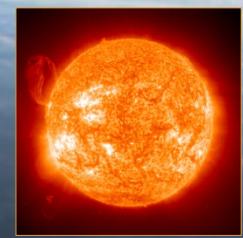


BRAM: Reanalysis of stratospheric chemical composition based on Aura MLS

Quentin Errera (quentin@oma.be), Simon Chabrillat, Yves Christophe and Sergey Skachko

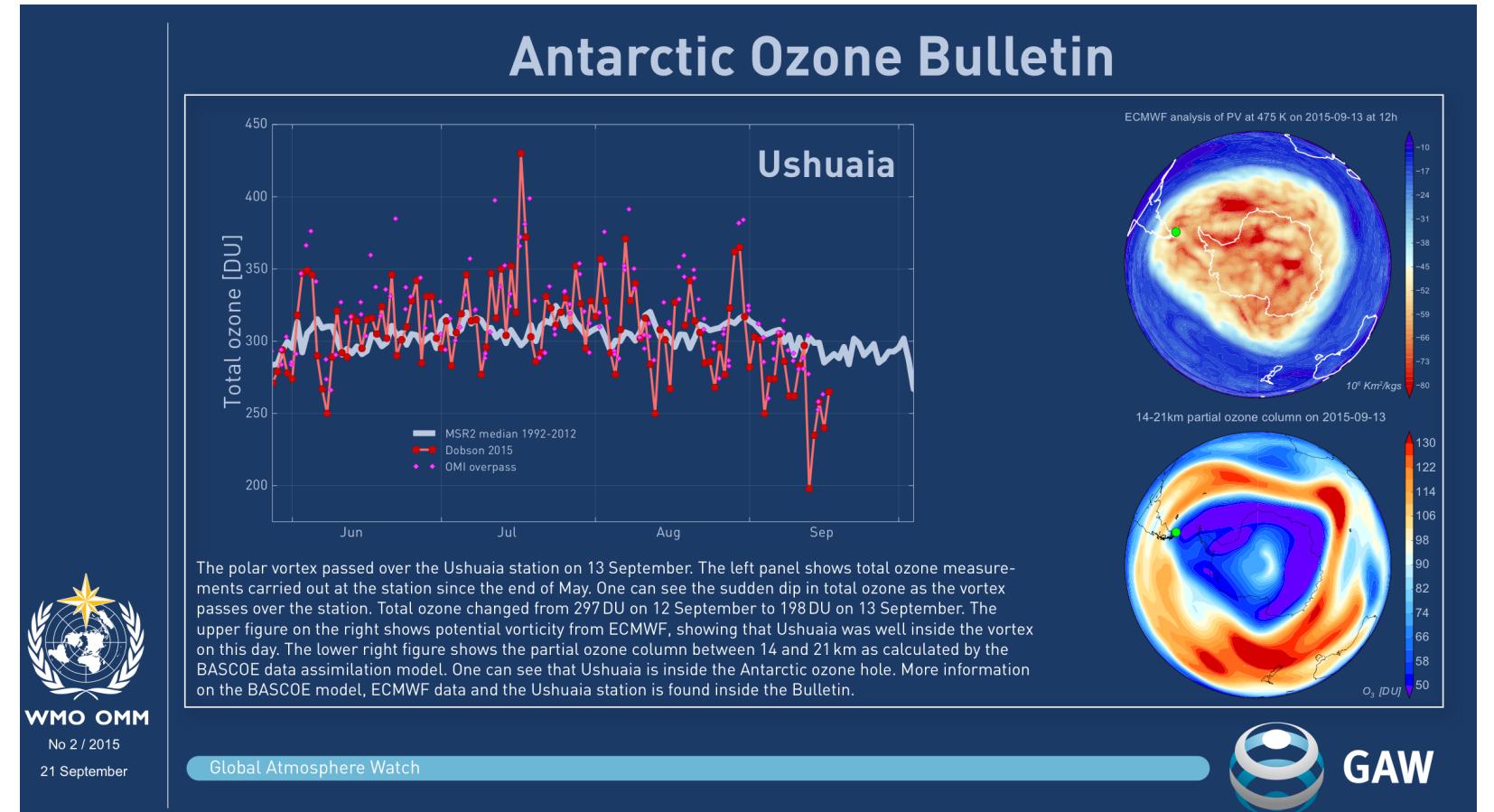
Royal Belgian Institute for Space Aeronomy (BIRA-IASB)

13th SPARC DA workshop, 25-27 Oct 2017, ECMWF, Reading, UK



Motivations

- BASCOE produces operational analyses of MLS since 2009 for the validation of MACC O₃ (Lefever et al., 2015)
- For this service, BASCOE assimilates O₃, H₂O, HNO₃, N₂O, HCl and ClO
- These analyses are used by WMO Global Atmospheric Watch (GAW) to monitor Ozone and related trace gases and to interpret ground-based observations
- A reanalysis of MLS was requested by WMO GAW
- BRAM: **BASCOE Reanalysis of Aura MLS 2004-2016**
(will be continued)



Outline

- BASCOE setup
- Observational setup
- Evaluation of BRAM
- Where to find BRAM dataset?
- Conclusions

Setup of BASCOE (Belgian Assimilation System of Chemical ObsErvations)



KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL

- CTM with 58 stratospheric species (Errera et al., ACP, 2008)
 - Advection: FFSL (Lin & Rood, MWR, 1996)
 - Chemistry: \approx 200 chemical reactions (gas phase, heterogeneous, photolysis)
 - Parameterization of PSC microphysics
 - Dehydration of H_2O in the stratosphere
- Dynamics (winds and T°) from ERA-Interim with resolution:
 - $2.5^\circ \text{ lat} \times 3.75^\circ \text{ lon} \times 37 \text{ levels}$ (surf to 0.1 hPa, 25 levels above 100 hPa)
- Time step: 30'
- DA method: **EnKF** (Skachko et al., GMD, 2014, 2016) chosen due to its better scalability on HPC than 4D-Var

Observations

- KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL
- Assimilated observations
 - Aura MLS Version 4.2x
 - O₃, H₂O, HCl, ClO, HNO₃, N₂O (190-GHz), CO, CH₃Cl
 - These are the species that do not need to be averaged
 - Prepare according to MLS Data Quality Document
 - Pressure ranges of validity, cloud screening, ...
 - Monitored independent observations (for validation)
 - **ACEFTS v3.6, MIPAS IMK, MIPAS ESA v6, WOUDC ozonesondes, O3_CCI L2 profiles, SMILES**
 - To be done: MIPAS ESA v7

BRAM vs other reanalysis

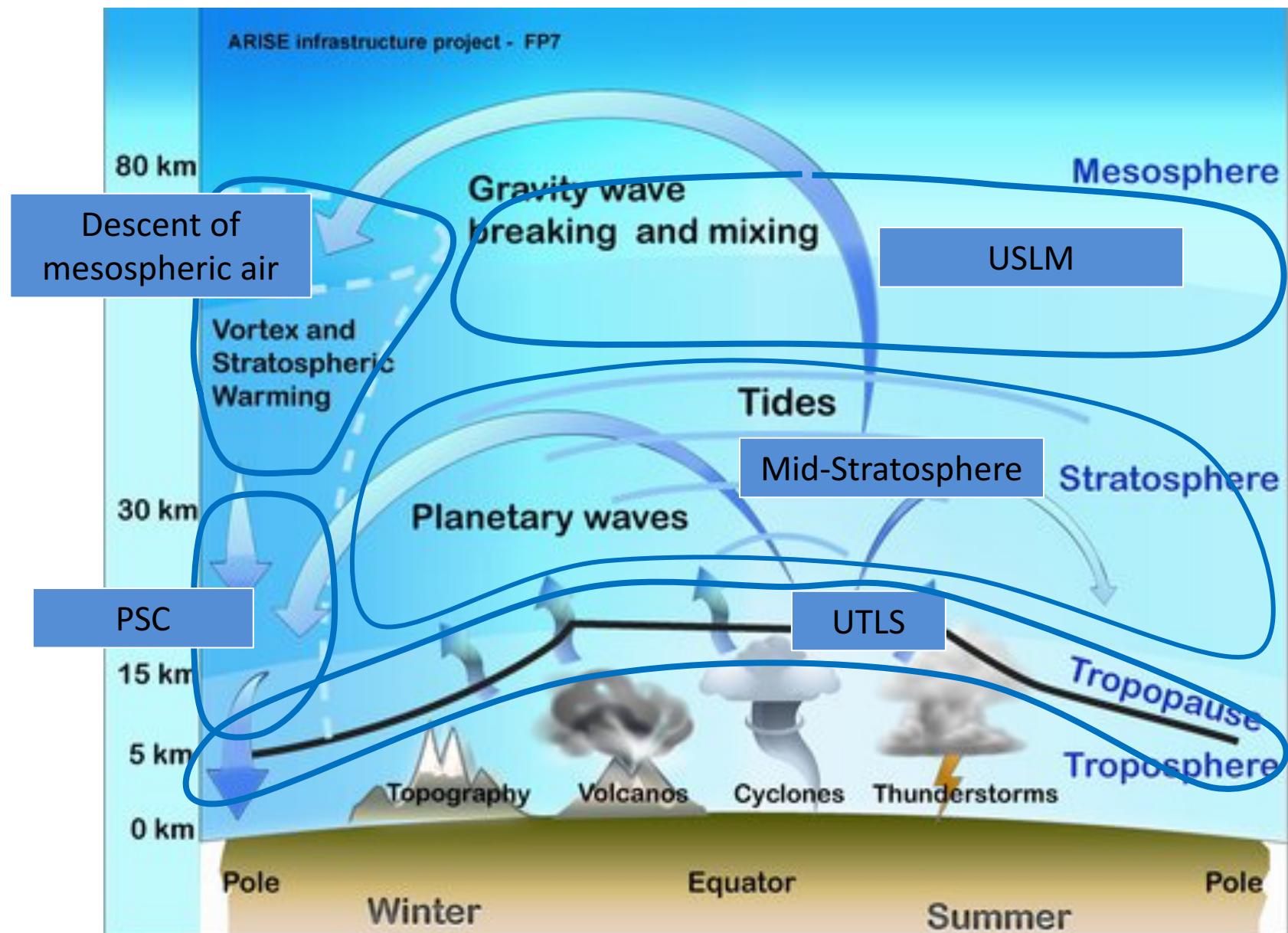
Status of existing constituents reanalysis

