BASCOE OZONE AND CL_Y ANALYSES PROVIDED IN THE FRAMEWORK OF PROMOTE

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ABSTRACT

The PROMOTE Stratospheric Ozone Profile Record service has been setup to deliver 3D global re-analyses of ozone and other related trace gas (www.gse-promote.org). Provided by DLR and BIRA-IASB, re-analyses will cover the period from 1992 until now. Both institutions are running their own systems and deal with different datasets, thus different periods. DLR is focusing on GOME-1 (1995-2003), MIPAS (July 2002-March 2004) and GOME-2 (beyond 2006) while BIRA-IASB is dealing with UARS/MLS (1992-1999) and MIPAS.

At BIRA-IASB, analyses are calculated using the Belgian Assimilation System for Chemical ObsErvations (BASCOE). This system is based on the 4D-Var method and a stratospheric Chemistry Transport Model (CTM) driven by ECMWF dynamical fields. In this contribution, we will review the BASCOE target species of this PROMOTE service, i.e., ozone and total inorganic chlorine (Cly) analyses.

Key words: UARS MLS; 4D-Var assimilation; BASCOE; ozone; inorganic chlorine.

1. INTRODUCTION

The PROtocol MOnitoring (PROMOTE) project provides numerous services for identified users in the framework of GMES (www.gse-promote.org) which cover many different fields: air quality, UV forecast, ozone monitoring... Within this portfolio, the Stratospheric 3D Ozone Record service (3DO3) aims at providing long-term assimilation of ozone profiles and related species. The Stratospheric Processes And their Role in Climate (SPARC) organization, within the Chemistry Climate Model Validation (CCMVal) initiative joined this service as a core user in order to better evaluate the three-dimensional representation of ozone in their model. On the other hand, the World Meteorological Organization (WMO) will use ozone re-analyses in the Global Atmospheric Watch (GAW) program.

They are two providers in the 3DO3 services, DLR and BIRA-IASB, both running their own system and having the own target as summarized on Table 1. At BIRA-IASB, it is planned to provide long-term analyses of ozone (O_3) and total inorganic chlorine (Cl_y) from the assimilation of UARS/MLS and MIPAS data.

In next section, the experimental setup of BASCOE is presented. Section 3 and 4 respectively discuss the BASCOE O_3 and Cl_y analyses.

Some of the analyses discussed in this paper are publicly available via: http://wdc.dlr.de/data_products/projects/promote/3D-Ozone/promote_3d-ozone.html.

2. EXPERIMENTAL SETUP

The BASCOE data assimilation system is based on the 4D-Var method dedicated to stratospheric chemical observations. The chemistry transport model advects 57 species using the ECMWF dynamical wind and temperature fields and calculates the chemical interactions using 199 chemical reactions. In the experiment conducted within PROMOTE, the system is run at a horizontal resolution of 5°in longitude by 3.75° in latitude and with 37 levels from the surface to 0.1 hPa.

Four runs of BASCOE have been performed for this paper and summarized in Table 2. The first one concerns the assimilation of the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS, Fischer et al., 2008) from July 2002 until March 2004, i.e., when the instrument was observing at its nominal resolution. During that period, around 85% of days have been observed by MIPAS. In this experiment, the six standard species were assimilated (O_3, HNO_3, NO_2, H_2O, CH_4 and N_2O) and the BASCOE CTM was driven by the ECMWF operational analyses. This experiment (BMIP) is discussed in detail by Errera et al. (2008).

The second experiment focuses on the assimilation of the Microwave Limb Sounder (MLS, Livesey et al., 2003) onboard the Upper Atmosphere Research Satellite (UARS) during the period 1992-1999. The MLS instrument records between September 1991 and July 1999

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Table 1. List of products, systems (and methods), datasets, providers and users of the 3DO3 PROMOTE service.

