Bridging the SAGE data gap: Toward a climate data product with ozone and water vapor data from NASA SAGE and Aura missions and NASA reanalyses

K. Emma Knowland

Morgan State University (MSU), GESTAR-II

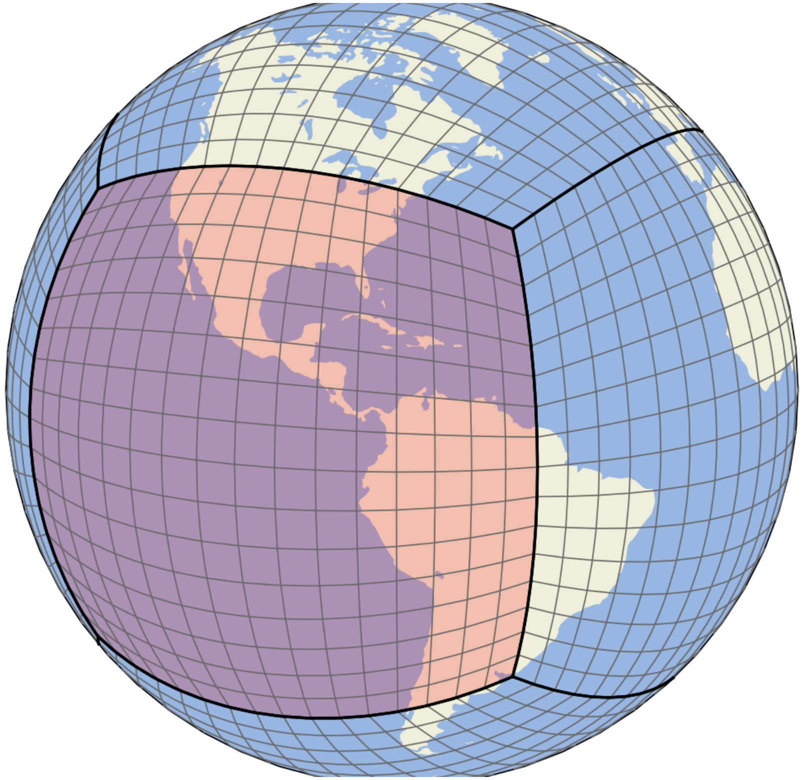
NASA Global Modeling and Assimilation Office (GMAO)

Co-Investigators

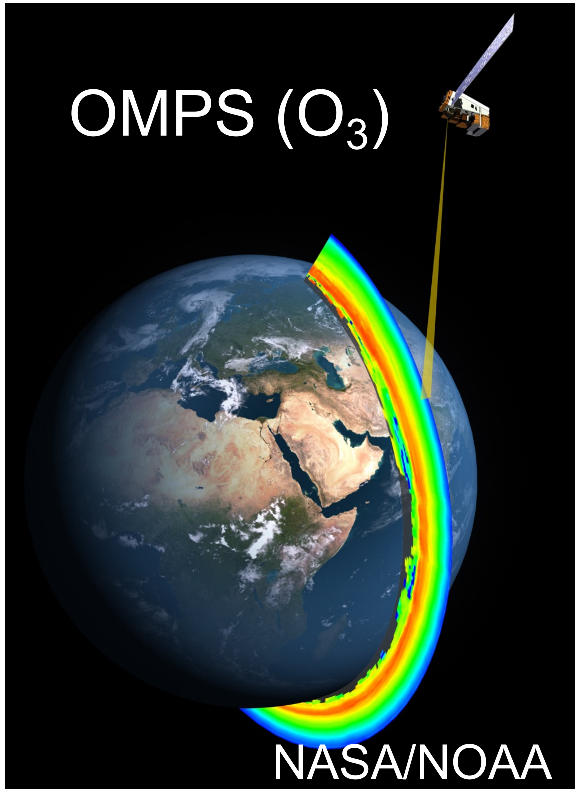
Steven Pawson (GMAO), Pam Wales (MSU/GMAO), Kris Wargan (SSAI/GMAO), Brad Weir (MSU/GMAO)

NASA GMAO global meteorology and chemistry products

GEOS



Bindle et al., 2021 GMD

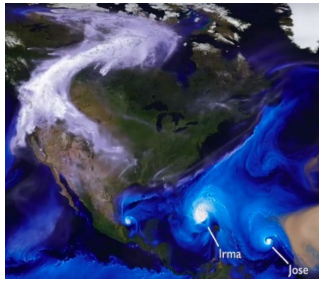


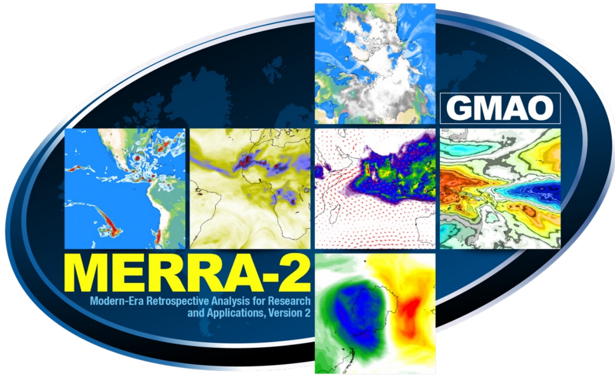
www.nasa.gov

NASA GMAO global meteorology and chemistry products

GEOS

- Forecasting
  - GEOS FP
  - GEOS FP-IT
    - GEOS-CF
- Reanalysis
  - MERRA-2
    - M2-SCREAM
    - MERRA2-GMI