- Meteorological reanalyses usually only consider O_3 in the stratosphere
- Same for MACC/CAMS reanalysis (Inness et al. 2013, Flemming et al. 2017)
- van der A et al. (2010) has produced a 30-year O_3 TC reanalysis (no profiles) based on multi-sensor assimilation
- Miyazaki et al. (2015) has produced a 7-year multi-species reanalysis for the tropospheric composition

BRAM is the first reanalysis that focus on the stratospheric composition with other species than O_3

Evaluation of BRAM reanalysis: strategy

- Evaluation of BRAM in different stratospheric region of interest
 - Mid-stratosphere
 - Winter pole in the lower stratosphere
 - Winter pole in the upper stratosphere
 - UTLS
 - USLM



Evaluation of BRAM reanalysis: strategy

KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL

Atm. Conditions	Vertical Ranges	Latitude ranges	Season	Species
Middel Stratosphere	3-70 hPa	60°S-60°N	-*	O ₃ , H ₂ O, HCl, ClO, HNO ₃ , N ₂ O, CH ₃ Cl
PSC	10-100 hPa	South pole region	JJA or SON	O ₃ , H ₂ O, HCl, ClO, HNO ₃ , N ₂ O
Descent of meso. air	0.1-6.8 hPa	South pole region	JJA	H ₂ O, HNO ₃ , CO
USLM	0.1-3 hPa	Tropics	-*	H ₂ O, HCl
Tropical UTLS	68-200 hPa	Tropics	JJA	O ₃ , H ₂ O, CO, CH ₃ Cl, (HCl?, HNO ₃ ?)
Mid-lat. UTLS	68-200 hPa	Tropics	-*	O ₃ , H ₂ O, CO, CH ₃ Cl, (HCl?, HNO ₃ ?)

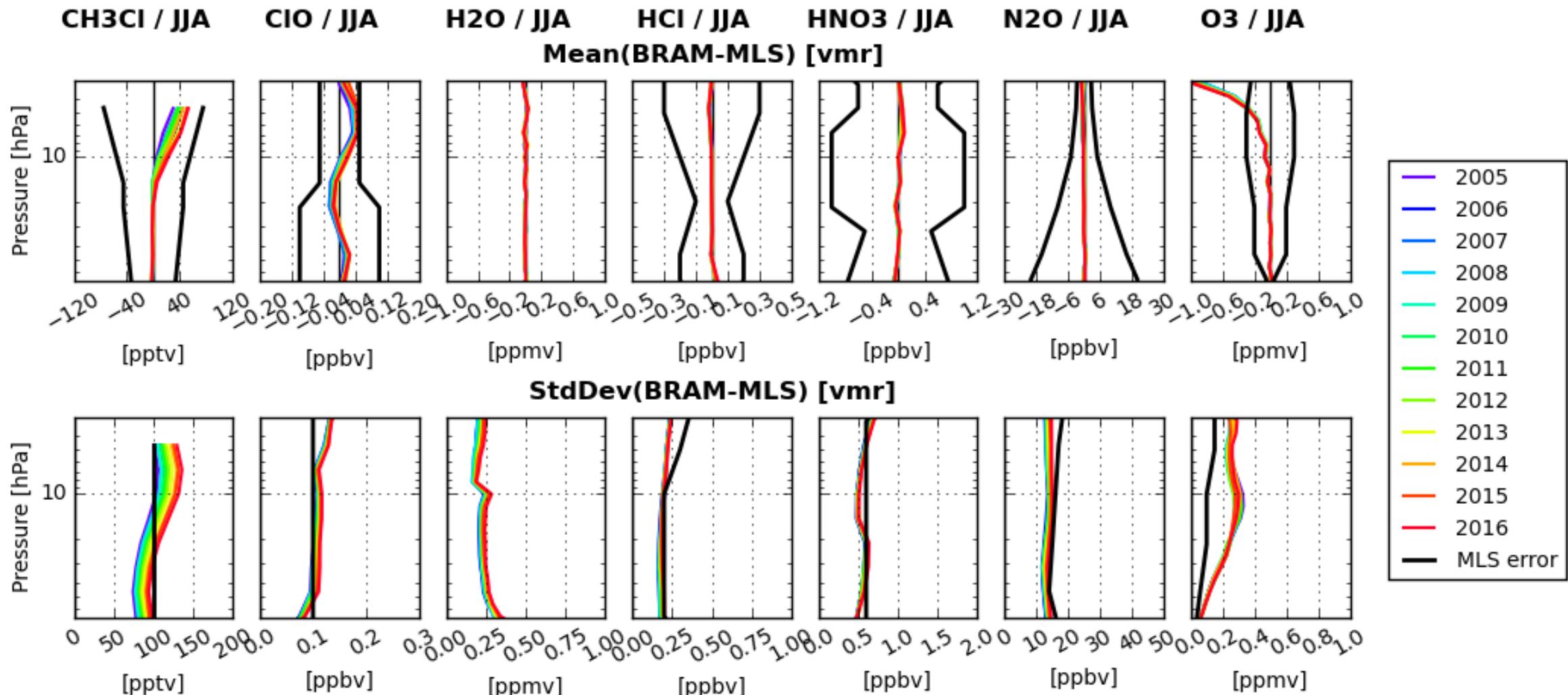
*: in these cases, JJA has been chosen arbitrarily

