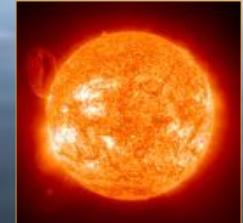


Comparison between BASCOE Reanalysis of Aura MLS (BRAM) releases 1 (BRAM-1) and 2 (BRAM-2)



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Outline

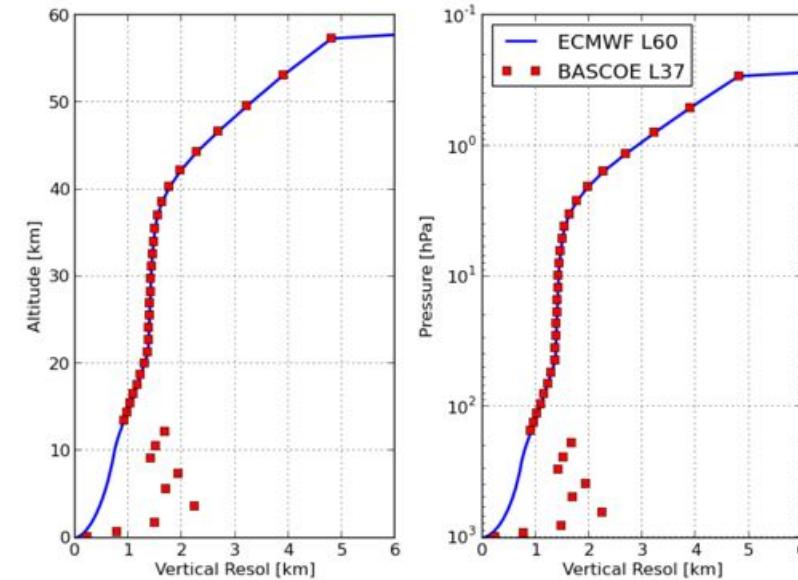
- Summary of BRAM Release 2 (BRAM-2)
- Differences between BRAM-1 and BRAM-2:
 - Model setup
 - Data Assimilation System (DAS) setup
 - Outputs
 - Observation setup
 - Stream setup
- What are the overall improvements from BRAM-1 to BRAM-2

- Reanalysis of the Microwave Limb Sounder (MLS) data (on board the Aura satellite) using the Belgian Assimilation System for Chemical ObsErvations (BASCOE).
 - BRAM-2 is a dataset of 6-hourly 3D fields of O_3 , HNO_3 , N_2O , H_2O , HCl , ClO , CO , CH_3Cl and Cl_2O_2 with an estimation of their uncertainties (based on the std dev of the ensemble – not available for Cl_2O_2) with the following resolution: 2.5° lat x 3.75° lon x 37 levels (surf to 0.1 hPa, 25 levels above 100 hPa)
 - This dataset is built based on data assimilation of MLS limb profiles of O_3 , HNO_3 , N_2O , H_2O , HCl , ClO , CO and CH_3Cl
 - BRAM-2 Period is Aug 2004 (when MLS starts to deliver observations) – Dec 2017. It will be continued with the availability of new MLS observations and new ERA-Interim dynamical fields.
 - BRAM-2 is produced from four streams running in parallel

BRAM-2: BASCOE Setup

- BASCOE is based on a Chemistry Transport Model (CTM) dedicated to the stratosphere
- The CTM includes 58 stratospheric species (Errera et al., ACP, 2008)
 - Advection: FFSL (Lin & Rood, MWR, 1996)
 - Chemistry: \approx 200 chemical reactions (gas phase, heterogeneous, photolysis)
 - PSC parameterization
 - Dehydration of H₂O in the stratosphere
 - No mesospheric source at the model lid
- Dynamics (winds and T°) from ERA-Interim with resolution:
 - 2.5° lat x 3.75° lon x 37 levels (surf to 0.1 hPa, 25 levels above 100 hPa)
- DA method: **EnKF** (Skachko et al., GMD, 2014, 2016) chosen due to its better scalability on High Performance Computer (HPC) than 4D-Var