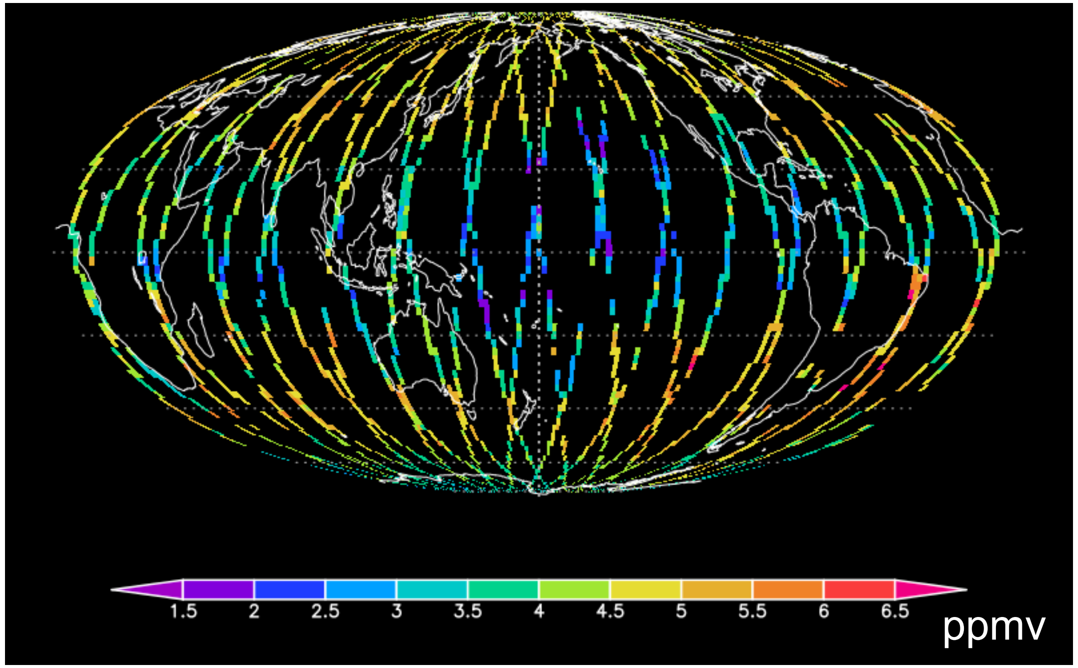


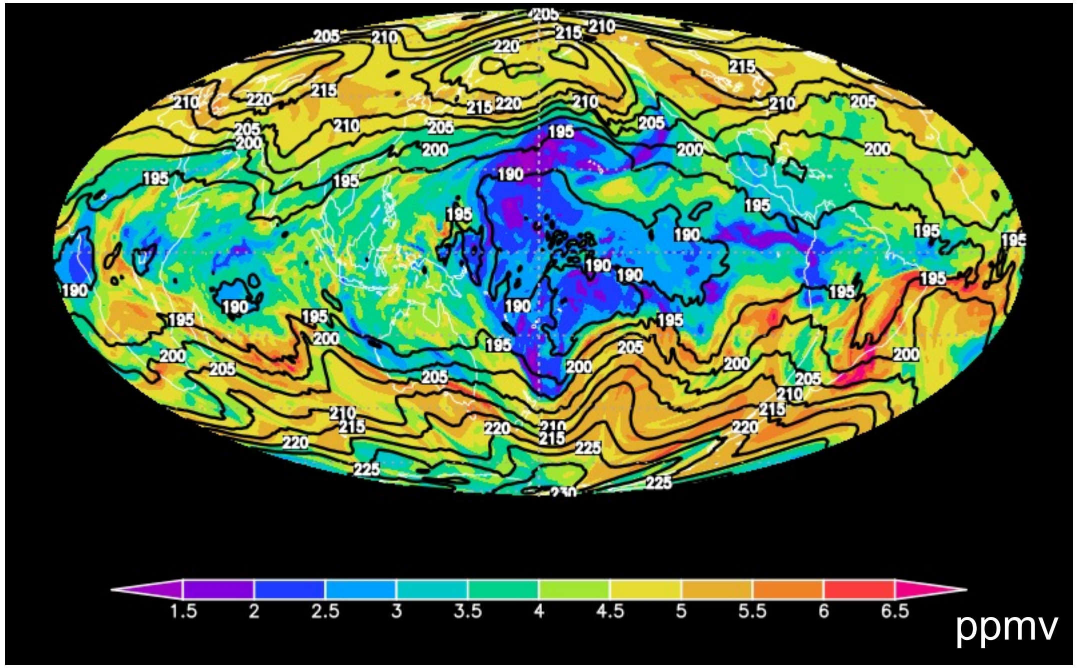


Constituent Data Assimilation

MLS water vapor at 100 hPa, 2 Jan 2016

Assimilated MLS water vapor and MERRA-2 temperature at 100 hPa, 2 Jan 2016

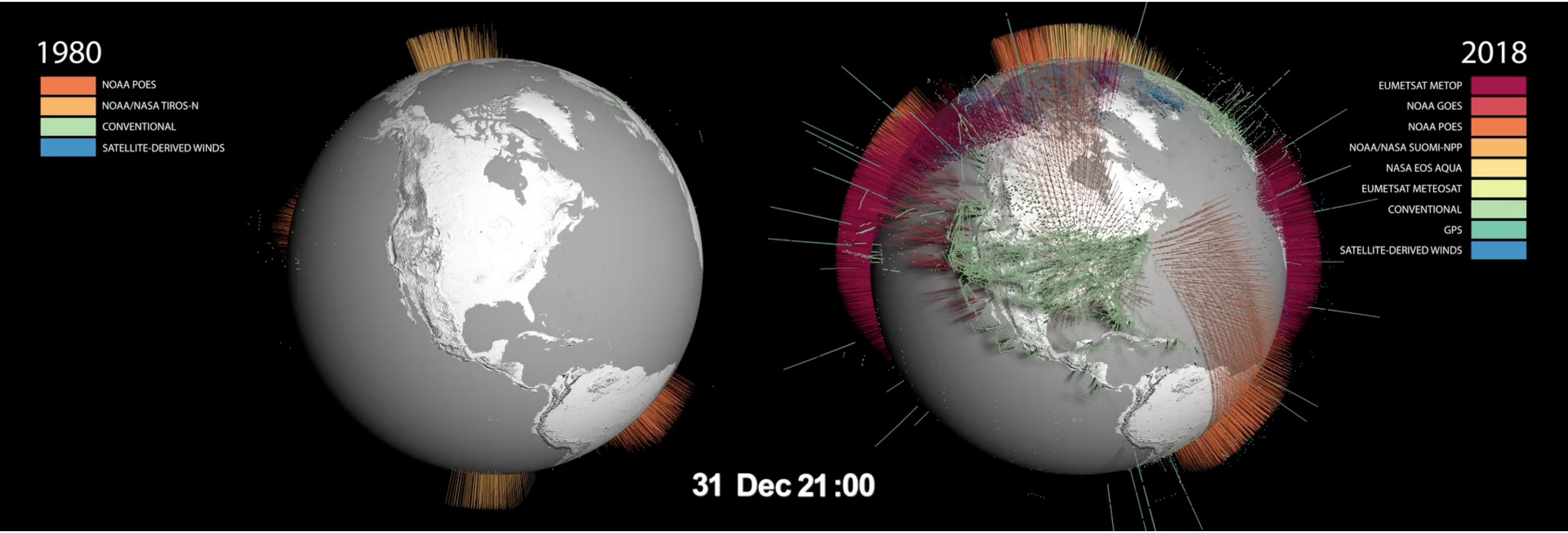




Data assimilation is a Bayesian method of combining and propagating information from observations in space and time using the governing equations and error estimates.

Figures courtesy of Kris Wargan

Changes to the observing system



https://svs.gsfc.nasa.gov/4654

NASA's MERRA-2 Reanalysis

- High resolution global data set
  - ➢ 50 km horizontal
    0.5º latitude x 0.625º longitude
  - ➢ 72 levels up to 0.01 hPa
- Available since 1980 to a few weeks behind present
- Product of GEOS data assimilation system
  - Assimilates meteorological observations, aerosols and ozone
  - **For the ozone observing system**
    - **1980-2004: SBUV**
    - **2004-present: Profiles from MLS, Total Column from OMI**
- **Ozone chemistry is simplified production and loss rates**

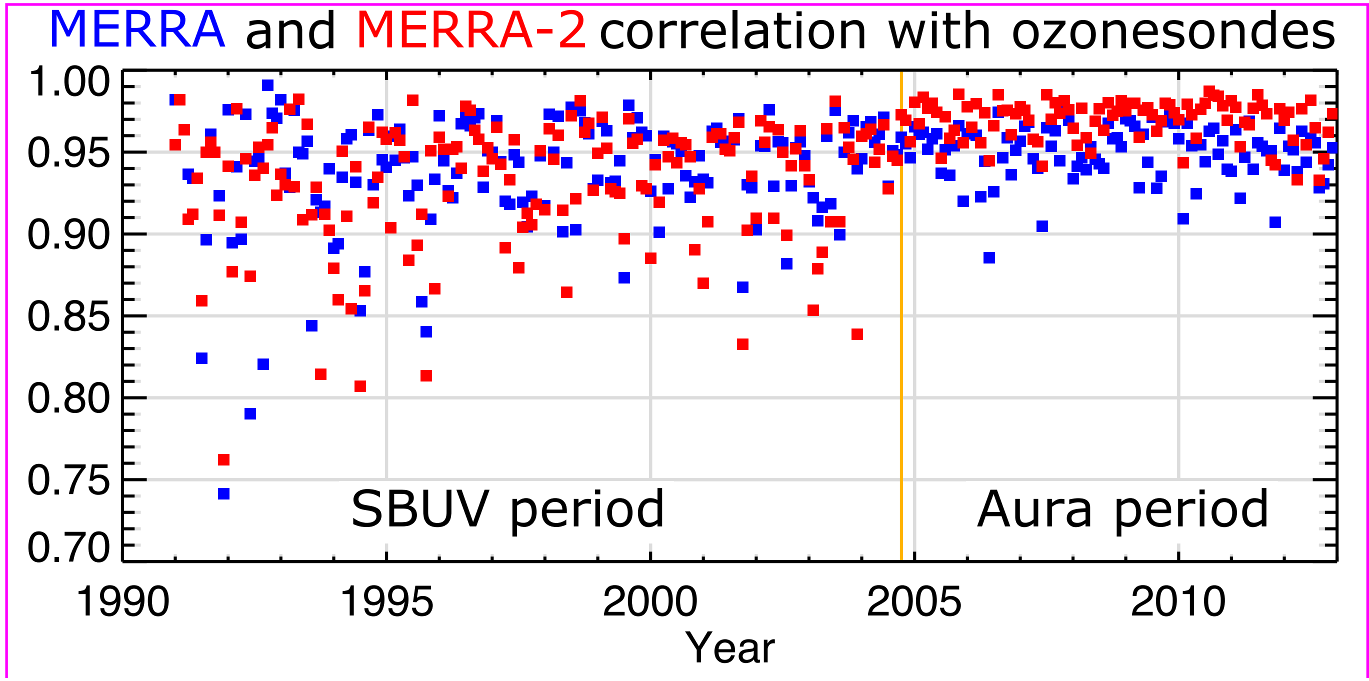
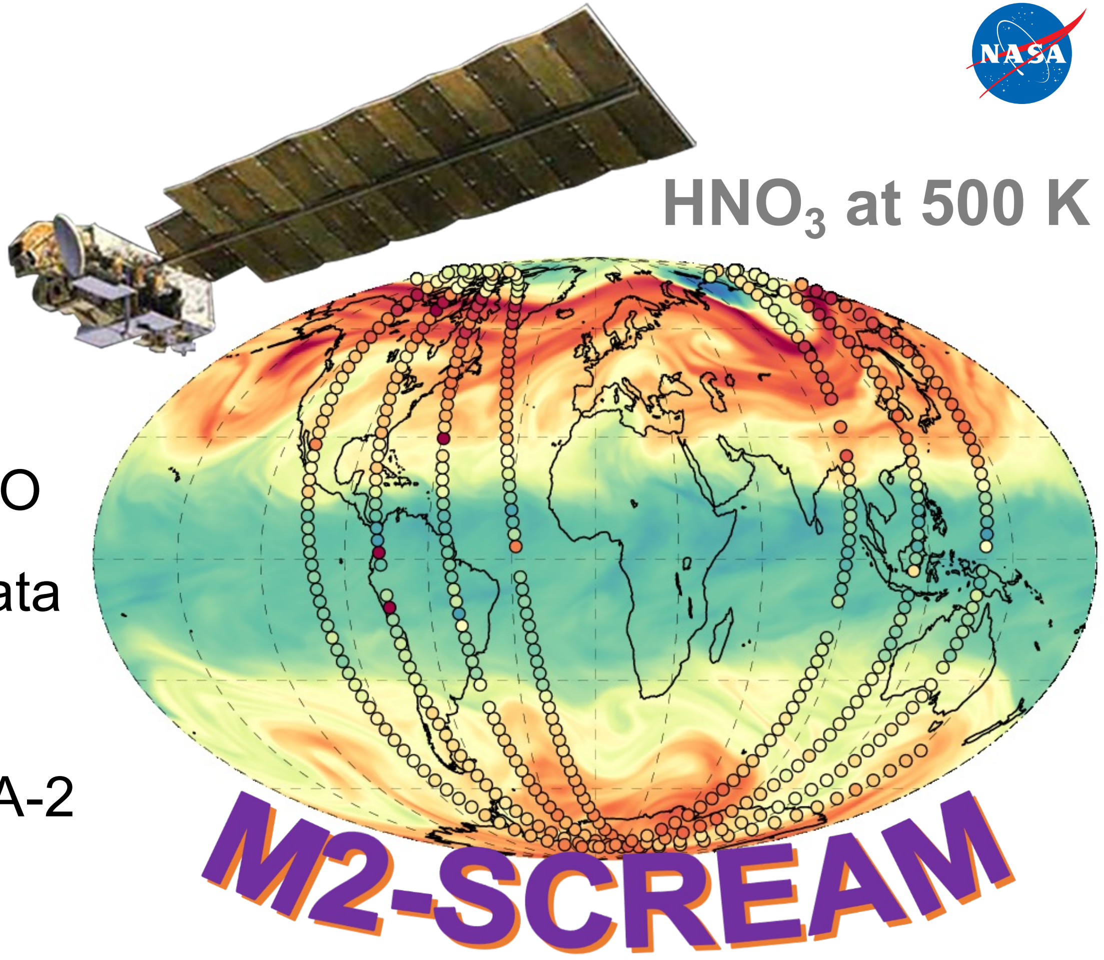


Figure from Wargan et al., 2017

MERRA-2 Stratospheric Composition Reanalysis with Aura MLS (M2-SCREAM)

Kris Wargan, Brad Weir, Gloria L. Manney, Stephen E. Cohn, Emma Knowland, Pamela Wales, Nathaniel J. Livesey and JPL colleagues