O₃ not assimilated in the USLM, see Jonas Debosscher's poster

Middle stratosphere

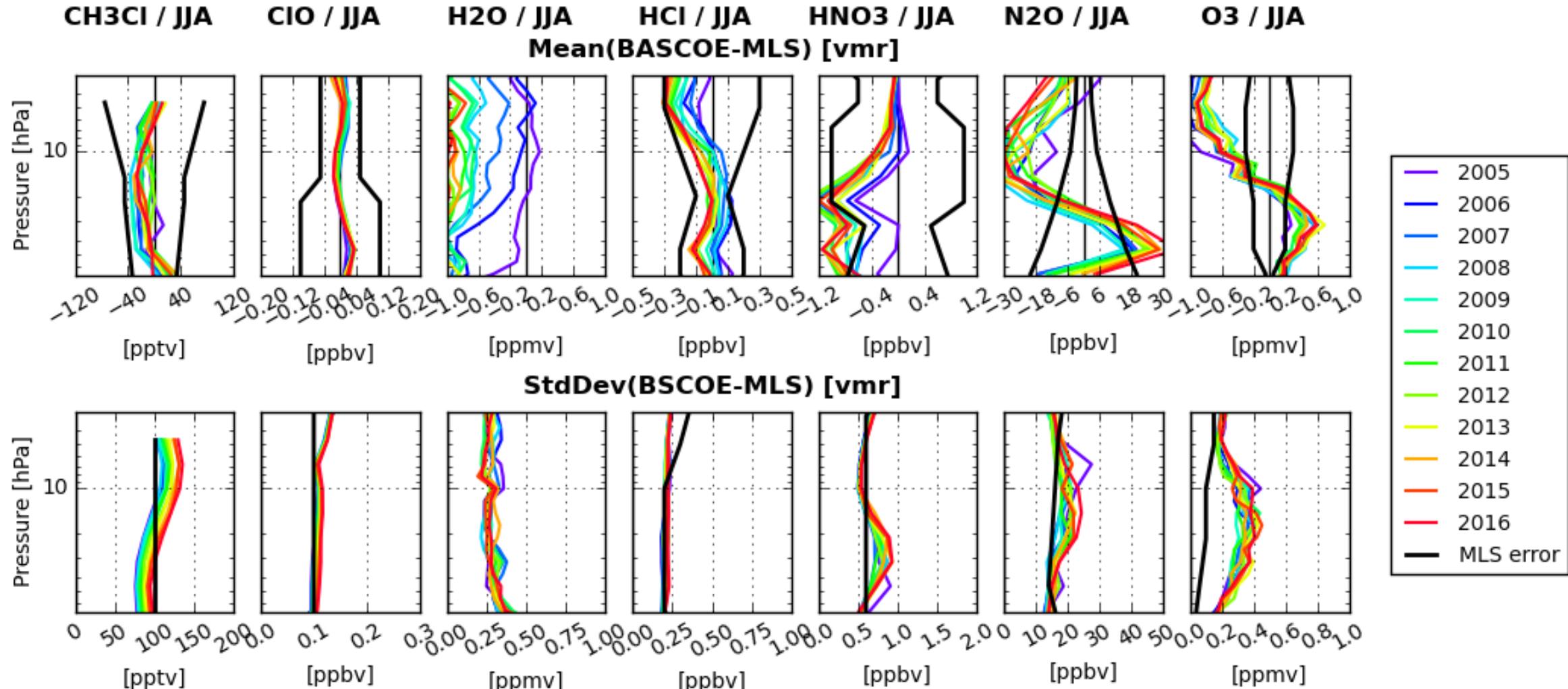
Middle Stratosphere: BRAM vs MLS

OmF statistics for BRAM vs MLS in the Middle Stratosphere



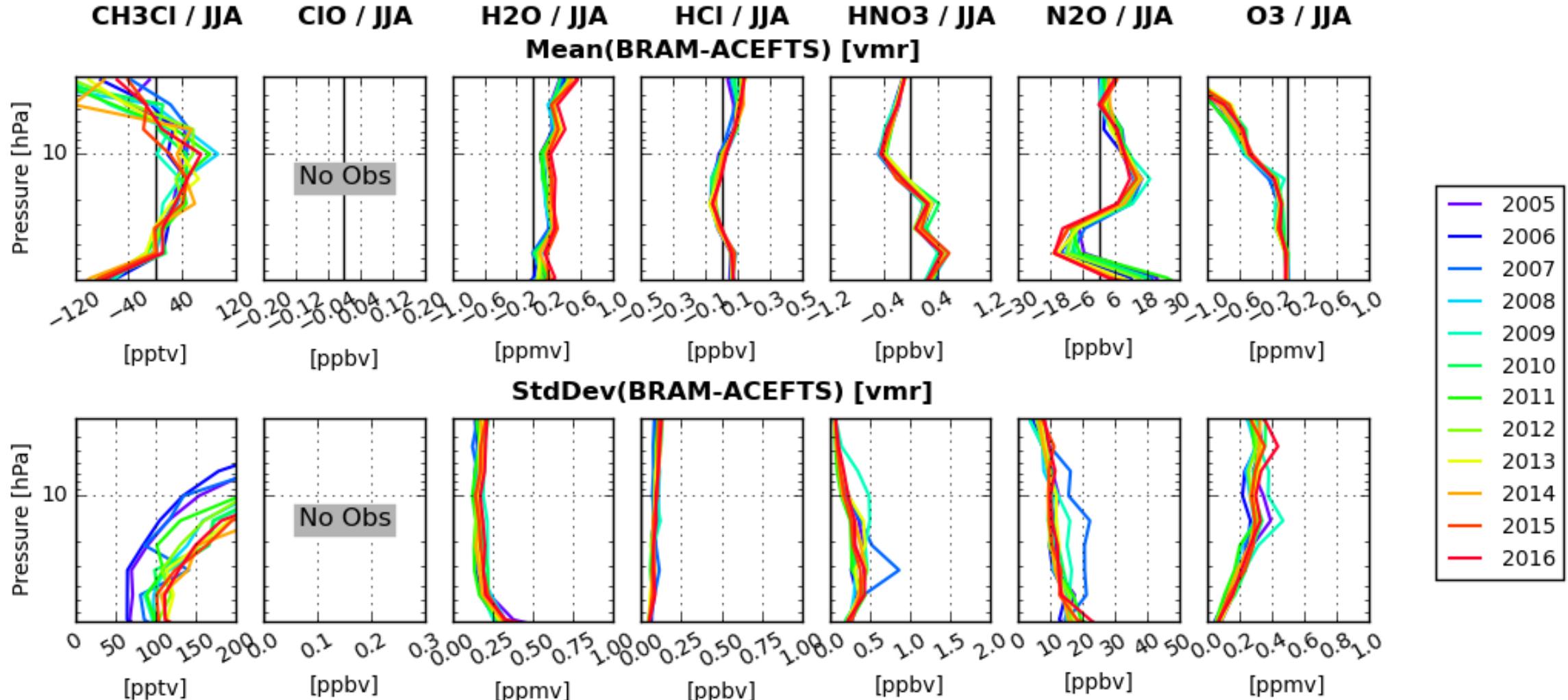
Middle Stratosphere: CTRL vs MLS

OmF statistics for CTRL vs MLS in the Middle Stratosphere



Middle Stratosphere: BRAM vs ACEFTS

OmF statistics for BRAM vs ACEFTS in the Middle Stratosphere



Error covariances in BRAM

- Forecast covariances estimated from ensemble covariances (20 members)
- For each species, observational variances scaled using Desroziers's method (Desroziers et al., 2005) which states:

$$s_o^2(z_o) = \frac{\sigma_o^2(z_o)}{\text{tr}(\mathbf{R}(z_o))}$$

Diagram illustrating the calculation of scaled observational variance:

```
graph TD; SF[scaling factor] --> Alt[Altitude]; Alt --> SOV[Observational (MLS) variances]; SF --> SOV; SOV --> S2OZo[s2o(zo)];
```

• Knowing that: $\sigma_o^2 = < (\mathbf{y}^o - \mathbf{H}\mathbf{x}^a)(\mathbf{y}^o - \mathbf{H}\mathbf{x}^b)^T >$