BRAM vertical resolution



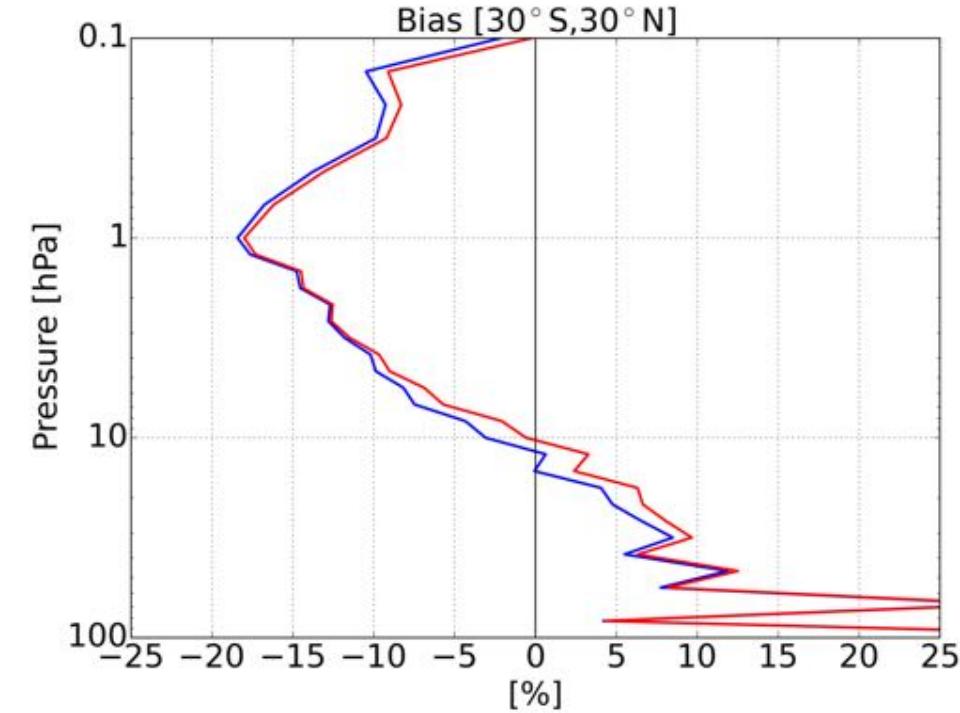
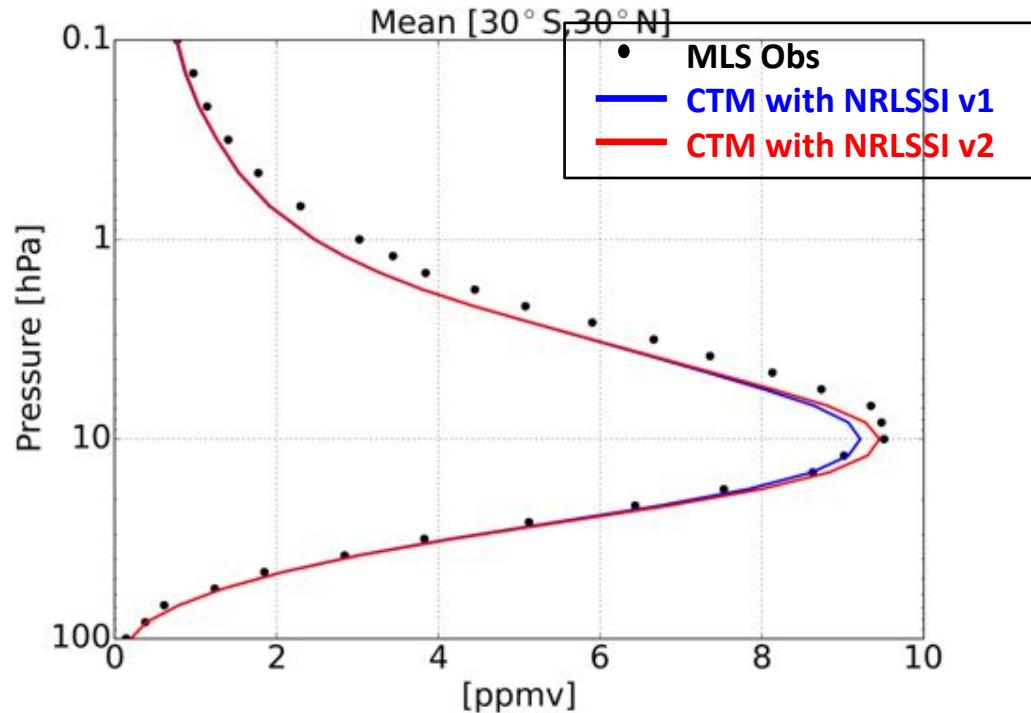
BRAM-1 vs 2: model setup