Products	System	Dataset	Provider	User
O_3, PSCs	ROSE (OI)	GOME Profiles 1996-2003	DLR	CCMVal
O_3, ClO_x, NO_x, PSCs	SACADA, 4D-Var	GOME Profiles 1996-2003	DLR	CCMVal
O_3, Cl_y	BASCOE (4D-Var)	UARS/MLS 1991-1999	BIRA	CCMVal
O_3, Cl_y	BASCOE (4D-Var)	MIPAS Jul02-Mar04	BIRA	CCMVal
O_3	SACADA (4D-Var)	GOME2 O_3 col. since 2006	DLR	WMO-GAW

(see Table 3) and provides profiles of O_3, HNO_3, H_2O (until April 1993) and ClO. Until 1993, the instrument measures nearly continuously. This starts to decrease in 1994 (65% of days are observed) and becomes critical in beyond 1995. Moreover, the temperature radiometer has been switched off on July 1997 to save spacecraft power. Following that data, retrieval of constituents used the temperature analyses produced by National Centers for Environmental Prediction (NCEP) or by the UARS temperature climatology whenever NCEP data were not available. Therefore, the quality of retrievals has been reduced afterwards. Livesey et al. (2003) recommends discarding those data after 1998 for scientific applications. For O_3, we present nevertheless the assimilation of MLS data over these last two years in order to evaluate the quality of BASCOE analyses when they are based on the assimilation of a dataset with poorer quality (see also Viscardy et al., submitted to JSTARS).

Another particular aspect of the MLS instrument is the yaw maneuver performed by the UARS satellite every 36 days. During this period, the instrument sounds one hemisphere (up to $\pm 80°$) and the tropical region (up to $\pm 34°$in the opposite hemisphere) and switches back to the other hemisphere after that time. Consequently, the BASCOE analyses in the opposite hemisphere cannot be considered as pure analyses. In this second experiment, the four MLS retrieved constituents are assimilated using ECMWF ERA-40 dynamical analyses.

Several studies have shown that ERA-40 wind fields enhanced the Brewer-Dobson circulation (van Noije et al., 2004) and produced too fast ascent across the tropical tropopause accompanied by too strong mixing between the tropics and the extratropics in the lower stratosphere (Meijer et al., 2004). Recently, ECMWF has released reanalyses from the ERA-Interim system that solved most of the issues in ERA-40 (Simmons et al., 2007; Monge-Sanz et al., 2007). Thus, in the third BASCOE experiment, UARS MLS data have been reassimilated using the dynamics precalculated by ERA-Interim. This experiment (BMLS-EI), which starts in late 1991 (four months before the second run), has now reached 1998 at the time of writing.

Finally, a fourth reanalysis has been carried out, though for a shorter period. Based on BMLS-E4, it assimilate for several time periods only UARS MLS O_3 data and is discussed in more details in Sect. 4.

The setup of the assimilation of MIPAS data and UARS MLS data are discussed in details in Errera et al. (2008)

Table 3. Number of observed days for every year of the UARS MLS mission.

Years	Nbr of Obs. days	% of obs. days
1991[a]	101	91
1992	338	93
1993	332	91
1994	237	65
1995	91	25
1996	122	33
1997	98	27
1998	68	19
1999[b]	32	9

[a]Only between September and December
[b]No data after August

and Viscardy et al., submitted to JSTARS, respectively. Note the use of a diagonal background error covariance matrix with constant value for its variances.

3. BASCOE O_3 ANALYSES

The analyses of ozone from the assimilation of MIPAS (BMIP experiment) and MLS (BMLS-E4 experiment) are extensively discussed in Errera et al. (2008) and Viscardy et al., submitted to JSTARS, respectively. We provide here a short summary and discuss the impact of the use of ERA-Interim in the case of assimilation of MLS (BMLS-EI experiment).

Figure 1 presents time series of ozone partial columns between 10 and 100 hPa derived from ozonesonde profiles at three NDACC stations (Ny-Alesund, Uccle and Amundsen-Scott) and compared to the corresponding BASCOE analyses. During the MIPAS period, BASCOE capture generally well the ozone seasonal variations seen by the ozonesondes while day to day variation shows significant discrepancies. Note that ozone during the 2002 vortex split is not very well reproduced and this could be partly explained by to the coarse horizontal resolution of BASCOE.

BASCOE ozone during the MLS period is generally not as good as during the MIPAS period. The analyses show periods of very good agreement against ozonesonde (e.g. 1994 above Uccle) followed by periods of large overestimation (e.g. 1995 above the same station). The ozone depletion during the ozone hole period is systematically

Table 2. List of BASCOE experiments discussed in this paper.