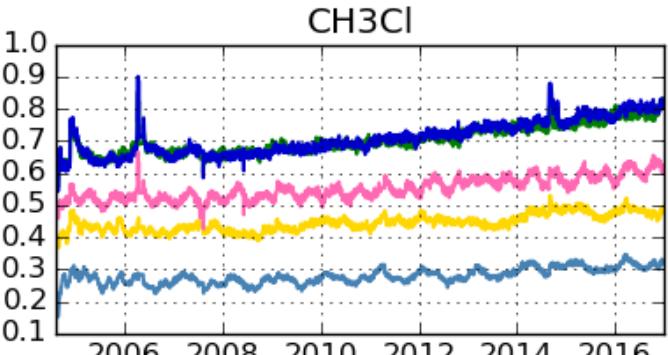
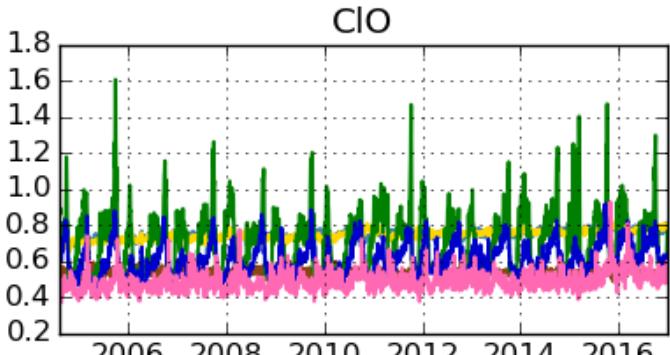
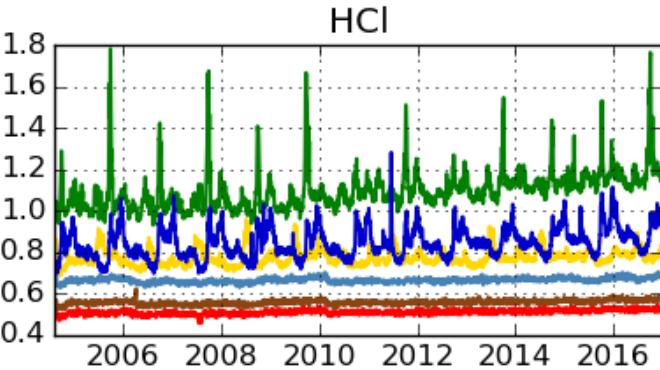
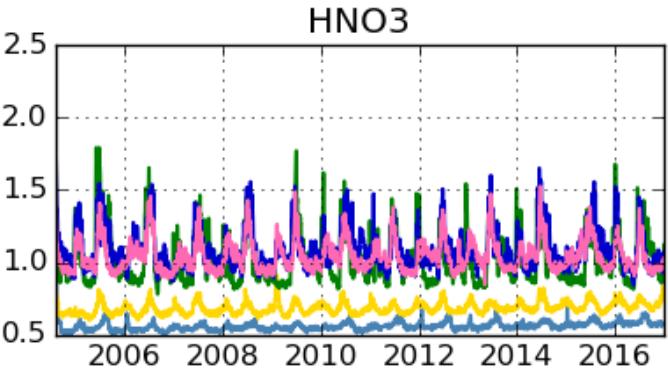
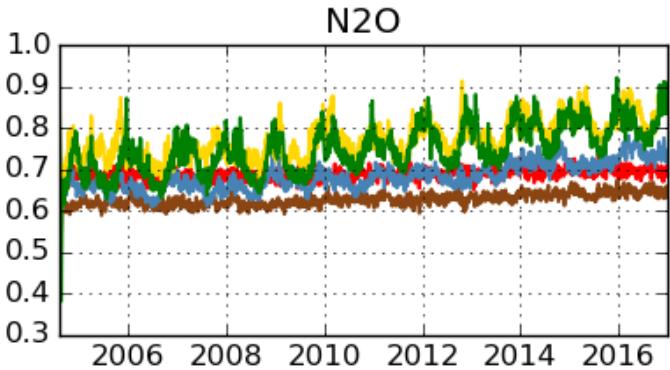
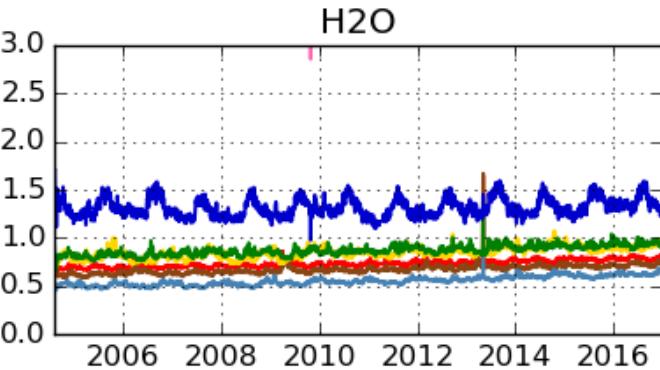
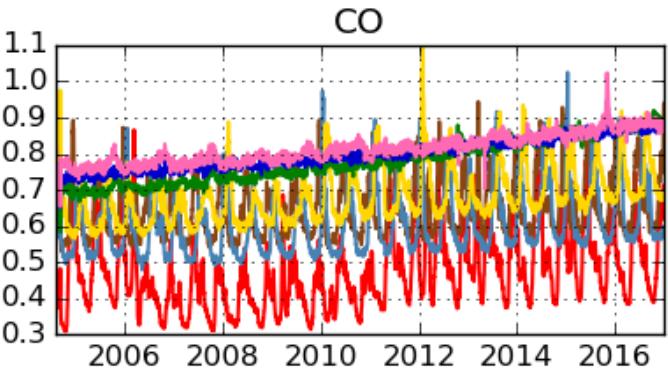
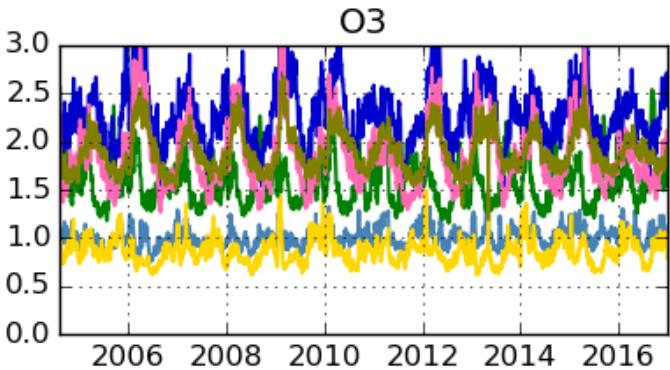
$\underbrace{\hspace{10em}}$ $\underbrace{\hspace{10em}}$

Analysis innovations

Forecast innovations

Error covariances in BRAM

KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL



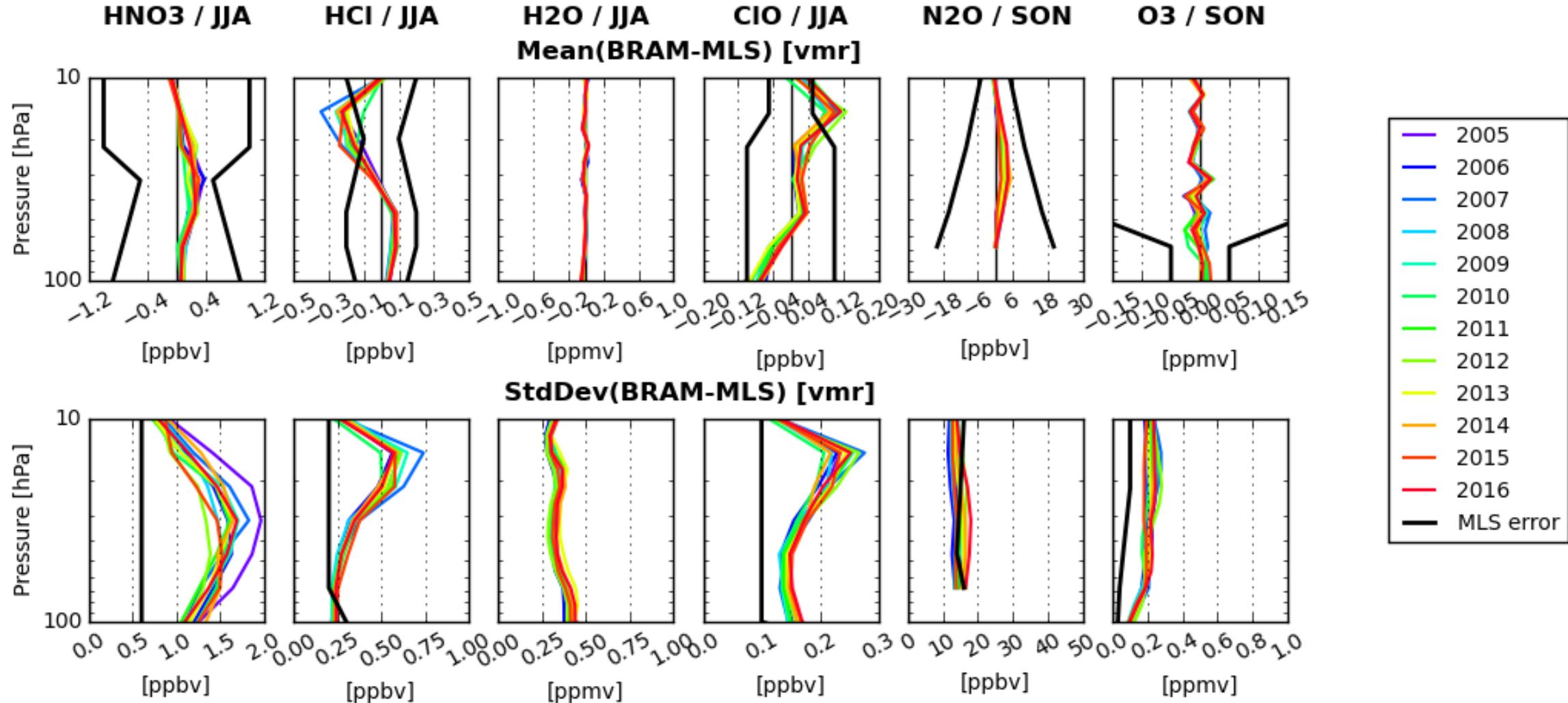
Time series of s_0
for assimilated
species at
several MLS
levels