	BRAM-1	BRAM-2
Version	5.13.2 (revision 9786)	07.00.00 (revision 10706)
Chemistry	sb15a (JPL 2011)	sb18 (JPL2015)
Solar flux	Lean 97 at SOLMIN	SOLVAR NRLSSI v2
Advection	FFSL	FFSL
Sulphate Aerosols Number Densities	Hitchman et al. (1994) divided by 5	Hitchman et al. (1994)
PSC param	CIFTS (Huijnen et al., 2017)	CIFTS (Huijnen et al., 2017)
Config of CIFTS	<ul style="list-style-type: none"> SSR NAT = 1 SSR ICE = 1 SAD NAT=2E-7 cm²/cm³ SAD ICE=2E-6 cm²/cm³ t_{loss} NAT by sedim=1/20 days t_{loss} ICE by sedim=1/9 days 	<ul style="list-style-type: none"> SSR NAT = 10 SSR ICE = 1.4 SAD NAT=1E-7 cm²/cm³ SAD ICE=2E-6 cm²/cm³ t_{loss} NAT by sedim=1/10 days t_{loss} ICE by sedim=1/9 days
Water dehydration	Same code but called in model.f90 after Chemistry	Same code but called in model.f90 between Advection and Chemistry

BRAM-1 vs 2: Solar Spectral Irradiance

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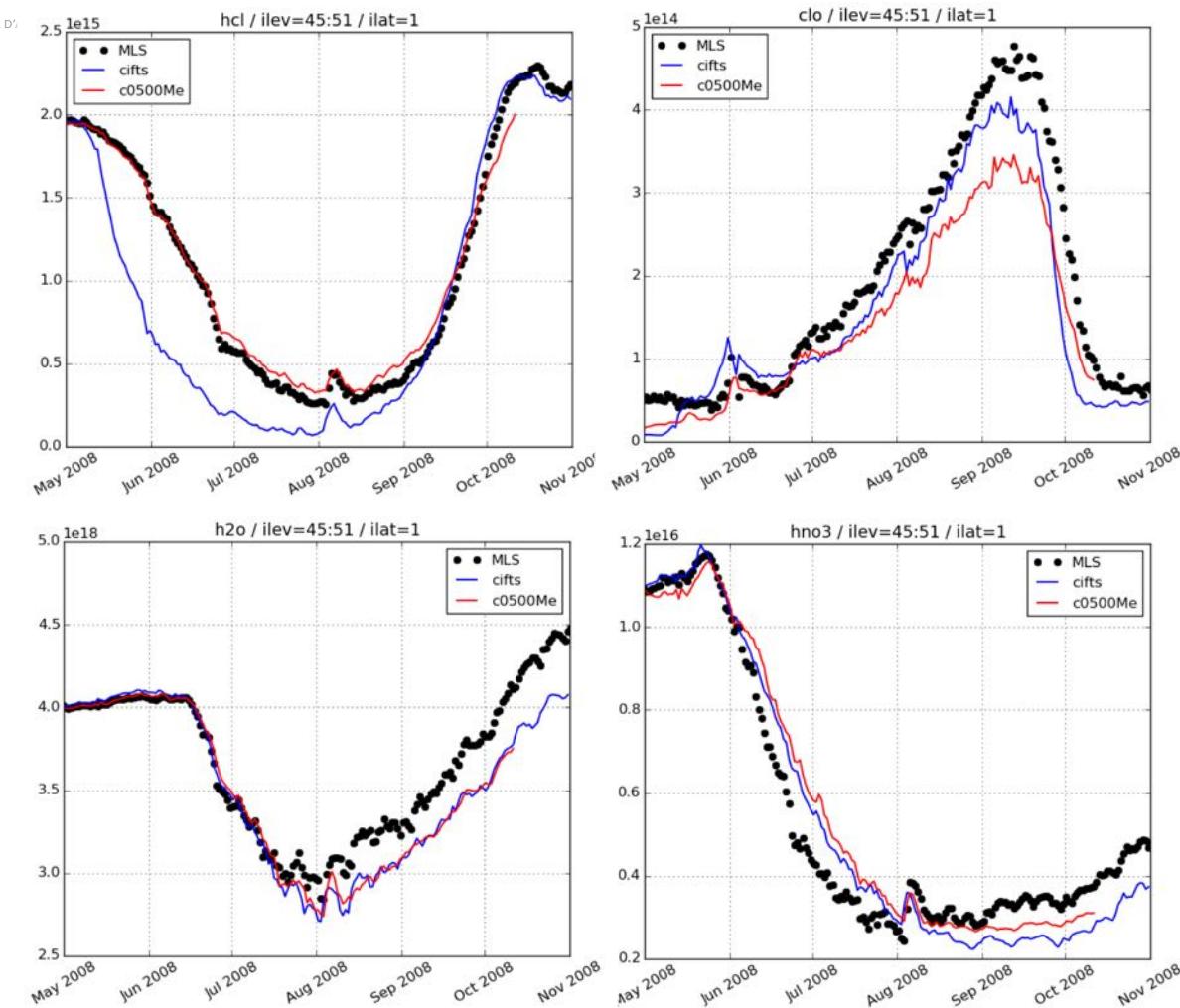
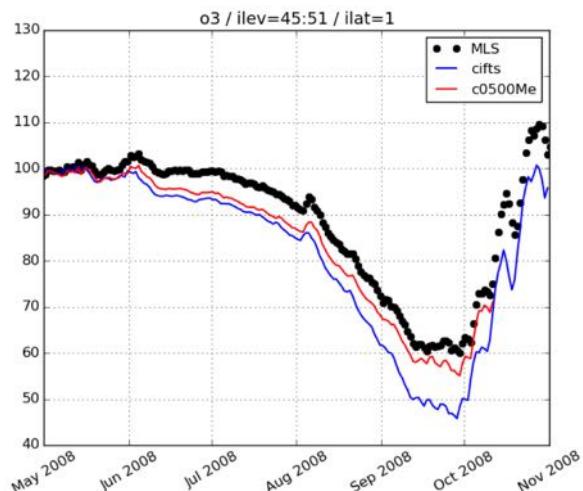
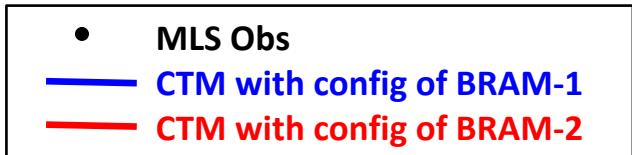
- Left figure shows zonal mean ozone (vmr) profiles between 30°S - 30°N on 1-Nov-2008 from MLS and two CTM simulations using Lean (97) and NRLSSI v2, respectively. Both simulations start on 1-May-2008.
- Left figure show the relative difference (%) between CTMs and MLS.
- BASCOE ozone deficit around 10 hPa is well reduced by the use of daily NRLSSI v2.