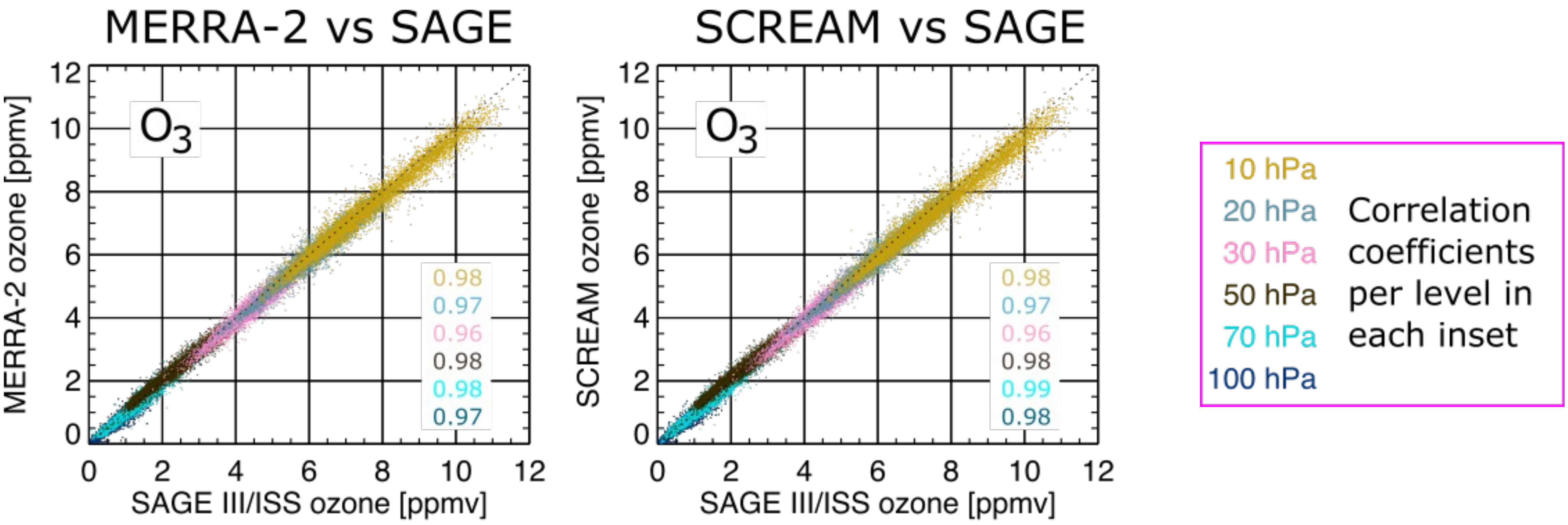


- Assimilating **MLS v4.2 ozone, H_2O**, HCl, HNO_3, & N_2O and OMI **total ozone** using the GEOS Constituent Data Assimilation System “CoDAS”
- Constrained by assimilated meteorology from MERRA-2
- GEOS “StratChem” stratospheric-only chemistry
- Period: September 2004 – August 2022+
  - ✓ Close agreement with ACE-FTS and GLORIA data and the BRAM2 reanalysis

Wargan et al (2022). M2-SCREAM: A Stratospheric Composition Reanalysis of Aura MLS data with MERRA-2 transport. *ESSOAr*, https://doi.org/10.1002/essoar.10512434.1
Coy et al. (2022). Stratospheric Circulation Changes Associated with the Hunga Tonga-Hunga Ha'apai Eruption. *ESSOAr*, https://doi.org/10.1002/essoar.10512388.1
Manney et al. (2022). Signatures of Anomalous Transport in the 2019/2020 Arctic Stratospheric Polar Vortex. *JGR*, https://doi.org/10.1029/2022JD037407
Wargan, K., et al (2020). The anomalous 2019 Antarctic ozone hole in the GEOS Constituent Data Assimilation System with MLS observations. *JGR*, https://doi.org/10.1029/2020JD033335

Motivation

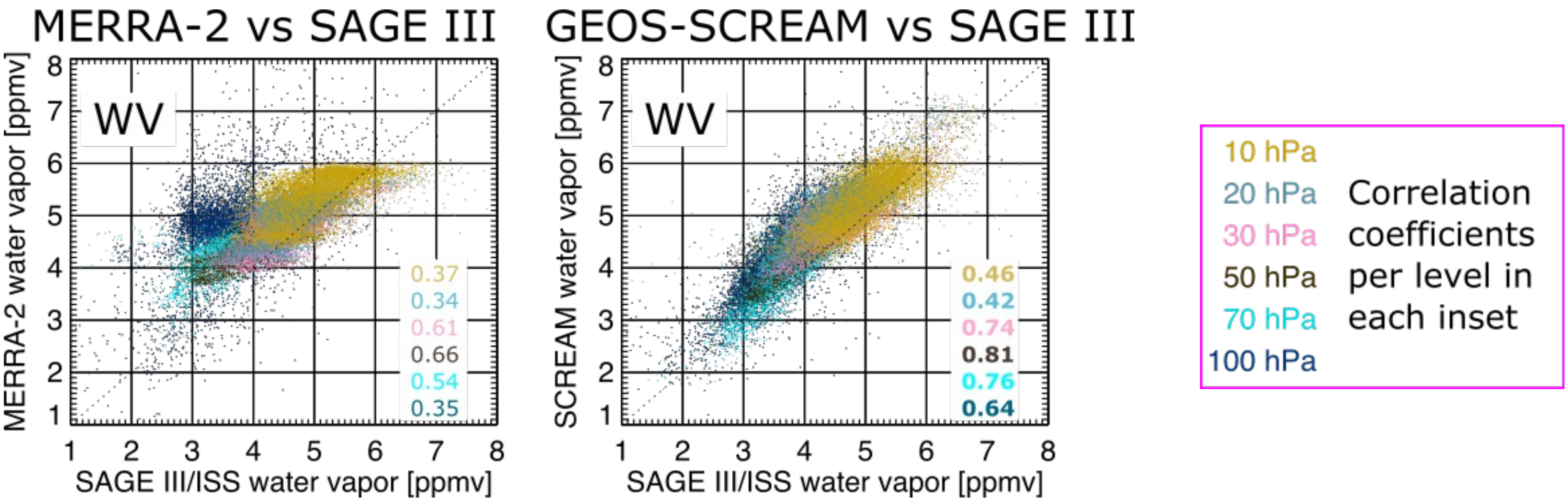
It is essential for trend and climate analysis to have consistent well-constrained data products such as reanalyses



1. Despite differences in the complexity of stratospheric ozone chemistry, the analyzed ozone in both reanalyses have near perfect correlation with co-located 2018 SAGE III/ISS ozone.

Motivation

It is essential for trend and climate analysis to have consistent well-constrained data products such as reanalyses



2. Reanalysis stratospheric water vapor ("WV") historically poor without an observational constraint (see Davis et al., 2020)

k.e.knowland@nasa.gov

Bridging the SAGE data gap

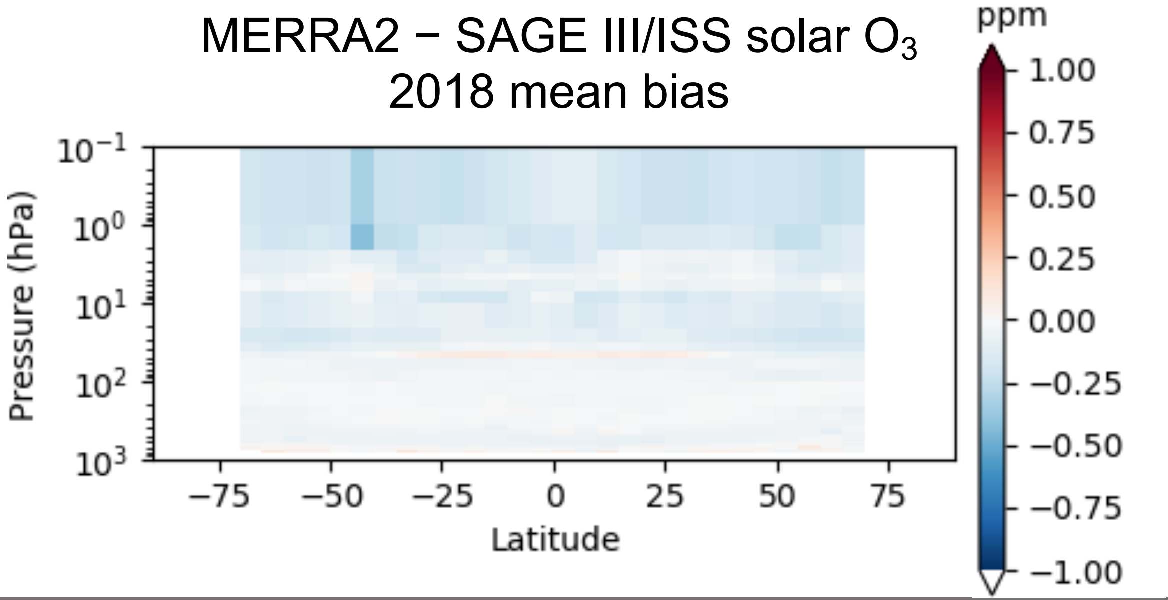
We will use NASA's uniformly-gridded, global GEOS model and DAS products to bridge the gap between the earlier SAGE missions and the SAGE III/ISS products.

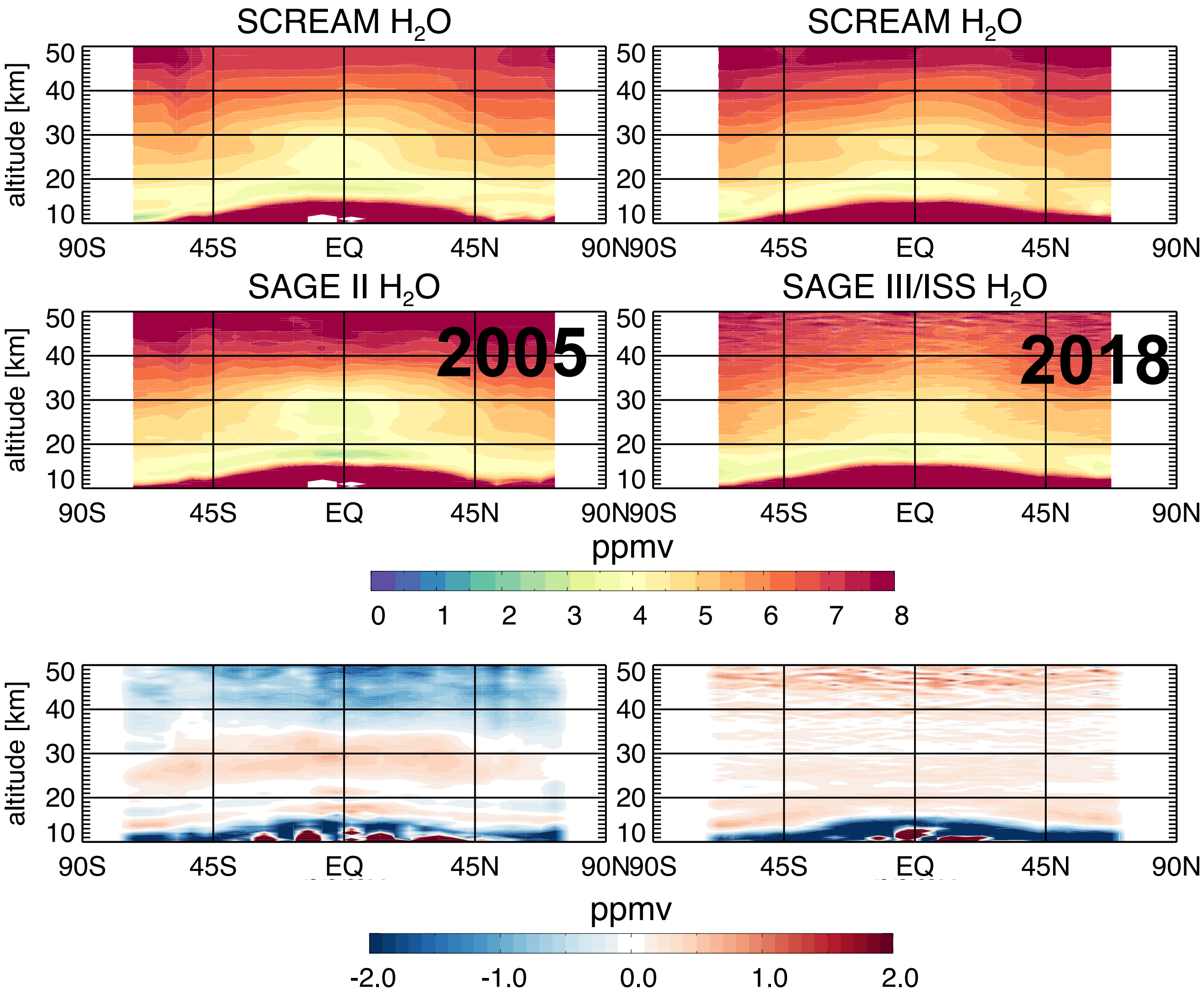
- A combination of GEOS model and DAS products constrained by satellite retrievals aboard NASA's Aura satellite, has great potential to characterize O_3 and water vapor (WV) distribution, trends, and variability from the SAGE II mission through SAGE III/ISS observations.
- The assimilation of SAGE WV and O_3 is now possible in the CoDAS framework to carry-on the trend and climate assessments after the Aura mission.