0.46 hPa	46.42 hPa
1.00 hPa	100.00 hPa
4.64 hPa	146.78 hPa
10.00 hPa	215.44 hPa

PSC conditions

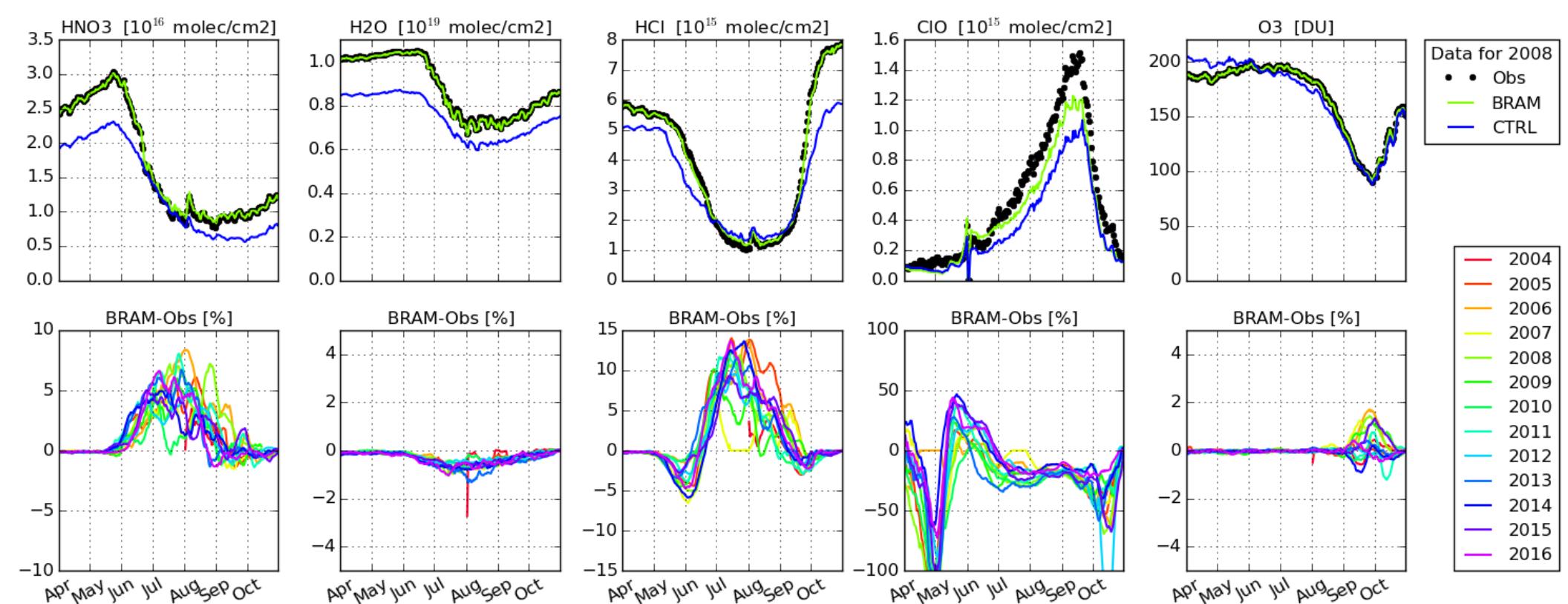
PSC conditions: BRAM vs MLS

OmF statistics for BRAM vs MLS in PSC conditions



Winter Pole in the lower stratosphere (South Pole)

KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INST:TUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL



Top: 2008
timeseries of MLS partial column [10-100] hPa averaged between 90°S-60°S for 5 key constituents involved in O₃ hole development and corresponding values of BRAM and CTRL

Bottom: Timeseries of the differences BRAM-MLS for 2004-2016

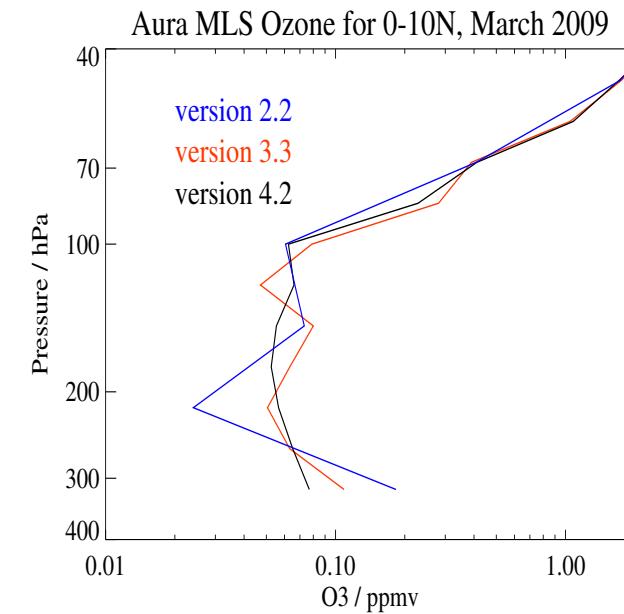
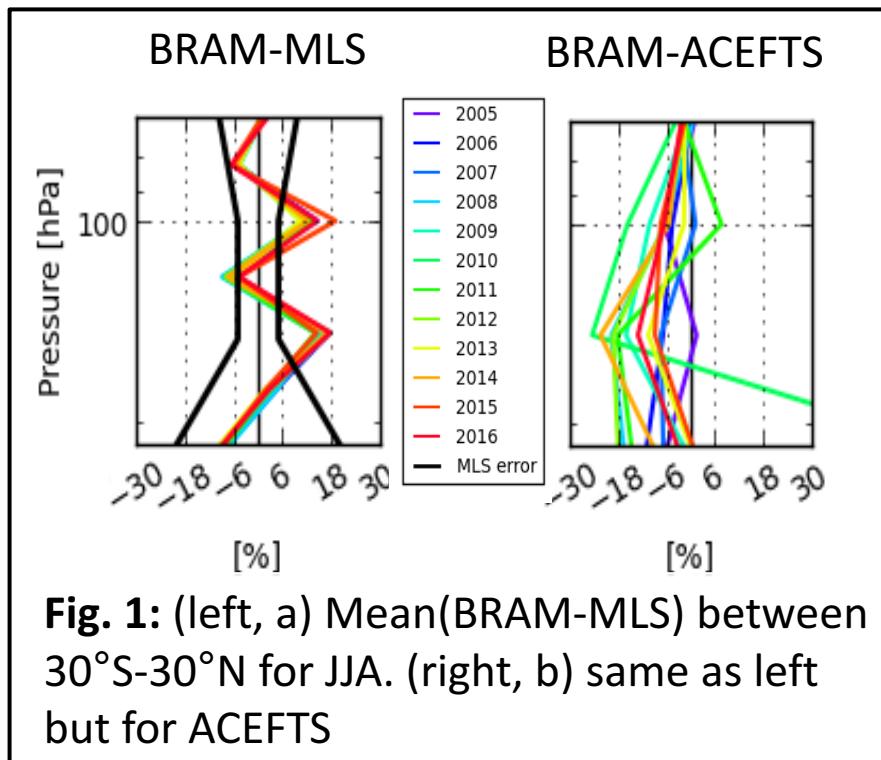
- BRAM corrects most of the deficiencies of the model (I.C. and physics)
- ... and highlights systematic errors in the PSC scheme of the model

Tropical UTLS

BRAM O₃ in the tropical UTLS

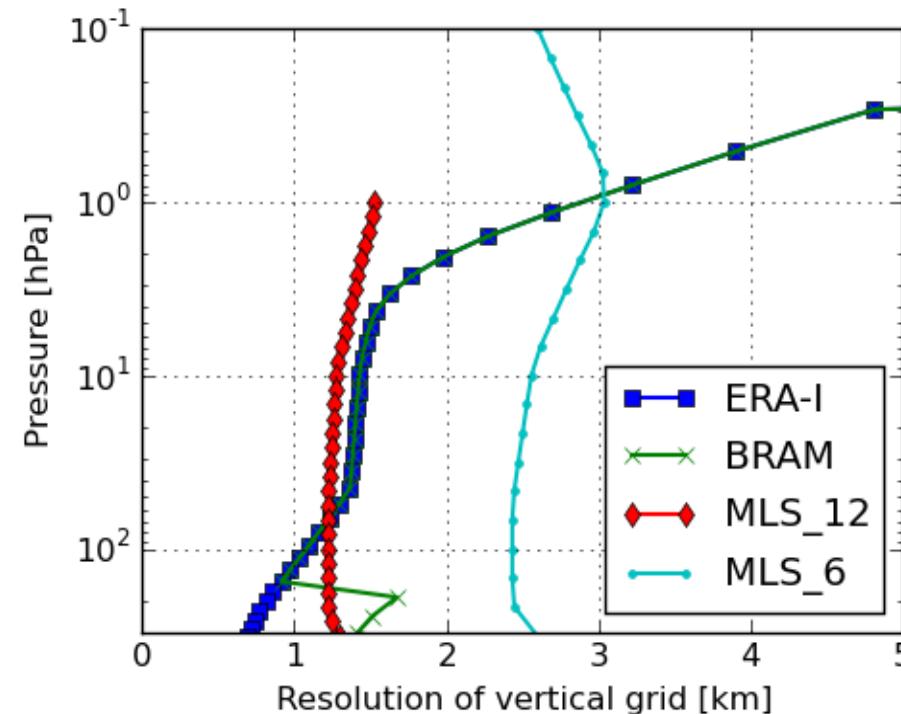
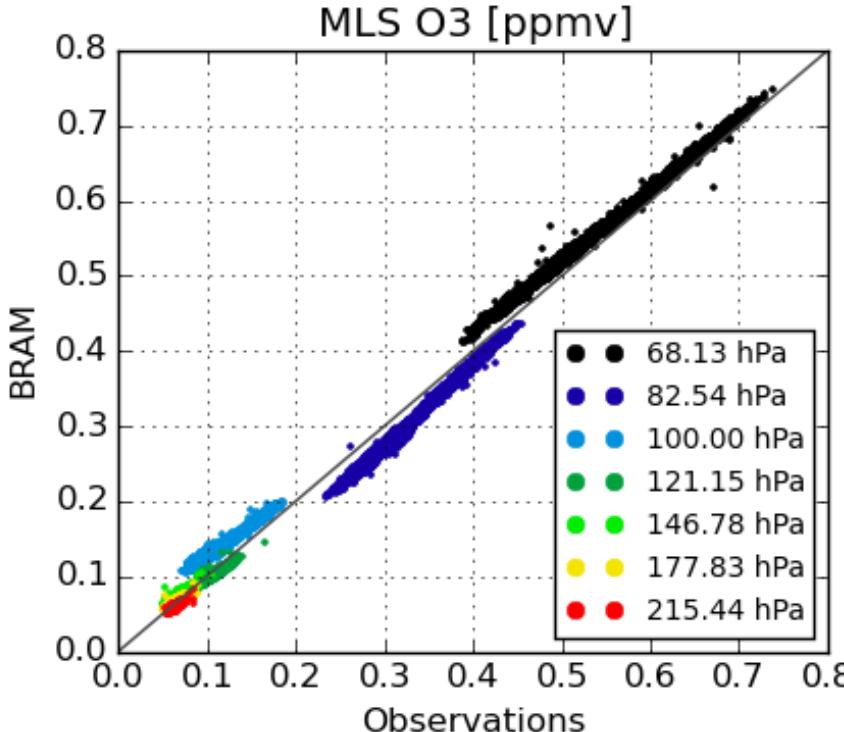
KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL

