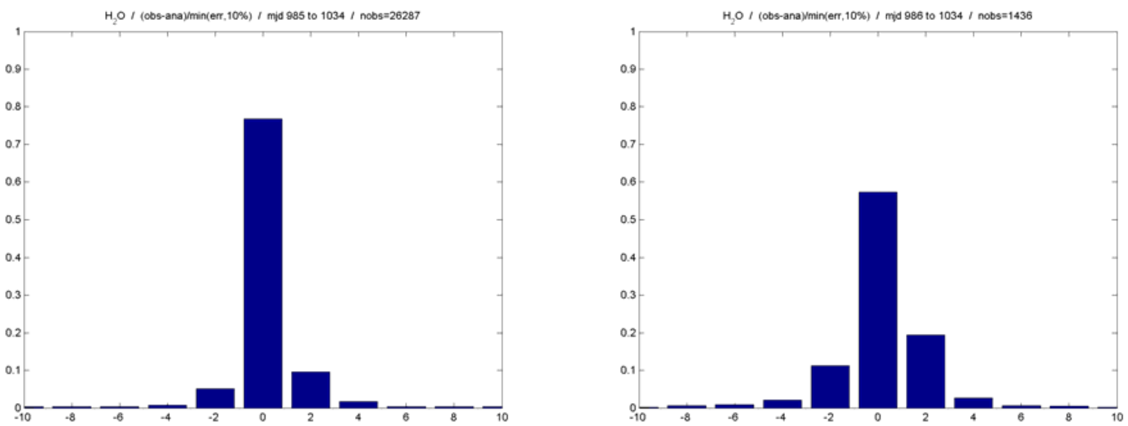
From the three chemical instruments onboard Envisat, the MIPAS instrument by its nature and history was able to provide data that could be used to constrain our assimilation system. During the Envisat Cal-Val, MIPAS provided on a daily basis a coverage that allowed operational chemical data assimilation. This was the Meteo product containing O_3 and H_2O. From late October, 2002 all species became available, N_2O, CH_4, HNO_3 and NO_2. This implies two versions of the obtained analyses. BASCOE v1b01 is the assimilation of MIPAS NLE data (O_3 and H_2O) until November 5. BASCOE v1b02 is the assimilation of NRT products (O_3, H_2O, N2O, CH_4, HNO_3 and NO_2), starting from December 1, 2002. In all cases BASCOE is driven by ECMWF analysed dynamical fields. The observational errors were somewhat relaxed to a minimal 10 % random error. MIPAS observations at altitudes lower than 90 hPa were by default rejected.

Typical for a Cal-Val period is the missing of data for some orbits. To optimize the use of the available observations, horizontal flow dependent correlations on background errors were introduced in the system for the long lived species [3].

The MIPAS data are the sole observations that constrain the assimilation system. It is thus important to show that the analyses are representative for the composition state as observed by MIPAS. This can be achieved by comparing the analyses with independent un-biased (relative to MIPAS) observations. Theoretically, this is very difficult but can easily be approximated by assimilating only a large part of the observations. The remaining non-constraining observations can thus be used as independent un-biased observations. BASCOE assimilates only 95 % of the MIPAS observations, the other 5 % are the un-biased independent observations. This procedure does not suffer from typical problems related to biases between different sets of observations. Figures 3-4 show the distribution of the relative difference between constraining (as reference), non-constraining observations and analysed fields in observations space.



Figuur 3: Distribution of (observation- co-located analysis)/error in the case of constraining ozone observations (left) and non-constraining ozone observations (right).



Figuur 4: Distribution of (observation-co-located analysis)/error in the case of constraining H_2O observations (left) and non-constraining H_2O observations (right).

The distribution of the relative differences between non-constraining observations and co-located analysed fields clearly indicate that the model does not introduce neither a significant bias nor increases the random error to a larger extend. This implies that the analysed fields are representative of the MIPAS observed state and thus that comparing the analyses to independent observations is representative of a MIPAS comparison with these independent observations.
Already a first conclusion can be drawn; all MIPAS observations can be assimilated by 4D-VAR assimilation system into a full chemical transport model. This indicates that no important inconsistencies in the MIPAS level 2 data are present.