Label	Dataset	Period	ECMWF Dyn.
BMIP[a]	MIPAS ESA OL	Jul02-Mar04	Oper. Ana.
BMLS-E4[b]	UARS MLS	1992-1999	ERA-40
BMLS-EI	UARS MLS	Sep1991-1998	ERA-Interim
BMLS-E4-O3	UARS MLS	1992; 1994; 1996-97	ERA-40

[a]Errera et al. (2008)
[b]Viscardy et al., submitted to JSTARS

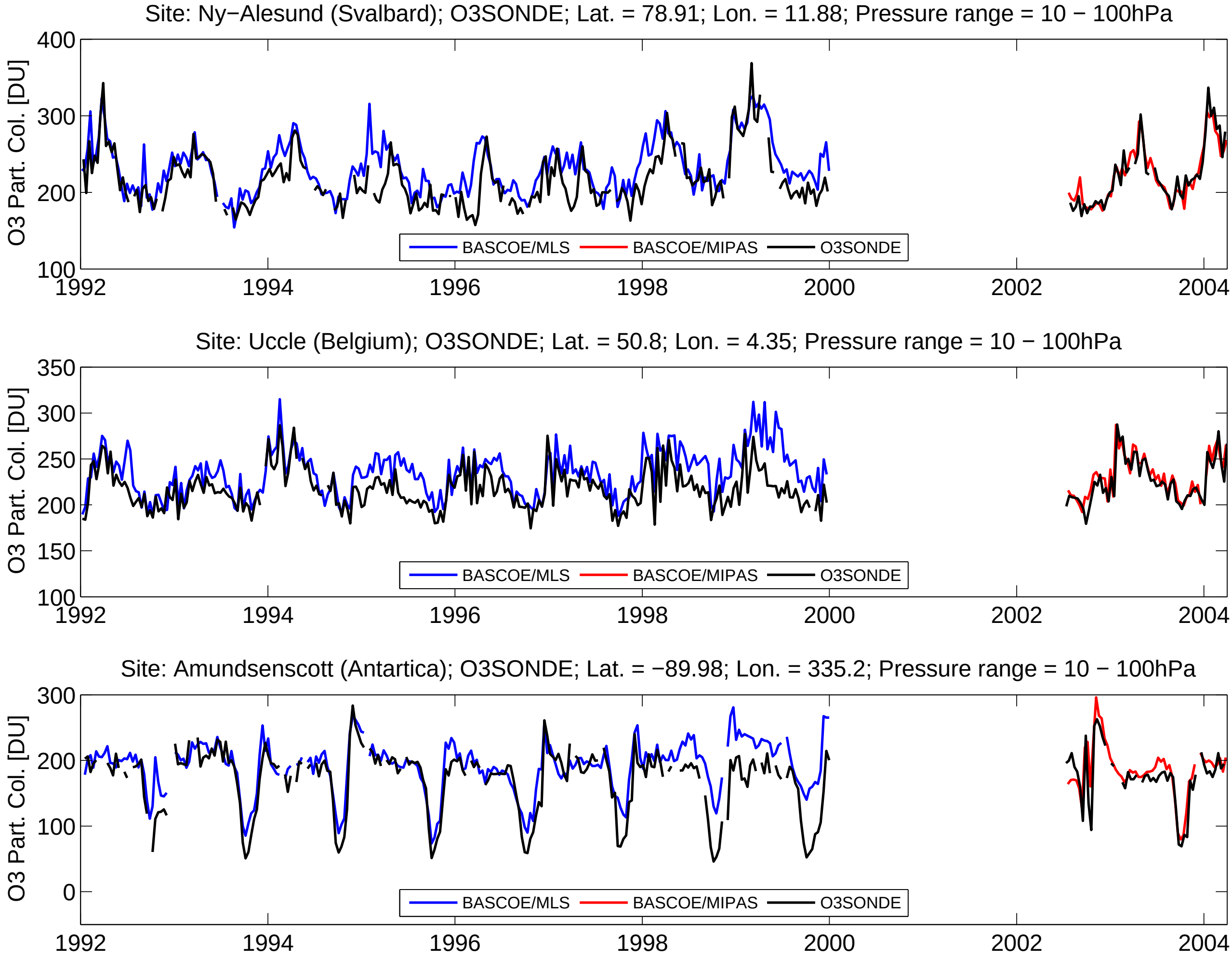

Figure 1. Time series of ozone partial columns between 10 and 100 hPa from January 1992 to April 2004 at three NDACC stations: Ny Alesund, Uccle and Amundsen Scott. Black line: ozone partial columns derived from ozonesonde profiles; blue line: ozone partial columns derived from BASCOE MLS (BMLS-E4) assimilation; red line: ozone partial columns derived from BASCOE MIPAS (BMIP) assimilation