- BRAM vs MLS in UTLS exhibits vertical oscillations for O₃ (Fig. 1a)
- Not seen in BRAM vs ACEFTS (Fig. 1b)
- Probably due to oscillation in MLS O₃ v4.2 (see MLS DQD), although improvements since v2.2 (Fig. 2)



BRAM O₃ in the tropical UTLS

KONINKLIJK BELGISCHE INSTITUUT VOOR RUIJMET-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIJMET-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIJMET-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL



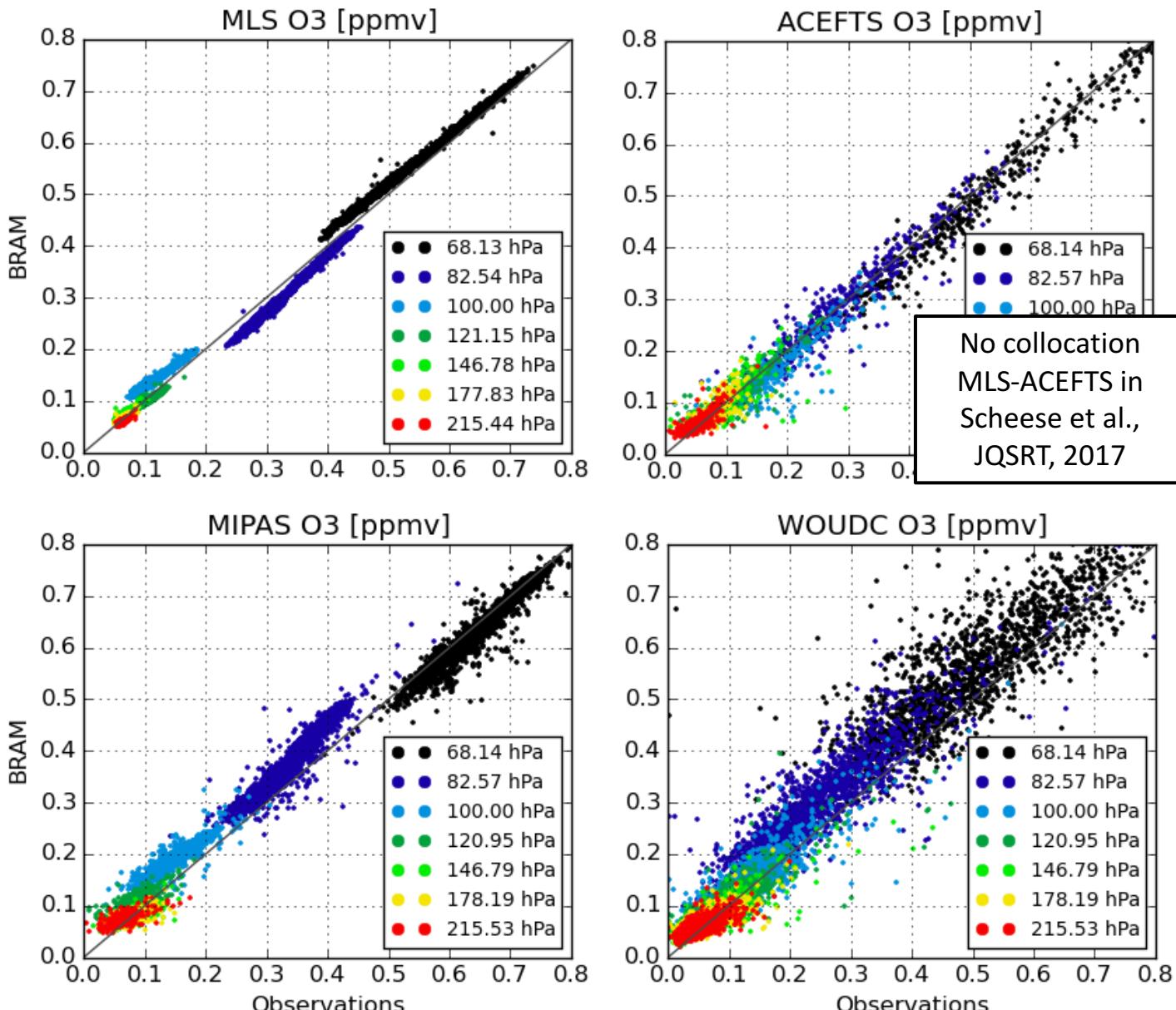
Left: Daily mean MLS O₃ in the tropical UTLS (30°S-30°N) and the BRAM corresponding values.
right: Resolution of vertical grid of ERA-I, BRAM, MLS 6 and 12 levels per decade of pressure

BRAM cannot reproduce MLS in tropical UTLS because:

- Vertical oscillation in MLS
- MLS and BRAM vertical grid have similar resolution

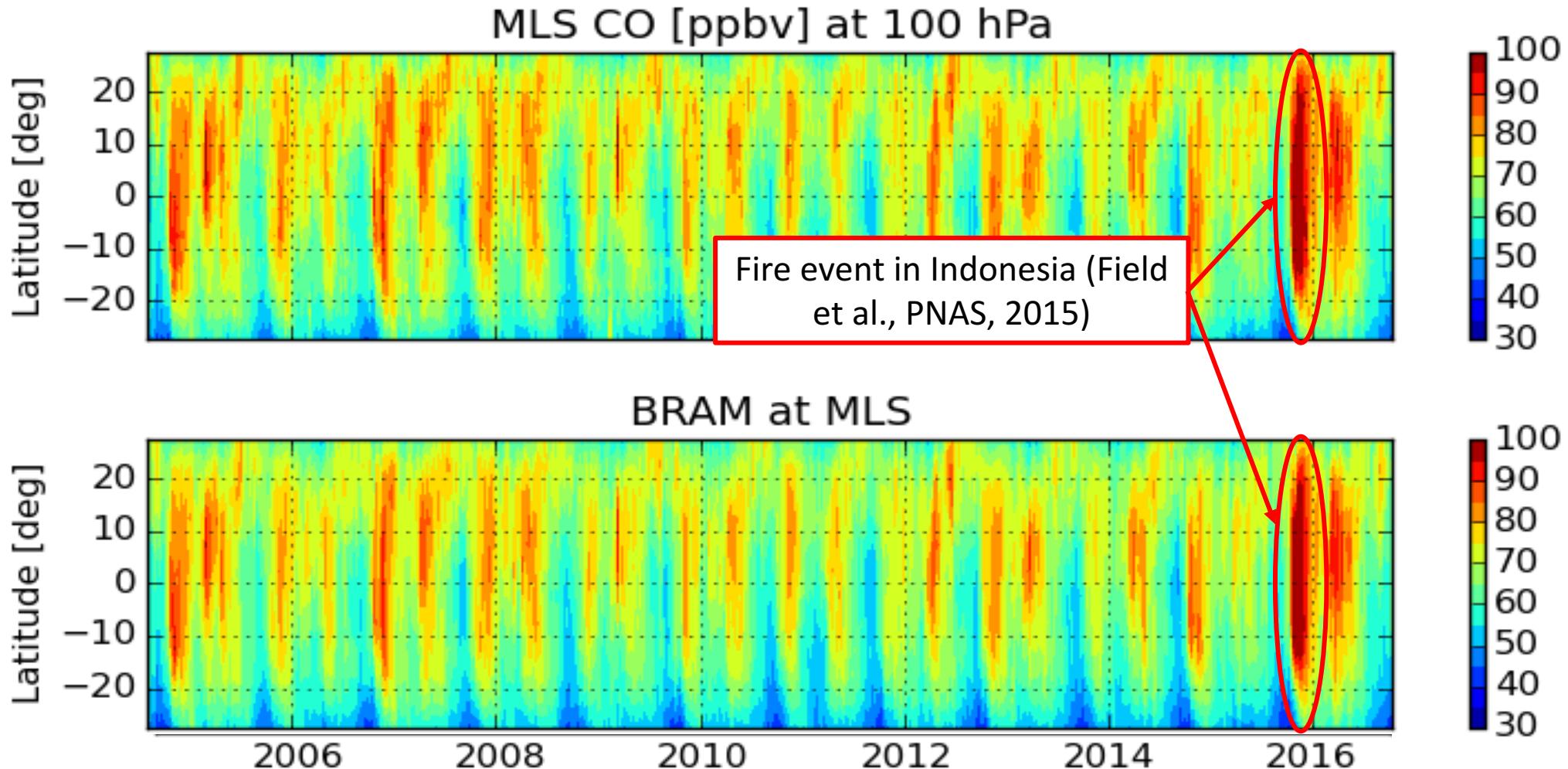
BRAM O₃ in the tropical UTLS

- BRAM highlight systematic differences between different instruments
- Good agreement with ACEFTS
- Could BRAM be used as transfer function between different observational datasets to estimate (and correct) their systematic differences?