BRAM-1 vs 2: impact of setup of aerosols and PSC

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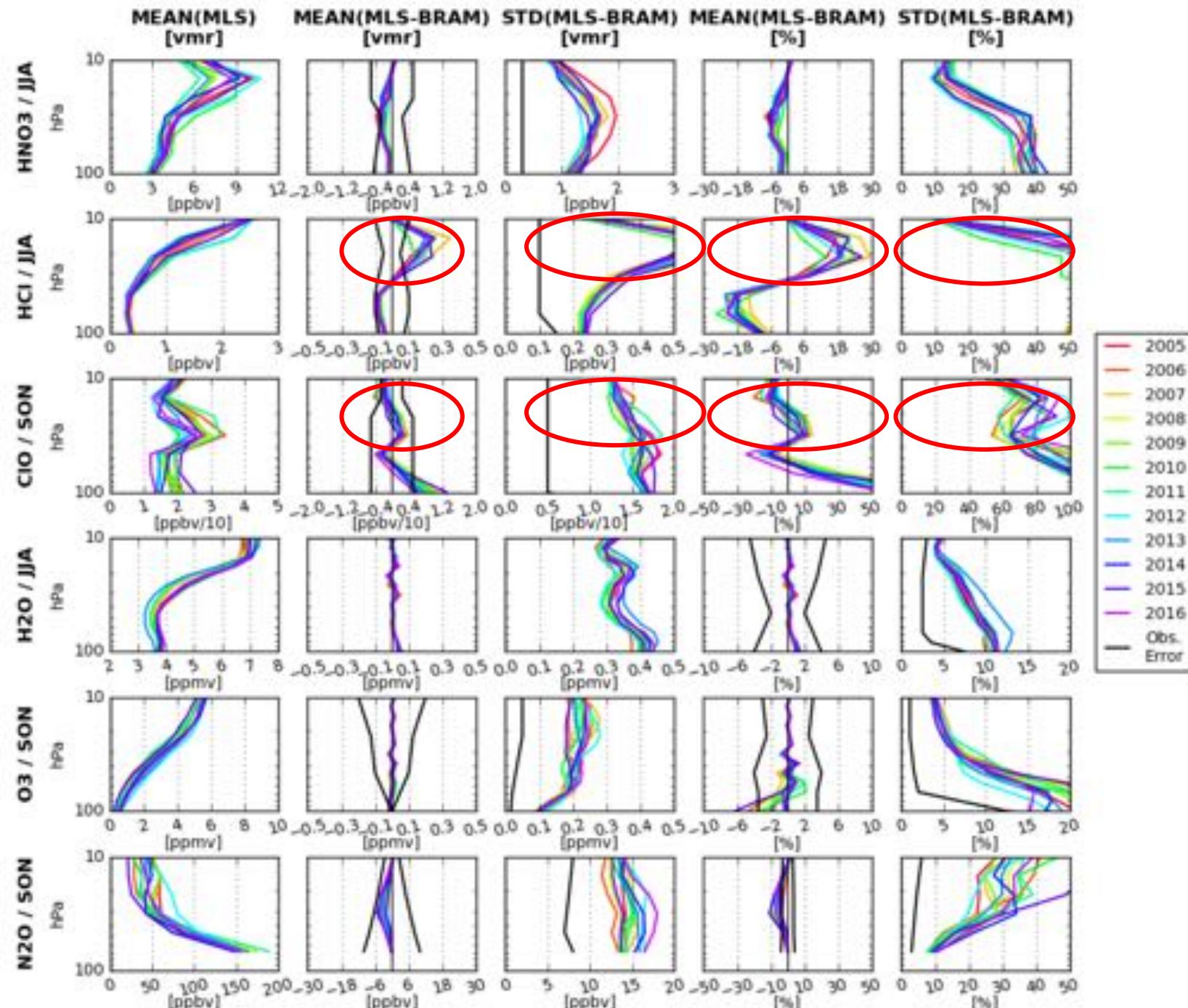
- Figs show time series of partial column between 90°S-60°S and 14-46 hPa of MLS observations and two CTM simulations based on the config of, respectively, BRAM-1 and 2
- By slowing NAT production (i.e. with SSR NAT=10), HCl is much closer to MLS
- Increasing NAT sedim is necessary to keep HNO₃ close to observation
- O₃ improved
- ClO degraded but DA will correct for that



BRAM-1 vs MLS

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- OmF statistics (**MLS-BRAM-1**) in the South Pole region (90°S-60°S) during the polar winter (JJA) or spring (SON), depending on the species
- Main differences between BRAM-1 and 2 occur for HCl and, to a lesser extent, ClO between 10-30 hPa