k.e.knowland@nasa.gov

Scientific Objectives

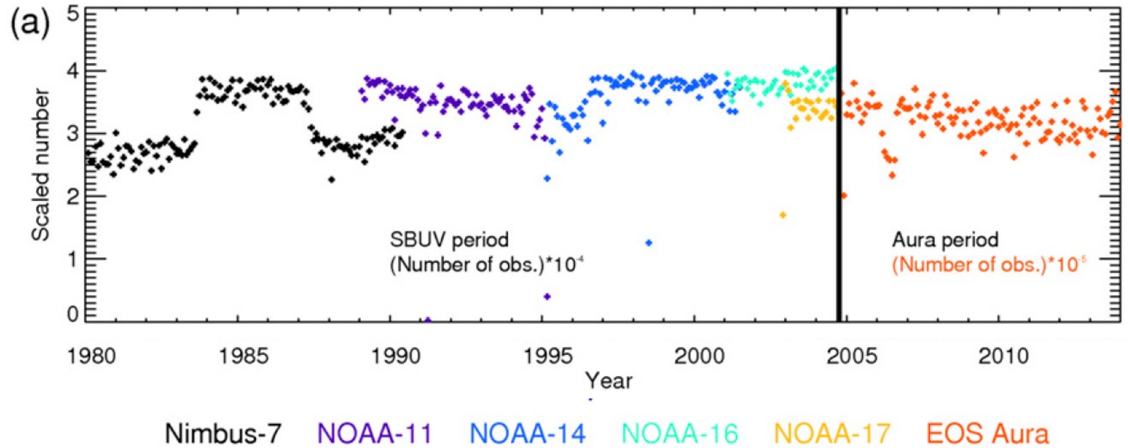
1. Statistical trend analysis of O_3 and WV profiles
   - We will conduct a statistical analysis of SAGE III and SAGE II observational data sets with the corresponding analyzed O_3 and WV from MERRA-2 and M2-SCREAM.





Statistical trend analysis of O_3

- Changes in assimilation observing system introduce discontinuities into MERRA-2 O_3 trends

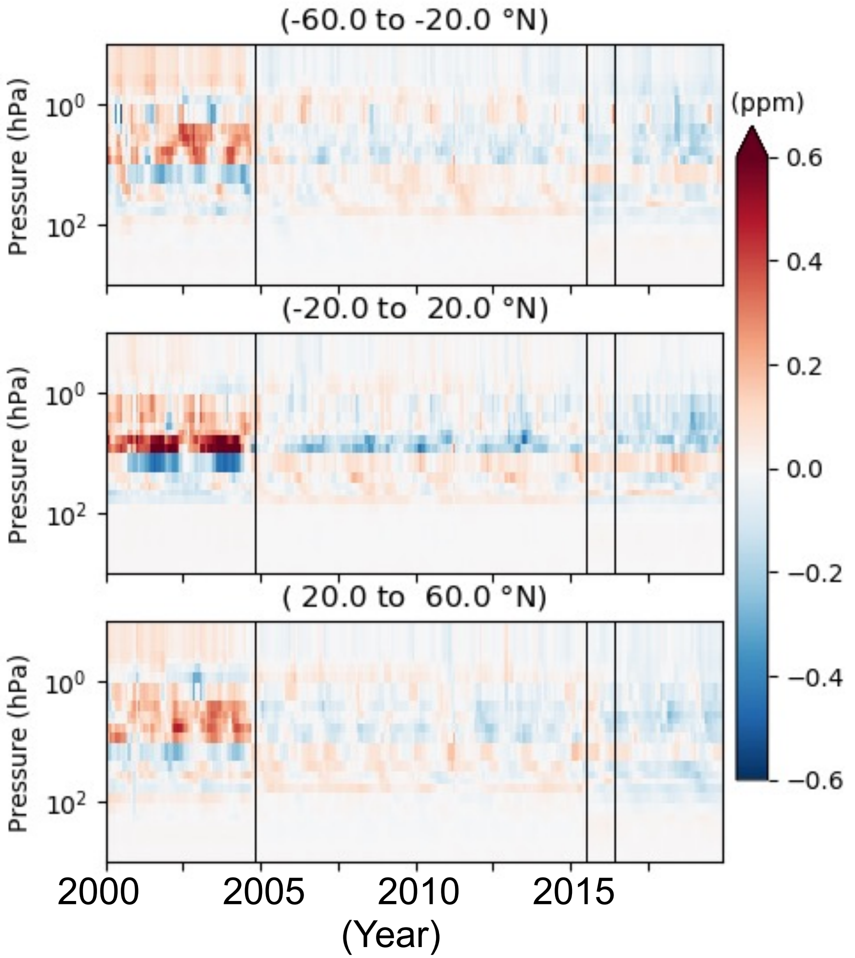


The monthly averaged number of total ozone observations per day from SBUV and OMI instruments assimilated in MERRA-2 as a function of time.

Colors denote different instruments indicated in the legend

Figure 1 from Wargan et al., 2017, J. Clim.

MERRA2 − M2GMI O_3 anomalies



- "MERRA2-GMI" (a.k.a. M2GMI) is a GMI chemistry simulation constrained by MERRA-2 meteorology

https://acd-ext.gsfc.nasa.gov/Projects/GEOSCCM/MERRA2GMI/

Statistical trend analysis of O_3

- Similar to Wargan et al., 2018, we plan to use M2GMI simulations as a transfer function for MERRA-2 O_3 discontinuities within the Aura period: 2004, 2015 and 2016

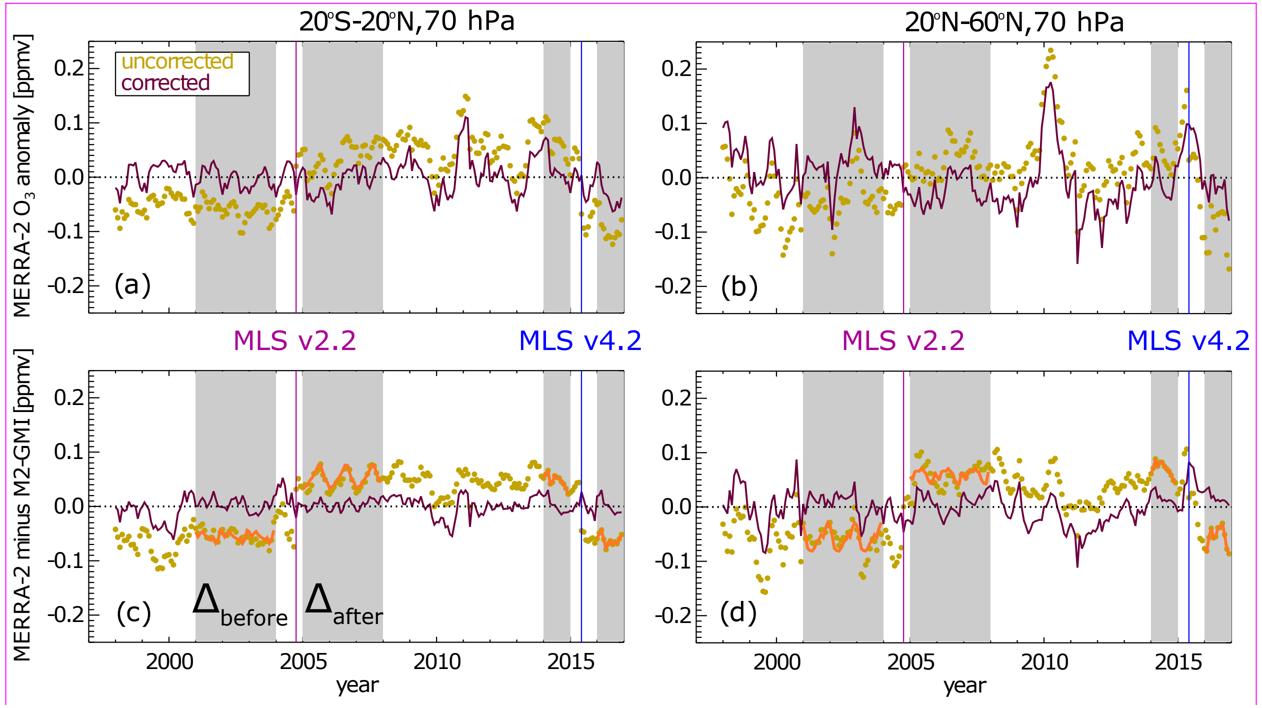
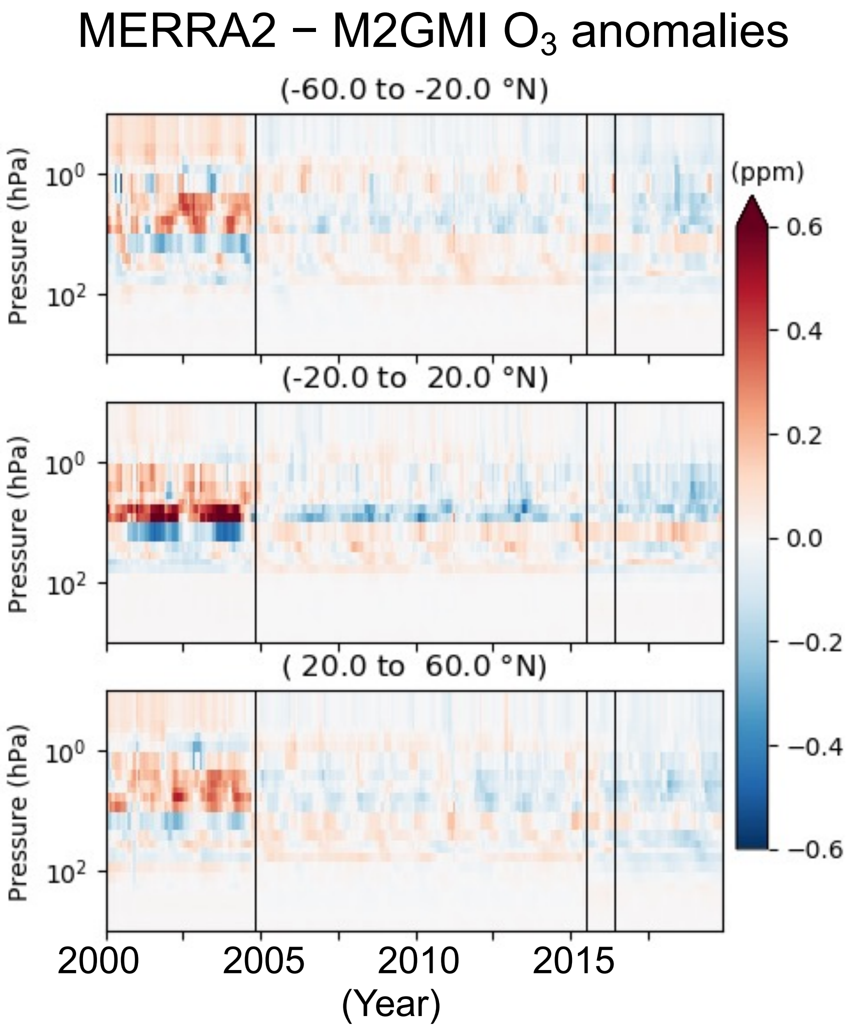