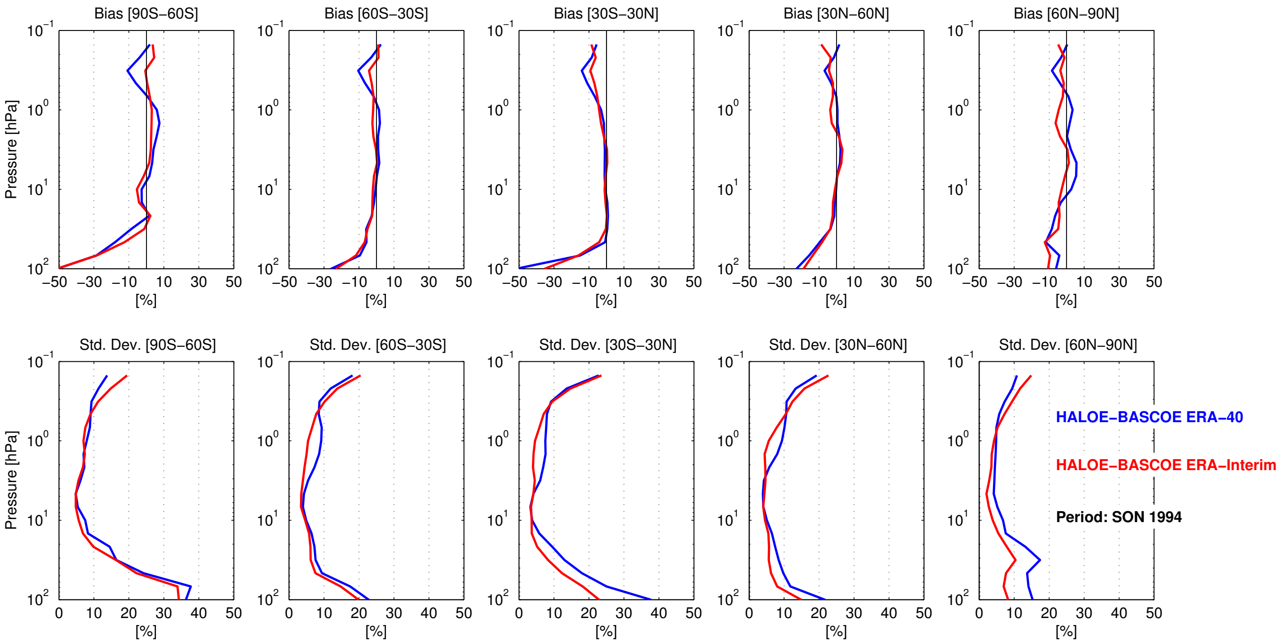

Figure 2. Bias and standard deviations for ozone between HALOE and BASCOE-MLS-ERA40 (blue line), HALOE and BASCOE-MLS-ERAInterim (red line) for the period September to November 1994.

underestimated. We also see that the general agreement decreases over the period, becoming critical after 1997 due to the lack of MLS data. We suggest two reasons explaining the differences of quality between BMIP and BMLS-E4: (1) the data coverage is much better in MIPAS including the fact that it has no yaw maneuver and (2) the quality of the driven ECMWF dynamical fields.

Recently, UARS MLS data have been reassimilated using the ERA-Interim dynamical fields. In order to evaluate the improvement made in the ozone analyses between the BMLS-E4 and BMLS-EI experiments, statistical comparison between HALOE and ozone analyses from these two experiments have been calculated. Figure 2 shows the mean differences and the associated standard deviations between HALOE and BASCOE for the period between September to November 1994 and for five latitude bands. The use of ERA-Interim allows to reduce the bias between HALOE and BASCOE in the mesosphere and in the lower stratosphere, including during the ozone hole period. Probably more important is the reduction of the standard deviation around 1 hPa and in the lower stratosphere.