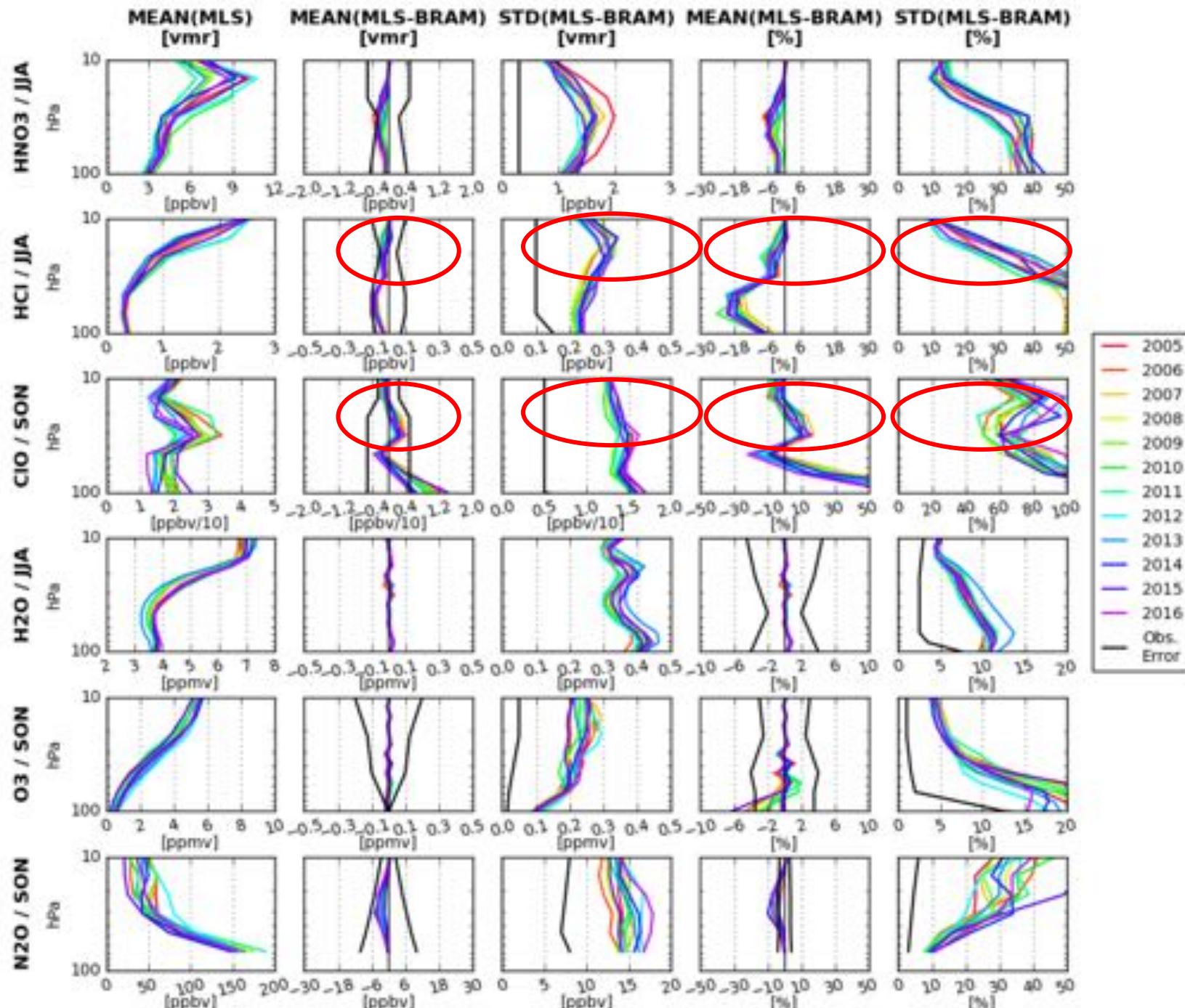


(press PageUp/PageDown to compare BRAM-1 and 2)

BRAM-2 vs MLS

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- OmF statistics (**MLS-BRAM-2**) in the South Pole region (90°S - 60°S) during the polar winter (JJA) or spring (SON), depending on the species
- Main differences between BRAM-1 and 2 occur for HCl and, to a lesser extent, between 10-30 hPa



(press PageUp/PageDown to compare BRAM-1 and 2)