Figure adapted from Wargan et al., 2018



- "MERRA2-GMI" (a.k.a. M2GMI) is a GMI chemistry simulation constrained by MERRA-2 meteorology

https://acd-ext.gsfc.nasa.gov/Projects/GEOSCCM/MERRA2GMI/

Statistical trend analysis of O_3

- Similar to Wargan et al., 2018, we plan to use M2GMI simulations as a transfer function for MERRA-2 O_3 discontinuities within the Aura period: 2004, 2015 and 2016

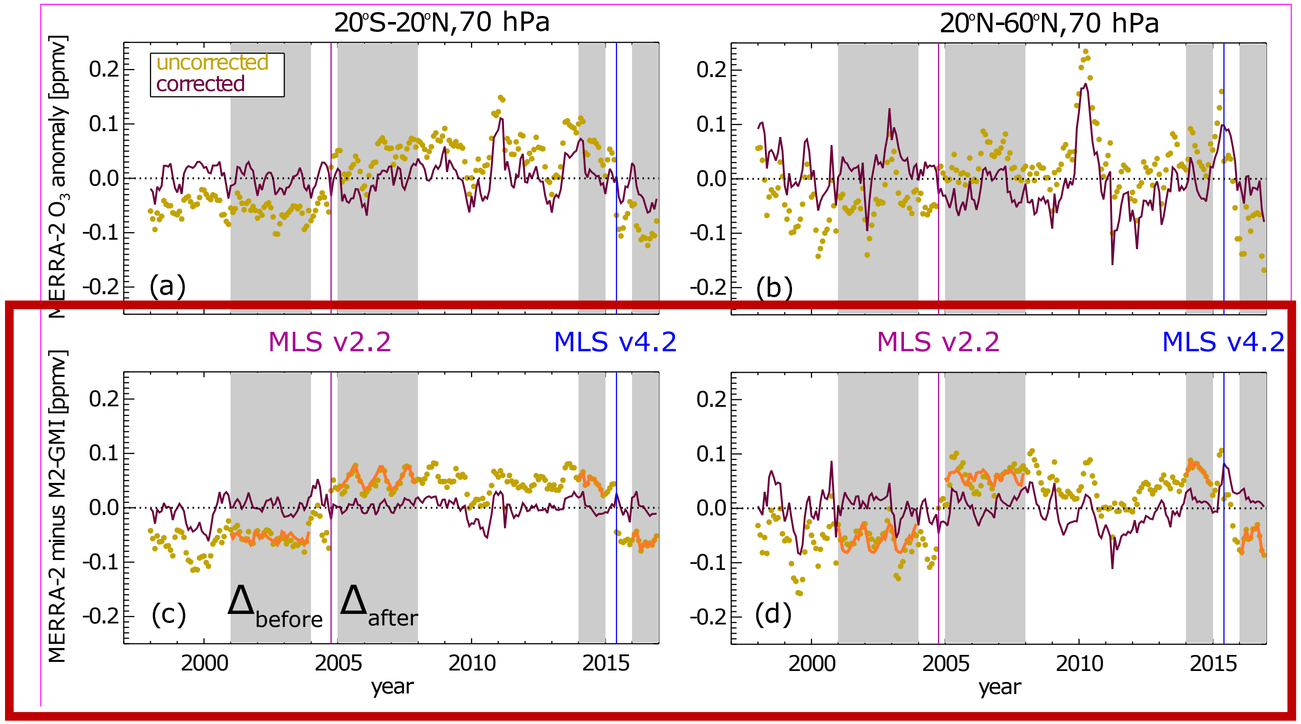
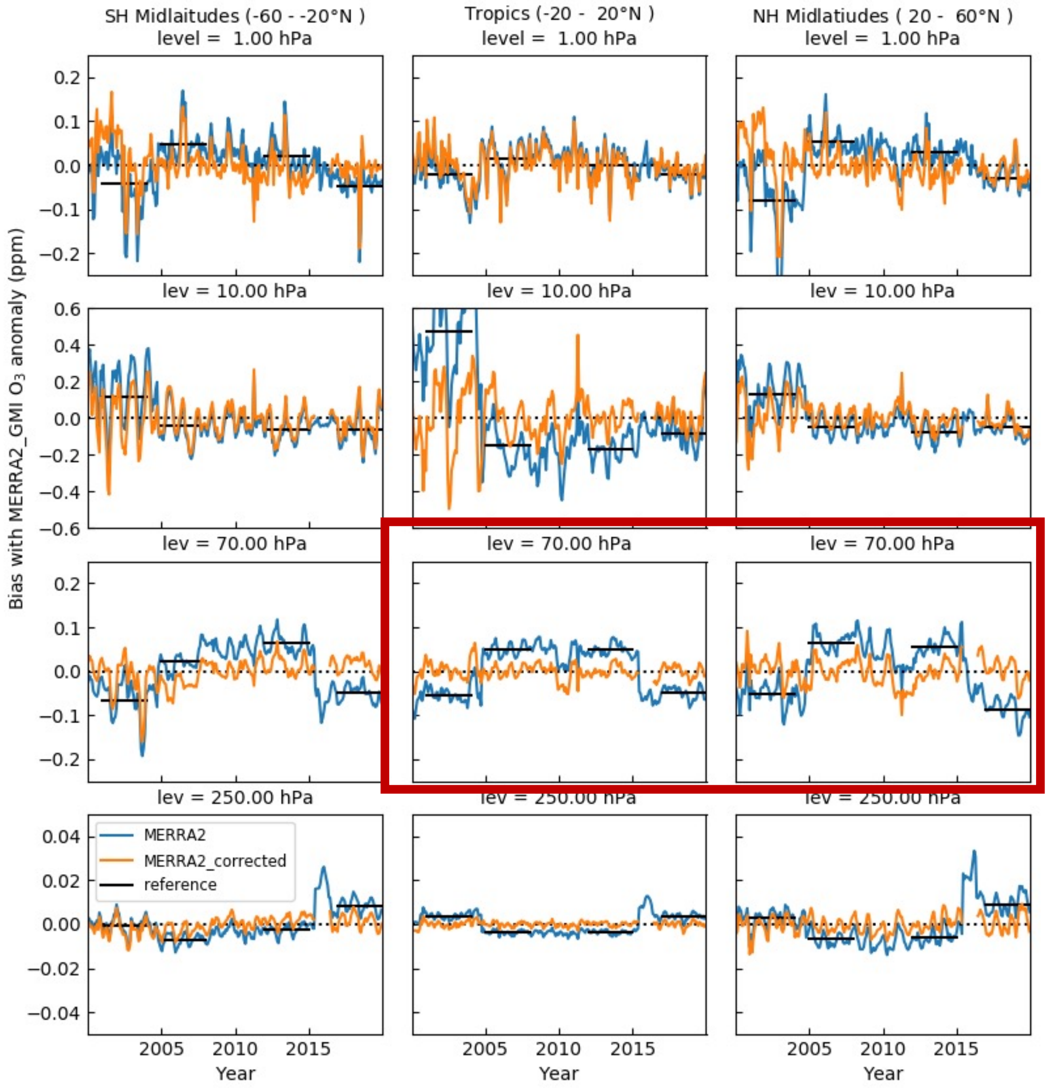
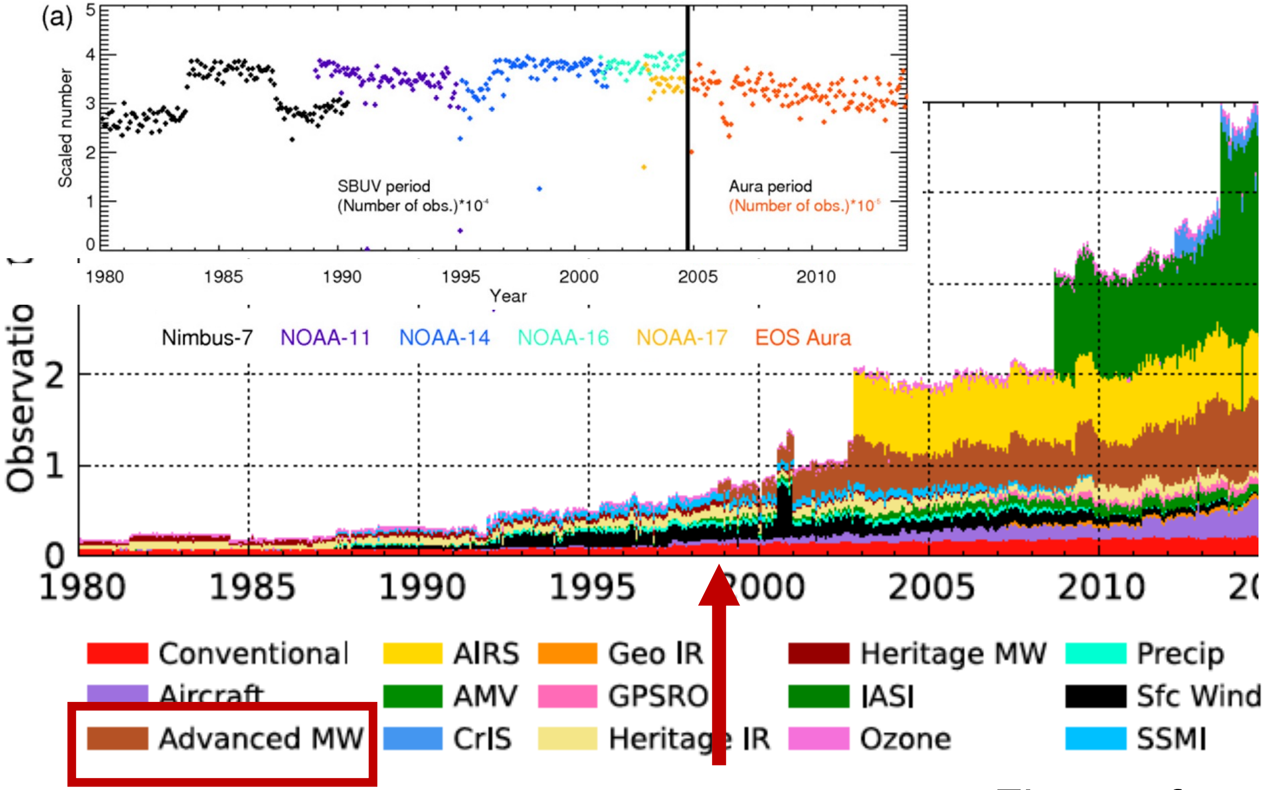