4. COMPARISON WITH INDEPENDENT OBSERVATIONS

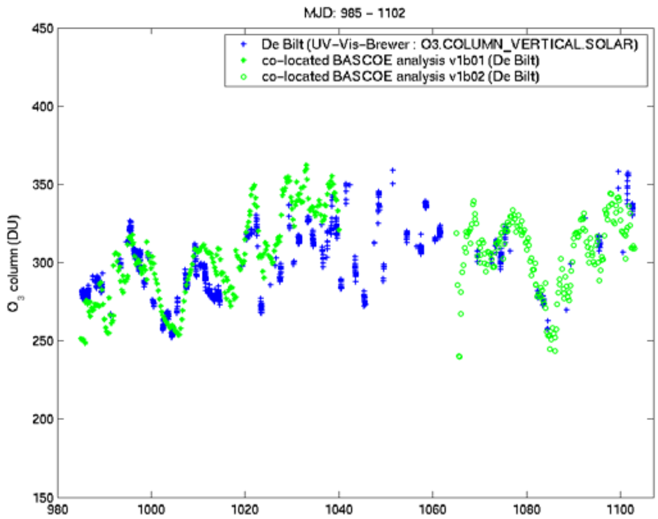
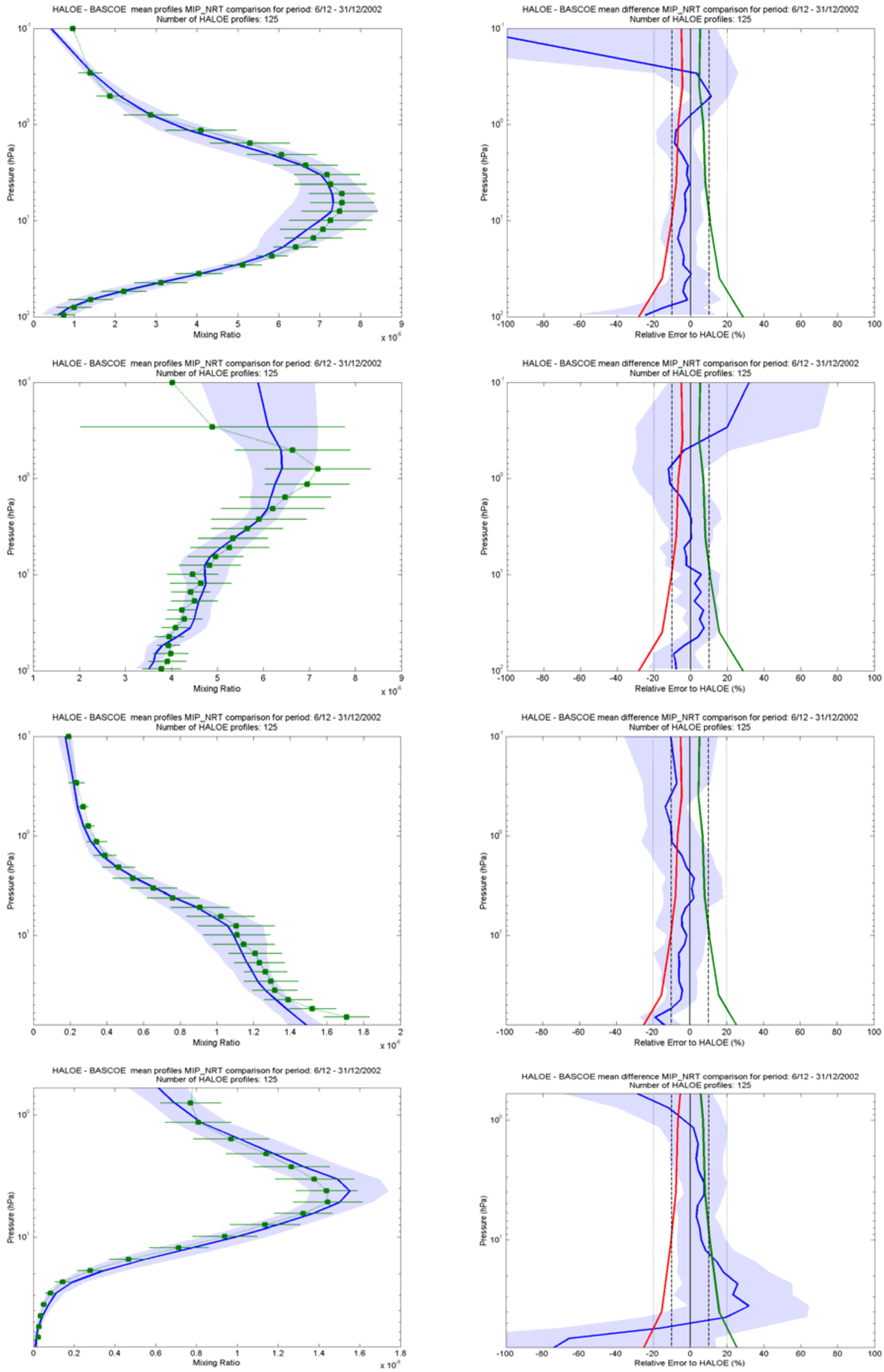


Figure 5: Time evolution of total ozone at De Bilt. See figure for legend.