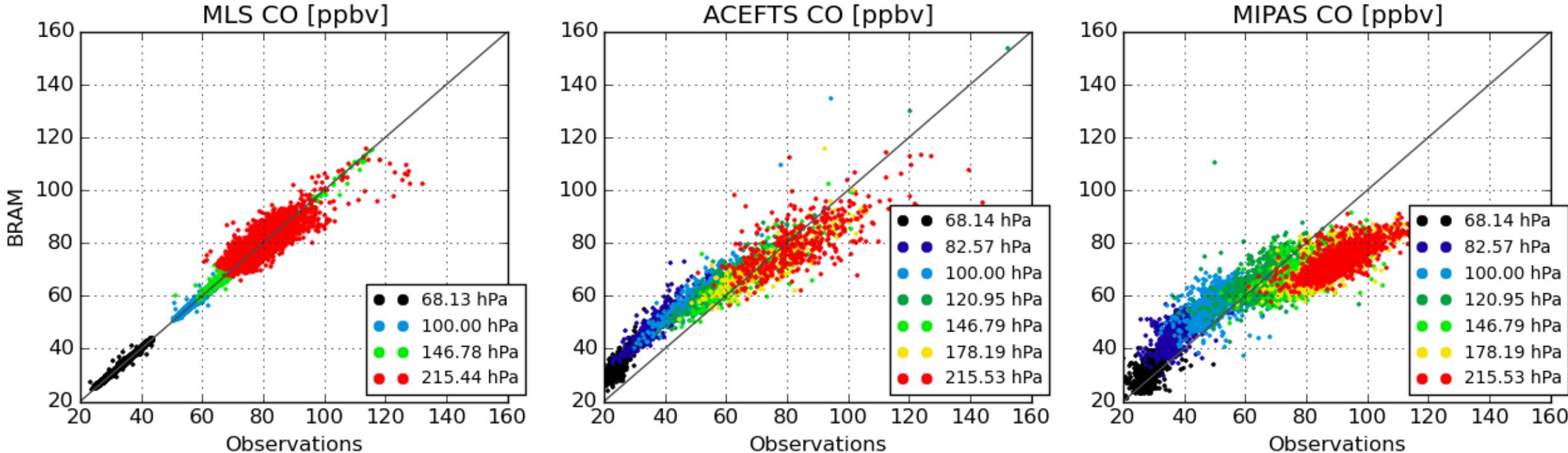


BRAM CO in the tropical UTLS

- CO at 100 hPa: very good agreement between BRAM and MLS



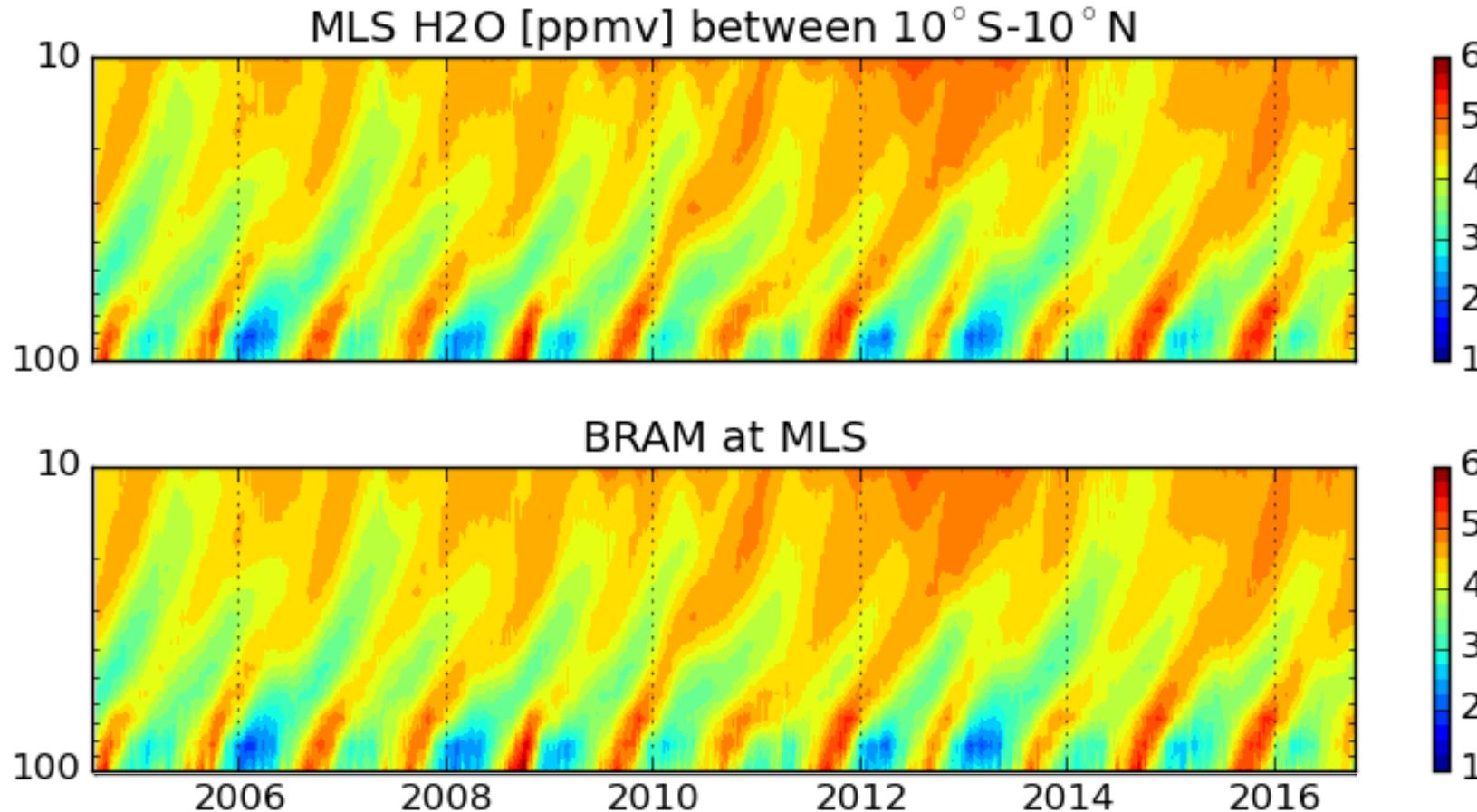
BRAM CO in the tropical UTLS



Daily mean CO in the tropical UTLS (30°S - 30°N) from observations and the BRAM corresponding values.
Left to right: MLS, ACEFTS and MIPAS

- BRAM highlight systematic differences between different instruments
- Could BRAM be used as transfer function between different observational datasets to estimate (and correct) their systematic differences?

BRAM H₂O Tape Recorder



Top: time series of mean MLS H₂O between 10°S-10°N
Bottom: Corresponding BRAM values

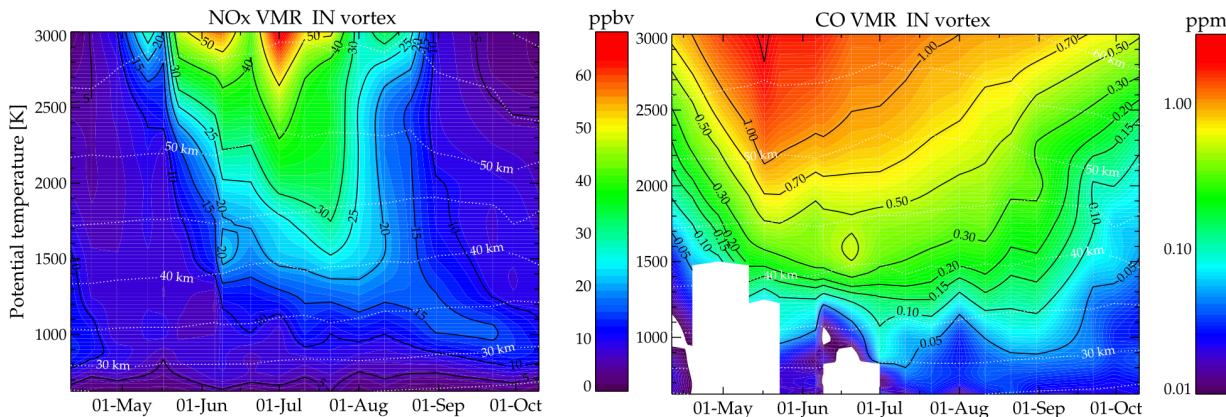
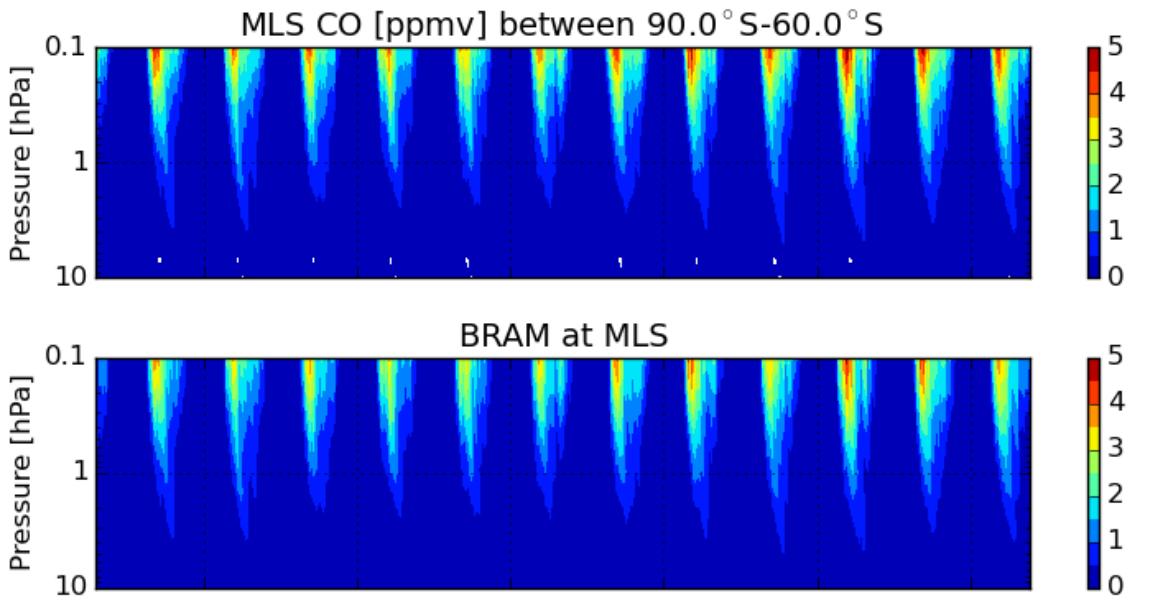
- H₂O Tape recorder (Mote et al., JGR, 1996)
 - Very good agreement between BRAM and MLS
 - Might be useful to evaluate vertical transport of CCMs/GCMs