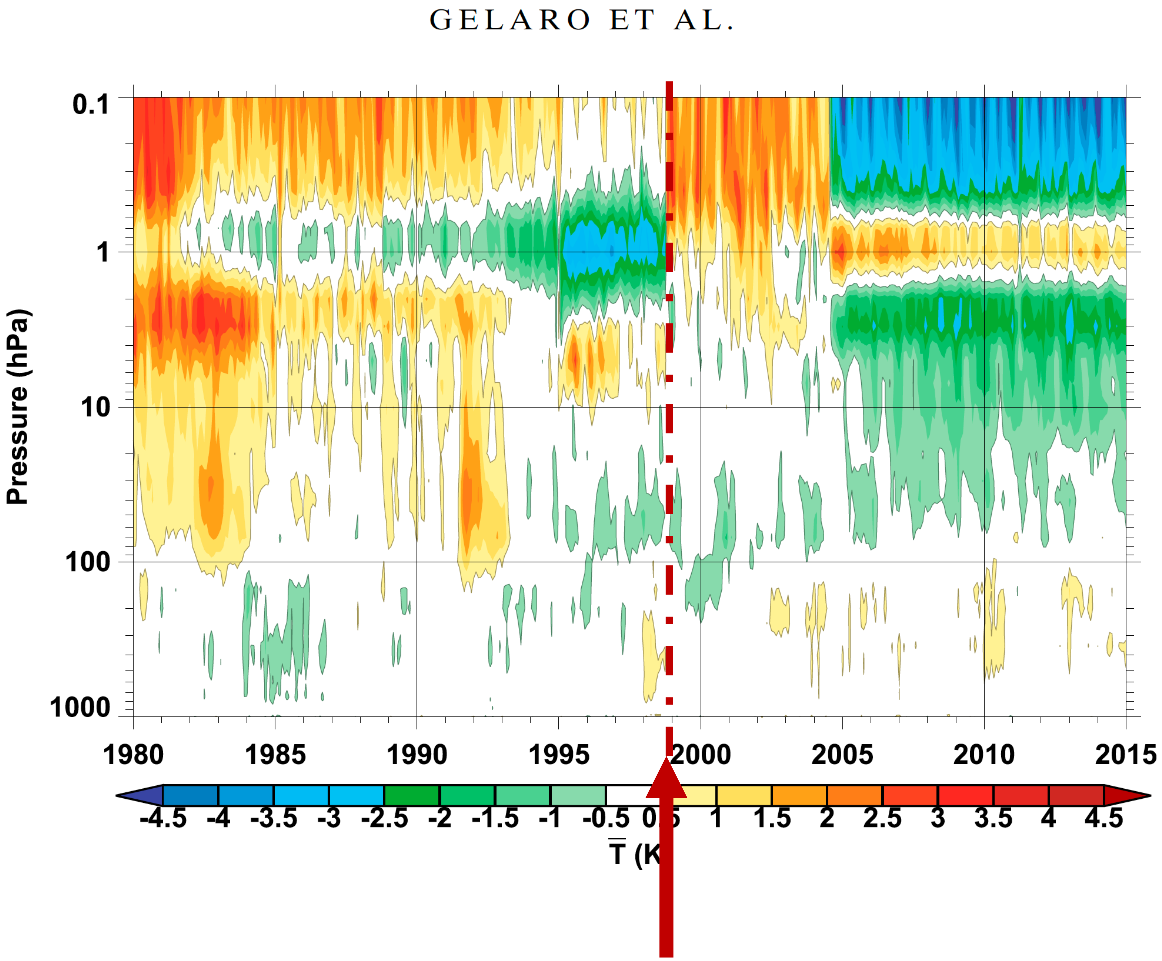
Figure adapted from Wargan et al., 2018



Statistical trend analysis of O_3
Next steps: pre-2000

- Changes in assimilation observing system introduce discontinuities into MERRA-2 O_3 trends





Figures from Gelaro et al., 2017

Scientific Objectives

3. Chemical data assimilation of O3 and WV profiles
    - SAGE data is likely suitable for assimilation into GEOS using the CoDAS framework.
    - Results will be evaluated against independent observations including other satellite retrievals, sonde and lidar measurements

k.e.knowland@nasa.gov

GEOS CoDAS Experiments

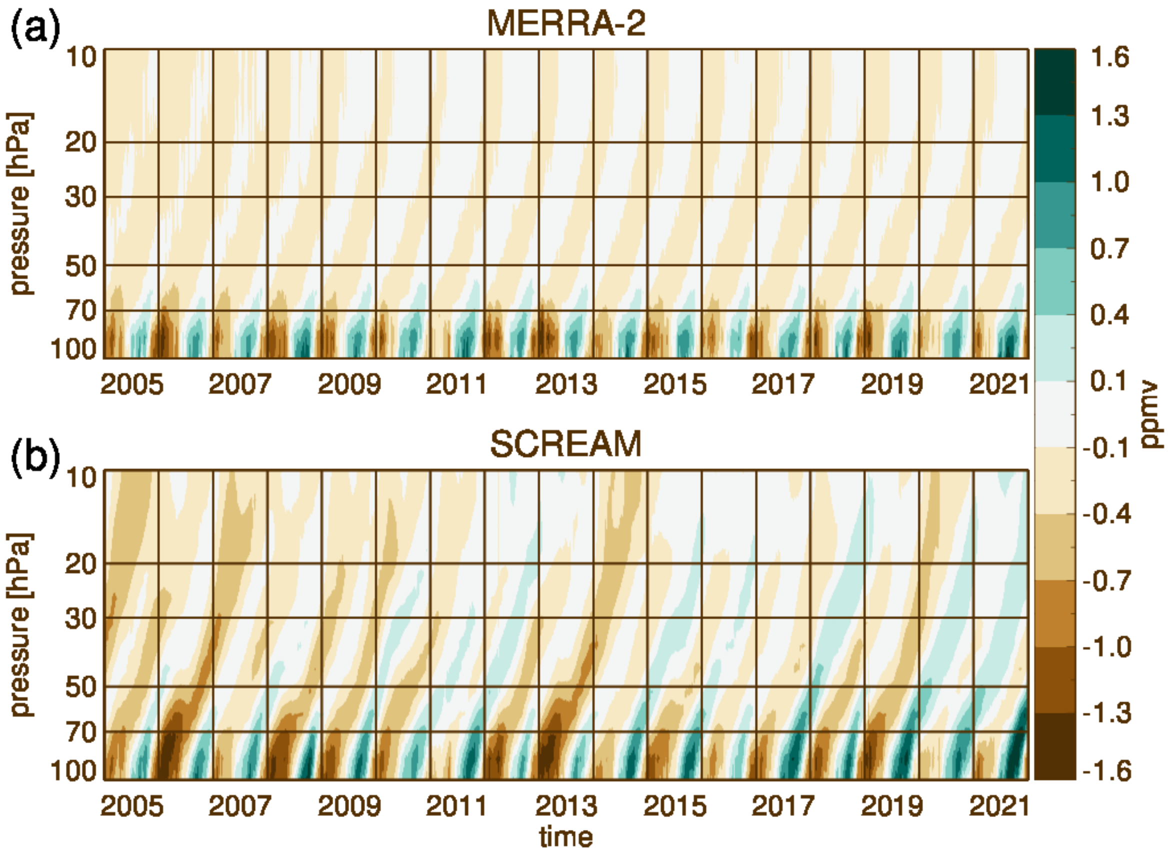
Same set up as M2-SCREAM

- ❑ Constrained by assimilated meteorology from MERRA-2
- ❑ GEOS "StratChem" stratospheric-only chemistry
- ❑ Period: July 2017 – August 2022+

Four experiments identified in the proposal:

1. SAGE + AURA: SAGE O3 and WV and MLS v5 profiles and OMI TCO
2. SAGE post-Aura: SAGE O3 and WV with alternative limb-sounding profiles and total ozone (e.g., OMPS)
3. SAGE-only post-Aura: SAGE O3 and WV
4. Control: Chemistry only with no CoDAS

Tropical "Tape Recorder"



15°S-15°N average water vapor anomalies (Figure 1, Wargan et al., 2022 ESSOAr)

GEOS CoDAS Experiments

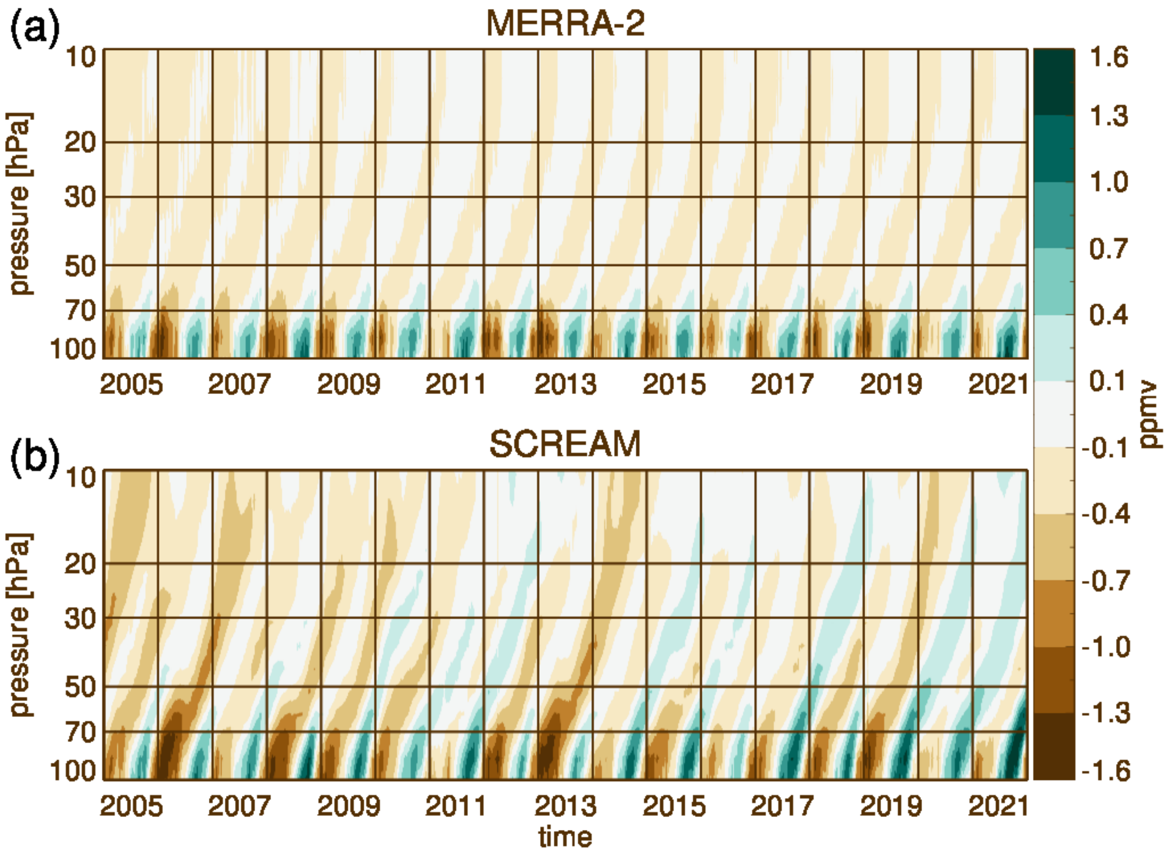
Same set up as M2-SCREAM

- ❑ Constrained by assimilated meteorology from MERRA-2
- ❑ GEOS "StratChem" stratospheric-only chemistry
- ❑ Period: July 2017 – August 2022+