The main goal of this study is the comparison with independent well validated observations to obtain a status of the MIPAS level 2 products. Two sets of independent observations have been used: ground based total ozone measurements and the HALOE data set. Practical reasons were the main limiting factors for not considering other data sets. In the course of the operational assimilation of MIPAS, the data were daily compared to ground based total ozone observations for control purposes. Figure 5 shows the evolution of both the observed total ozone and co-located BASCOE total ozone, for both versions. Although MIPAS does not contain full tropospheric information, nevertheless the BASCOE total ozone agrees very well with the observations. Despite the coarse horizontal resolution, both absolute values as temporal evolution are in good agreement. Other ground based observations exhibit the same behaviour. But this does not constitute a quantitative comparison due to the unconstrained troposheric composition in BASCOE.
HALOE onboard UARS still provides valuable observations that allow a quantitative comparison for O_3, H_2O, CH_4 and NO_2. The comparison is performed by co-locating the analyses by horizontal interpolation, and interpolating the HALOE data on to BASCOE vertical grid, using the BASCOE output time resolution. Sunrise and sunset events are treated independently, and, no latitudinal differentiation is performed. The HALOE products are disseminated in files per event type for periods of approximately 30 days. Means are taken for 1 file and event type and differences between HALOE and BASCOE are averaged. The mean of the respective profiles will be shown with their standard deviation as well as the mean of the differences. Instead of comparing NO and NO_2, their sum (NO_x) is compared which is longer lived than the individual species. Although HALOE measures each individually, MIPAS only observes NO_2. Using a 4D-VAR system the NO_2 observations immediately influences NO through the tight chemical couplings.
The mean profiles also show the standard deviation, in this case the variability in the data set. This variability for BASCOE and HALOE are for all species in good agreement. This indicates an overall consistency between HALOE and BASCOE. The results of this comparison are shown in figure 6 for the given period and sunrise events. Other periods and/or event type show similar results. But using a solar occultation experiment to compare with only gives a reasonable number of cases if no latitudinal differentiation is done. Therefore, the following figure is representative but is only indicative and deriving a systematic bias would require assimilation over at least 6 months to be statistical relevant.
In the main part of the stratosphere BASCOE ozone overestimates HALOE, by less than 10 %. Although in very good agreement, the water vapour results show more variable behaviour, more noisy. Methane and NOx are also in very good agreement with HALOE.



Figuur 6: Mean profiles (left): full line (HALOE) and symbols (BASCOE) with shading and bars representing variability over data set. Mean relative differences HALOE - BASCOE(right) with standard deviation shaded. Species from top to bottom: O_3, H_2O, CH_4 and NO_x.

5. CONCLUSION

Both NLE and NRT MIPAS products can be assimilated into a 4D-VAR chemical assimilation system. This is already an important conclusion on its own, showing that no major inconsistency between model chemistry and dynamics and observations is present. Although some species observations (water vapour for example) exhibit sometimes a ‘noisy’ behaviour, the possible causes of this behaviour have been identified and the proposed modifications will certainly improve the individual profile quality.
For the MIPAS product assimilation it is shown that BASCOE is representative of the MIPAS observed state, and, thus comparisons between other independent observations relate directly to the MIPAS level 2 products. Thus data assimilation can provide substantial support for the validation of atmospheric instruments. The comparison of BASCOE and HALOE is thus meaningful in this framework.
The agreement of BASCOE with HALOE is very satisfactory. In most of the stratosphere for all species the average difference is less than 10 %. At the high and lower stratosphere this difference may be higher, and, is also related to a larger standard deviation. This should be viewed in the context of both instruments and their error budget taking into account the influence of the data assimilation on the propagation of the instrumental and random errors.
This work will continue on an operational basis. With a longer time series even more detailed analyses can be made taking into account error budgets. (More information will be made available on WWW: bascoe.oma.be).

6. REFERENCES

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