Descend of mesospheric air

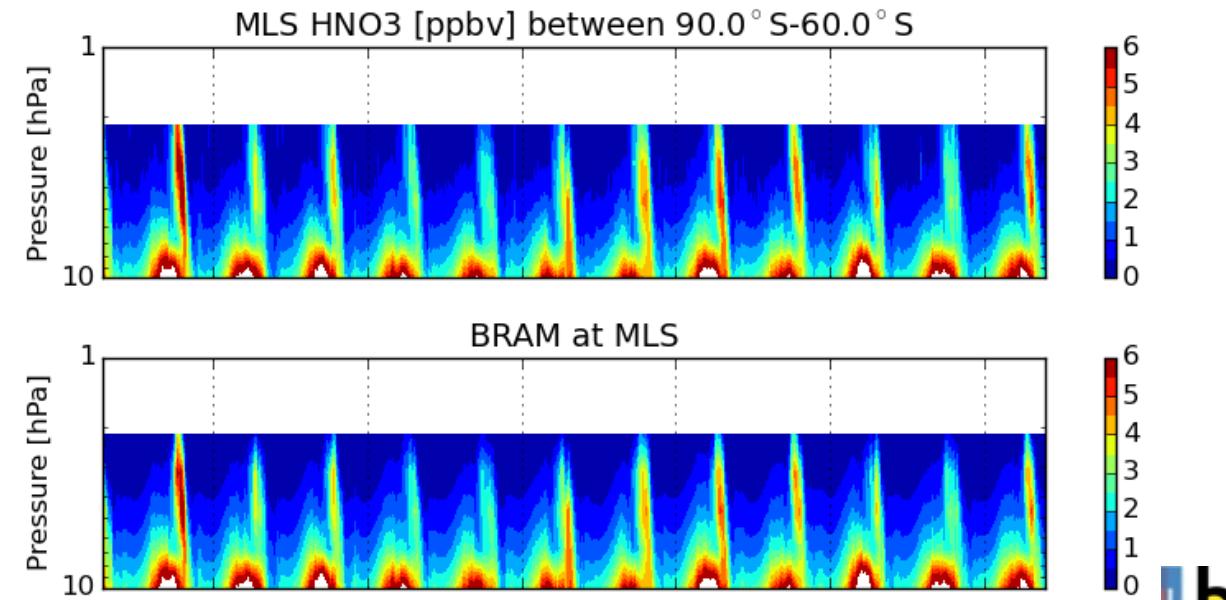
Winter Pole in the upper stratosphere (South Pole)

KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL

- USLM polar winter characterized by descend of mesospheric air in the stratosphere (CO, NO_x, H₂O)
- Good representation of CO descent by BRAM while no source of CO at model lid
- HNO₃ enhancement (due to NO_x descent) well capture by BRAM
- Nevertheless, EnKF cannot correct NO_x (not shown)



Time evolution of NO_x and CO in May-Aug 2003 measured by MIPAS IMK (Funke et al., JGR, 2005)



Getting the BRAM dataset

KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL

- BRAM Release 1 **is available**
 - Only assimilated species plus Cl₂O₂ will be delivered:
 - O₃, H₂O, HCl, ClO, Cl₂O₂, HNO₃, N₂O, CO, CH₃Cl
 - File format: NetCDF-CF, one file per year per species
 - BRAM datasets available on BIRA-IASB ftp site
 - To get login/pw, contact quentin@aeronomie.be
 - Website: strato.aeronomie.be -> Datasets -> BRAM

Conclusions and perspectives

- BASCOE EnKF successfully assimilate MLS observations of O₃, H₂O, HCl, ClO, HNO₃, N₂O, CO, CH₃Cl for 2004-2016
 - ... but also highlight:
 - Model deficiencies (PSC microphysics, model O₃ deficit, ...)
 - Instrumental issues (O₃ vertical oscillations in MLS, MLS CO bias...)
 - Could BRAM be useful to correct systematic differences between different instruments (MLS, ACEFTS, MIPAS, O3 sondes)?
 - Would the replacement of ERA-Interim by ERA5 improve BRAM?
 - This work also suggests themes for DAWG 2019-2022
 - Assessing (and correct) systematic difference between instruments using DA

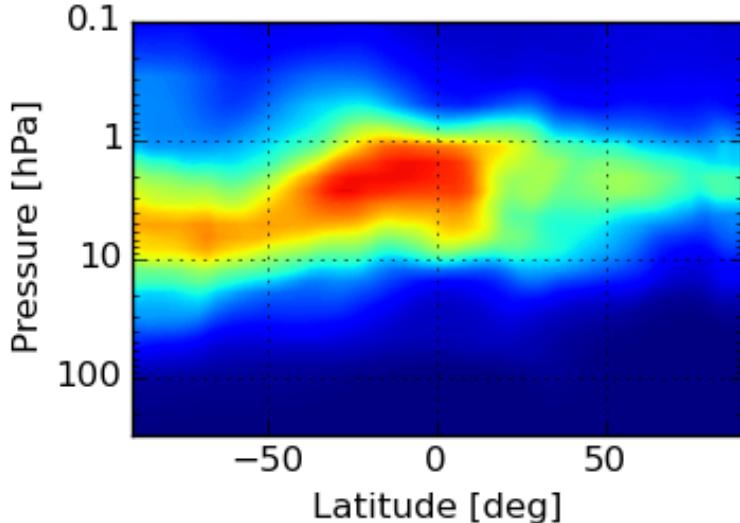
Thank you for your attention!

What about unobserved species?

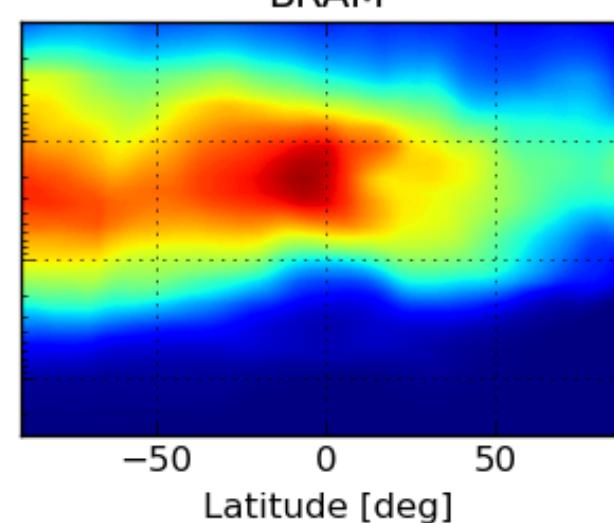
KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL BELGIAN INSTITUTE OF SPACE AERONOMY KONINKLIJK BELGISCHE INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT ROYAL D'AERONOMIE SPATIALE DE BELGIQUE ROYAL

- Little attention yet given to other species than: O_3 , H_2O , HCl , ClO , HNO_3 , N_2O , CO , CH_3Cl
- Here, example for NO_x ($NO+NO_2$)
 - BRAM overestimates MIPAS ESA and is closer to a CTM

BASCOE Assim of MIPAS ESA
including NO_2 observations



BRAM



BASCOE CTM run