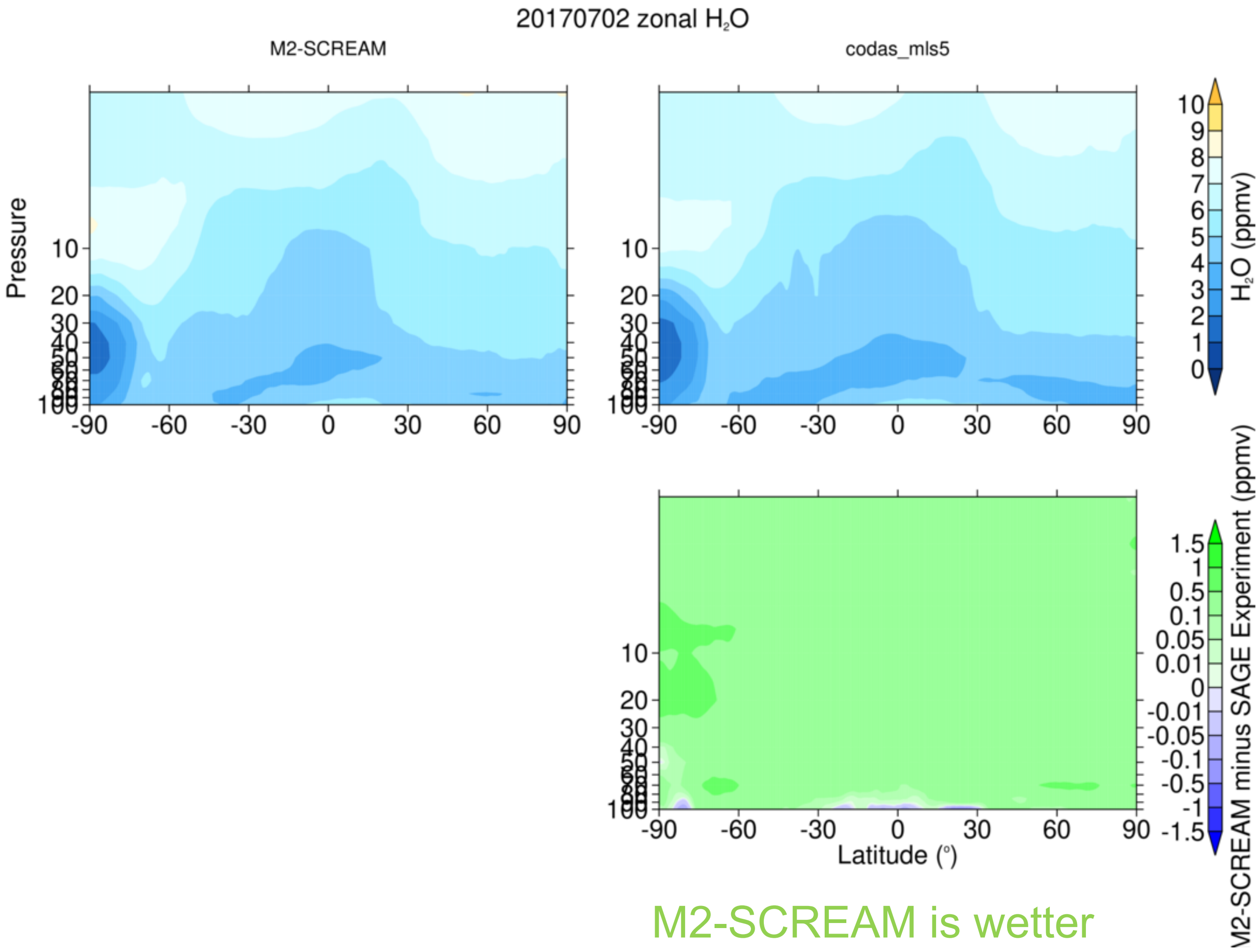
Experiments running:

3. **SAGE-only post-Aura: SAGE WV**
    1. "codas_sage3h2o". Initialized July 1, 2017
4. **Control: Chemistry only with no CoDAS**
    1. "replay_stratchem_201602-201803". Initialized Feb 1, 2016
    2. "replay_stratchem_201707". Initialized July 1, 2017
5. **Aura: MLS v5 profiles and OMI TCO**
    1. "codas_mls5". Initialized July 1, 2017

Tropical "Tape Recorder"



15°S-15°N average water vapor anomalies (Figure 1, Wargan et al., 2022 ESSOAr)



M2-SCREAM is wetter
SAGE Experiment is wetter

GEOS CoDAS experiments

5. Aura: MLS v5 profiles (O3 and WV) and OMI TCO

Assimilating MLS v5 water vapor results in uniformly decreased concentrations in stratosphere (100 to 1 hPa) compared to M2-SCREAM.

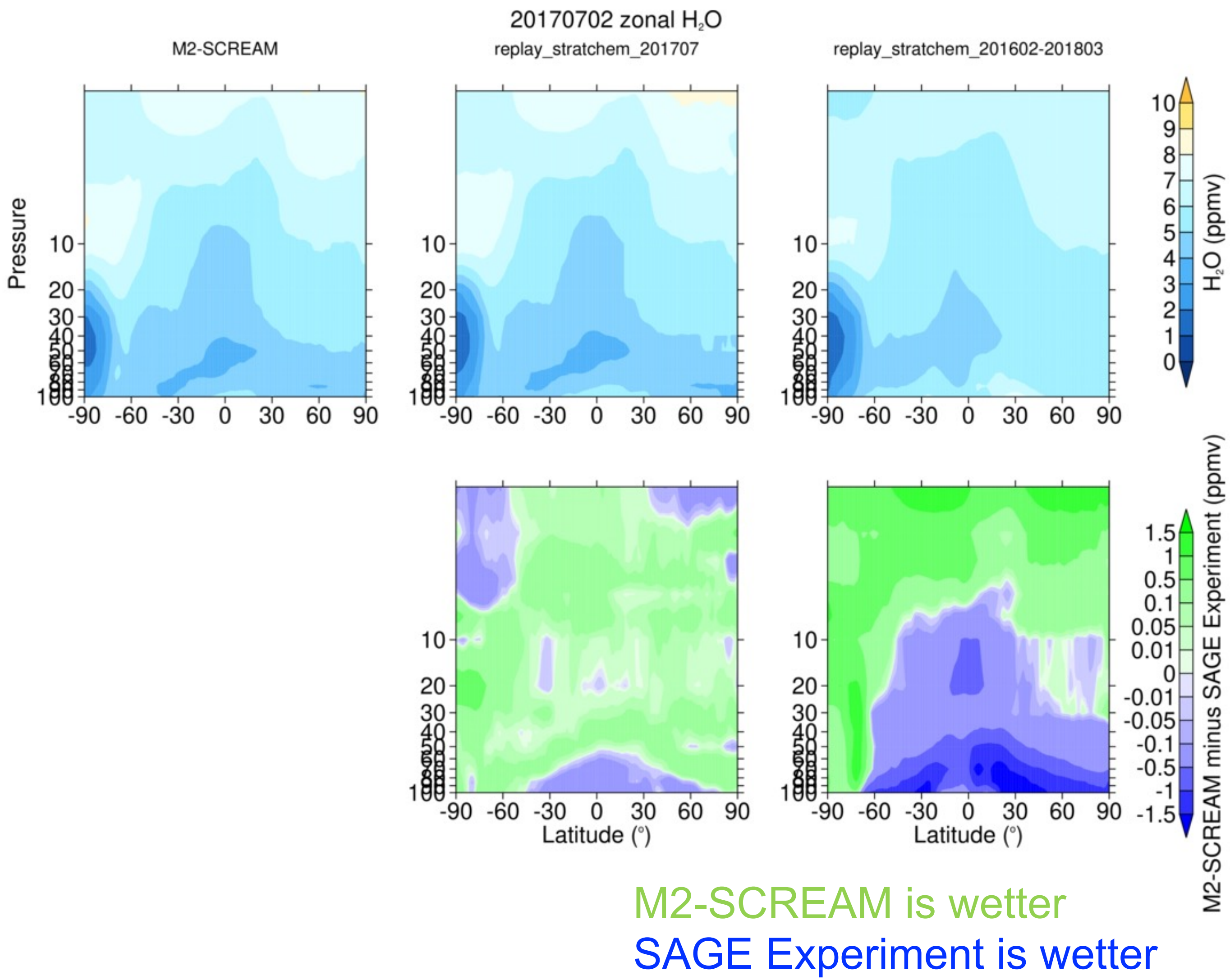
This is expected as v5 corrects for the bias during the entire record, see Livesey et al., 2021, ACP https://doi.org/10.5194/acp-21-15409-2021.

k.e.knowland@nasa.gov

GEOS CoDAS experiments

4. Control: Chemistry only with no CoDAS

Without chemical data constraints, the chemistry-only control run exhibits greater concentrations of water vapor than in M2-SCREAM, especially in the lower stratosphere, and the bias continues to increase over time.