4. BASCOE CL$_Y$ ANALYSES

In the effort for evaluating the different Chemistry Climate Model involved in the SPARC CCMVal initiative, Eyring et al. (2006) have used only two observations of Cl_y in the South Pole lower stratosphere in October: one in 1992 and the other one in 2005. More recently, Lary et al. (2007) have estimated Cl_y from HALOE HCl using a neural network method. In this paper, we would like to evaluate the constrain of assimilated species on unobserved modeled species through the adjoint model of BASCOE.

First, we check to which degree BASCOE chlorine analyses benefit from the assimilated observations. In order to achieve this, we check at the innovation of the analyses, i.e., the differences between the assimilated and the background fields. Figure 3 shows the zonal mean of the innovation of the BMLS-E4 run on the 1^{st} September 1993 on Cl_y (upper left). The Cl_y innovation shows two regions constrained by the MLS data at that time: (1) the South Pole lower stratosphere which results from the assimilation of MLS ClO (not shown) and (2) the middle-higher stratosphere which cannot be constrained by MLS ClO data because of their large uncertainties in this region. Figure 3 also shows how the individual chlorine species are constrained by MLS data. HCl and $ClONO_2$ are mostly constrained in the mid-high stratosphere where they represent together almost the total inorganic chlorine. ClO_x is innovated in the South Pole lower stratosphere (as expected) and in the mid stratosphere, as HOCl but to a lower extend.

Several calculations of the influence of ozone data on the other modeled species have been made using the adjoint model of BASCOE and following the method of Fisher and Lary (1995). They show that ozone data are able to weakly constrain HCl, $ClONO_2$, ClO_x and HOCl in the mid-high stratosphere (not shown). Thus, a new BASCOE experiment (BMLS-E4-O3) has been setup, based on the BMLS-E4 experiment but for selected period only and where only MLS O_3 is assimilated. Figure 4 shows the time series of HALOE at 0.5 and 5 hPa averaged over 15 days and between 60°S and 60°N. The positive trend

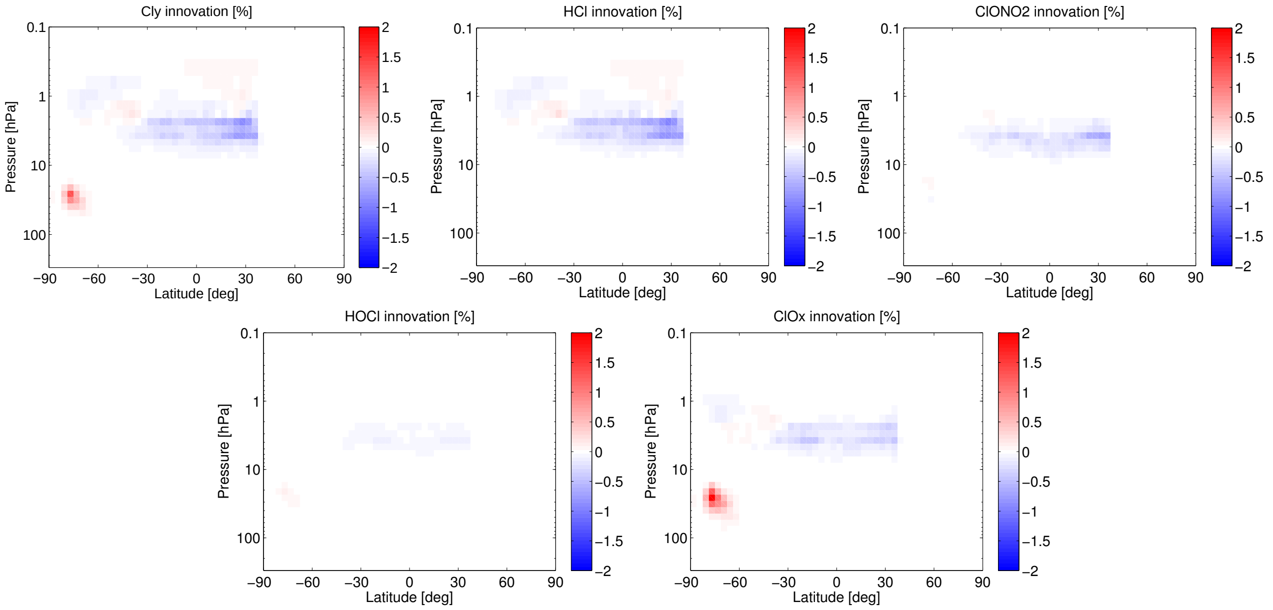

Figure 3. Zonal mean of the innovation of Cl_y, HCl, HNO_3, HOCl and ClO_x ($ClO+2\times Cl_2O_2$) from the BMLS-E4 run on the 1st September 1993.