BRAM-1 vs 2: DAS setup

	BRAM-1	BRAM-2
Version	5.13.2 (revision 9786)	07.00.00 (revision 10706)
Method	EnKF but: <ul style="list-style-type: none">• obs. perturbation $\approx \mathcal{N}(0, \sigma^2)$• B matrix = $X_k'(X_k')^T$	EnKF but: <ul style="list-style-type: none">• obs. perturbation $\approx \mathcal{N}(0, \sigma)$• B matrix = $X_k'(X_k')^T / N-1$
Background Quality Control	<ul style="list-style-type: none">• Yes for CH₃Cl, ClO, CO, N₂O, O₃• No for H₂O, HCl, HNO₃	<ul style="list-style-type: none">• Yes for CH₃Cl, ClO, CO, H₂O, HCl, N₂O, O₃• No for HNO₃
Ensemble perturbation	If any MLS observations found for the day, noise is added to all assimilated species in the whole model domain at each time step	Noise is added to assimilated species only at time step with observations and only around levels with observations
Config for observations*	Some obs were rejected at their top/low levels*	Updated to get obs at their top/low levels

* MLS DQD provides valid pressure levels with limited precision, e.g. 1.5-215 hPa for HNO₃ instead of 1.467-215.4433. Since we used pressure ranges from DQD for BRAM-1, several species were rejected at their top/low levels of validity (e.g. HNO₃ at 1.467 and 215.4433). These species are (with the missing level in R1): O₃ (261 hPa), H₂O (316 hPa), HNO₃ (1.5 and 215 hPa) and CO (215 hPa). This issue is corrected in BRAM-2 but the improvement is limited.

BRAM-1 vs 2: Outputs

	BRAM-1	BRAM-2
Chi2	No	Yes
Std Dev of ensemble	No, not setup properly	Yes
Model_at_observations (see next slide)	Online (MLS), offline	mostly online

- The χ^2 between the assimilated observations and BASCOE is calculated during the assimilation run. However, it was not properly saved in BRAM-1 and was lost. With some additional work, it has been possible to recalculate it but only for the 2nd day of each month. This issue has been resolved for BRAM-2.
- The same kind of issue append with the standard deviation of the ensemble in BRAM-1, and resolved in BRAM-2.
- Model_at_observations are saved to evaluate BRAM. Here, observations stand for MLS (assimilated), and many other independent datasets (ACEFTS, MIPAS_IMK, WOUDC, ...)

BRAM-1 vs 2: Observations

	BRAM-1	BRAM-2
MLS (assimilated)	v4.2x, online => file 04q	v4.2x, online => file 04r (correct flag for valid levels – see)
ACEFTS	v3.5 (online), v3.6 flagged (offline)	v3.6 flagged (online)
MIPAS IMK	V5R, offline	V5R, online
WOUDC	As in database, offline	Regridded with averaged value every 100m, online
ESA O3 CCI	Same version, offline	Same version, online
SMILES	Same version, offline	Same version, online

- “Online” means that the ensemble mean is interpolated at observation at the closed time step during the assimilation
- “Offline” means that BASCOE CTM was rerun every day, initialized by ensemble mean at 0 UT, and interpolated at observation as in online
- In BRAM-2, BASCOE fields are interpolated online for all independent set of observations but we do not expect significant impact on the O-F calculations due to this difference.

BRAM-1 vs 2: Streams

	BRAM-1	BRAM-2
Nb of streams	3	4
Starting date of streams	1-Aug-2004, 1-Apr-2008, 2012	1-Aug-2004, 1-Apr-2008, 2012, 2016
Overlap between streams	1 month	1 month
Init conditions	From BASCOE assimilated fields of MLS and MIPAS valid at the same day than the starting date of streams but for 2008	30 y CTM simulation (sc0706B) with LBC for CMIP6; CTM forced by MERRA2 with perpetual year 2000

Significant differences between BRAM-1 and 2

- BRAM-2 improves HCl and ClO in polar winter, above 30 hPa due to updated setting for aerosols and PSC parameterization.
- BRAM-2 provides the std dev of the ensemble as an estimation of the analysis uncertainties (not provided in BRAM-1 because not properly saved during BRAM-1 production).
- BRAM-2 extended for 2017