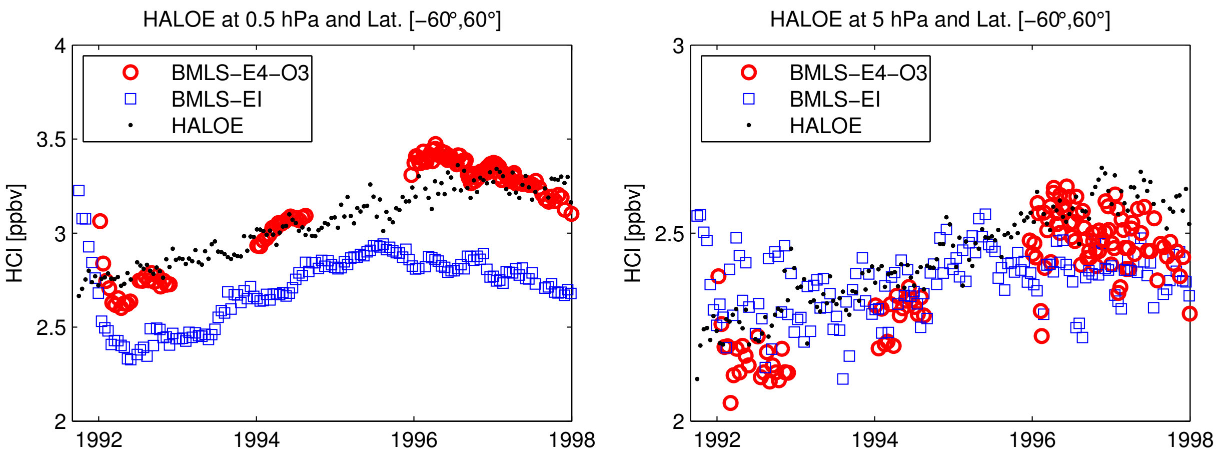

Figure 4. Time series between September 1991 and December 1998 of HALOE HCl (black dots) averaged over 15 days and between 60°S and 60°N. The corresponding BASCOE analyses BMLS-E4-O3 and BMLS-EI are given, respectively, by the red circles and blue squares.

of HCl until 1997 due to the anthropogenic emission of CFCs is clearly visible from HALOE at both altitudes. BASCOE BMLS-E4-O3 reproduces well the observed trend until 1997 at both levels while analyses present a higher variability at 5 hPa. The effect of the spin up is also clearly visible: while starting the assimilation on the 1^{st} January 1992 with HCl field overestimating the HALOE observations, the assimilated O_3 data are able to correct the BASCOE HCl during the first month of 1992 to reach values closer to HALOE. However, BMLS-E4-O3 reverses the HCl trend well before the observations. Similar results have obtained when all MLS species are assimilated (not shown).

The Figure 4 also shows the HCl trend obtained by the BMLS-EI experiment. At 0.5 hPa, the HCl trend is similar to HALOE until 1995 while biased low. The effect of the spin up is also clearly visible. As for the BMLS-E4-O3 run, the HCl trend also reverse earlier than observed in 1997. While showing higher variability and though less biased, similar behavior is observed at 5 hPa.

From these experiments, the following conclusions can be draw. First, middle and upper stratospheric ozone observations are able to constrain HCl, the most abundant inorganic chlorine in this region. Unfortunately, this constrain appear to be weak since it need several months of spin up. Thus, when the data coverage significantly decreases (after 1994), the analyses are more difficult to interpret: they are not coming from a pure CTM run neither a full constrained data assimilation system.

Also important is the impact of the dynamical field used to drive BASCOE. While Figure 4 suggests a better agreement between HALOE and BASCOE when ERA-40 is used, one could not conclude that ERA-40 are better than ERA-Interim in this particular experiment. The low bias between HALOE and BMLS-EI is probably due to the way O_3 and HCl are balanced in the chemical scheme of BASCOE. When ERA-40 drives BASCOE, the too fast vertical transport lift HCl from the lower part of the model and thus minimize the bias against HALOE.

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