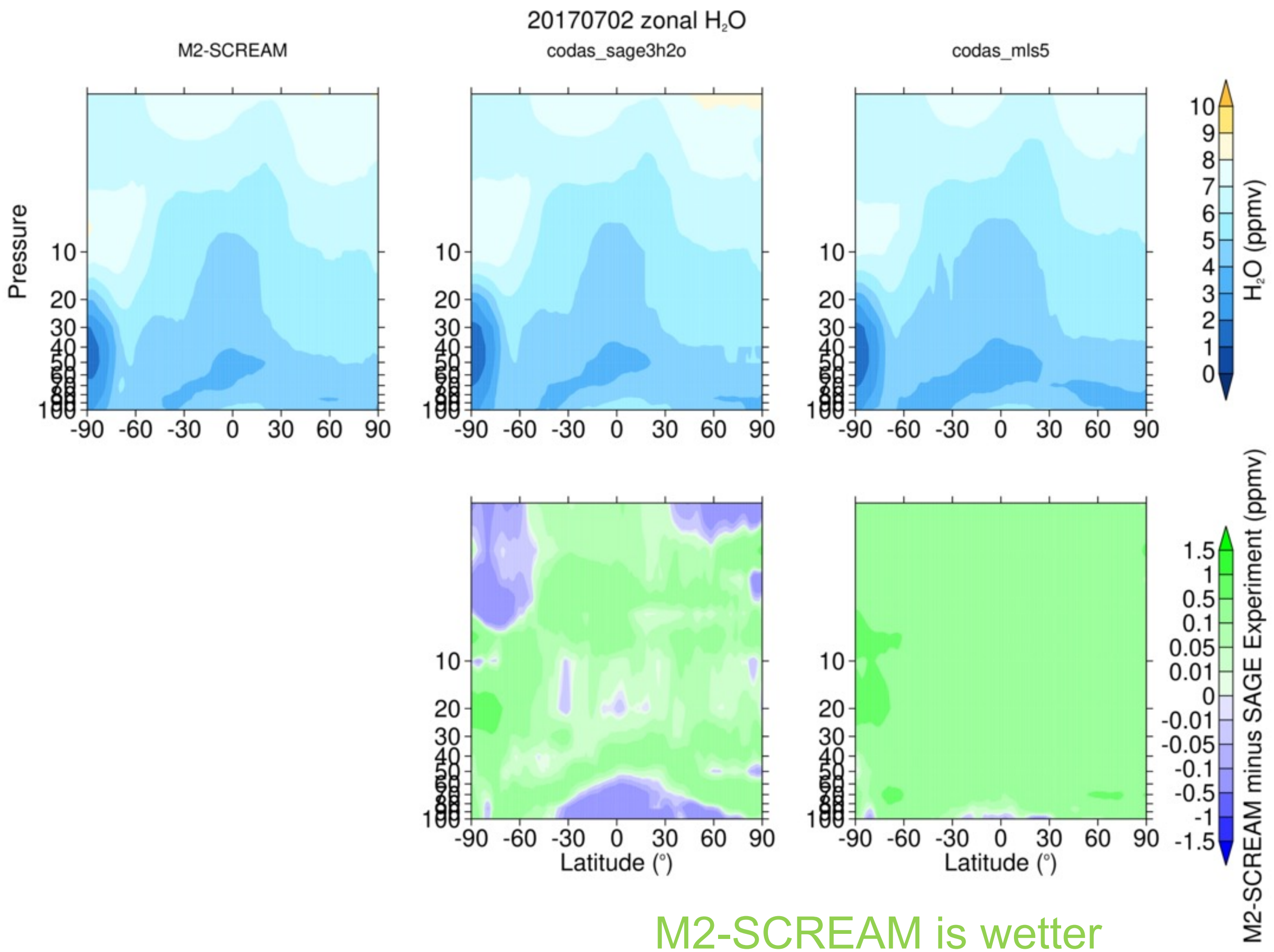


"replay_stratchem_201707"
Initialized July 1, 2017

"replay_stratchem_201602-201803"
Initialized Feb 1, 2016

GEOS CoDAS experiments

3. SAGE-only post-Aura: SAGE WV



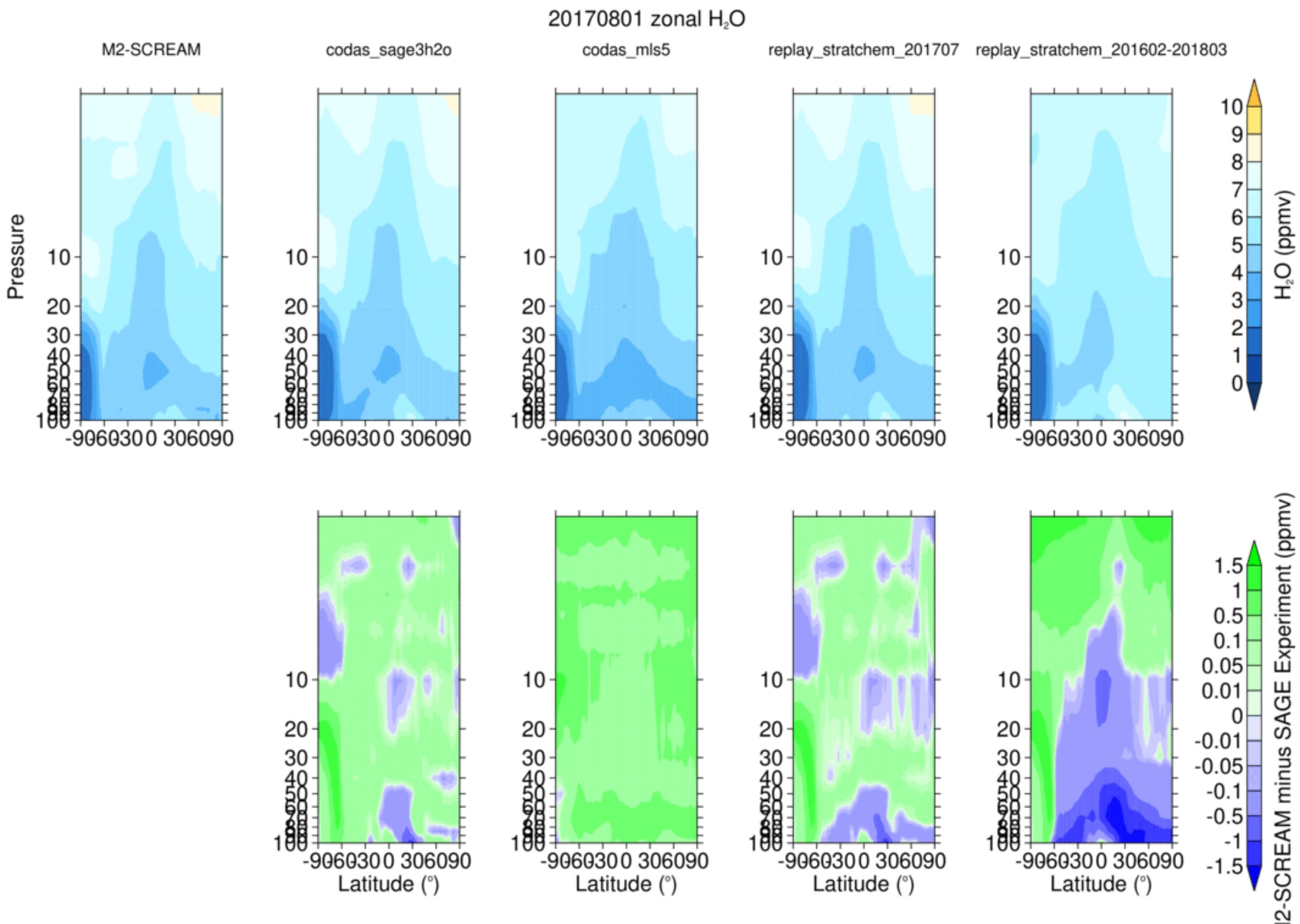
M2-SCREAM is wetter

SAGE Experiment is wetter

Assimilating SAGE III/ISS water vapor profiles at first looks to make very little impact.

k.e.knowland@nasa.gov

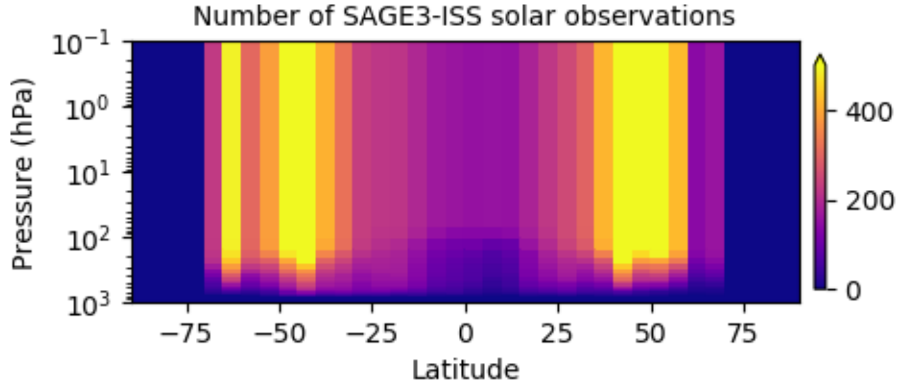
Snapshot First day of each month August 2017 to Feb 2018



M2-SCREAM is wetter SAGE Experiment is wetter

But after a few weeks, **assimilating only SAGE III/ISS water vapor profiles results in water vapor fields more consistent with experiments that assimilated MLS v5 than chemistry-only controls.**

However, in polar regions where SAGE III/ISS observations are not available, the simulated values are determined by the chemistry mechanism only.

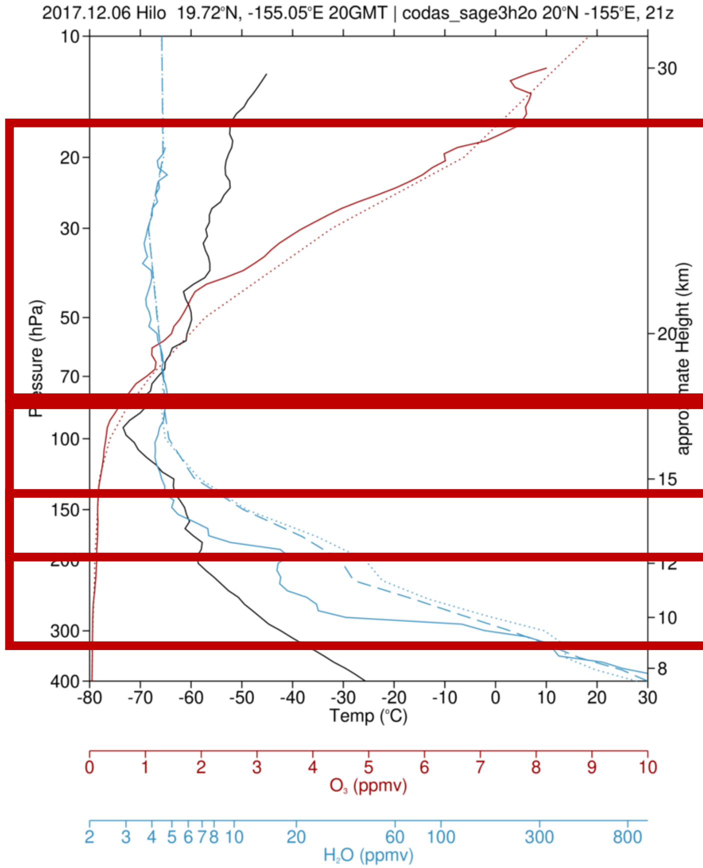


This is a very encouraging result. **There is a clear benefit to assimilating the less frequent SAGE III/ISS observations.**

k.e.knowland@nasa.gov

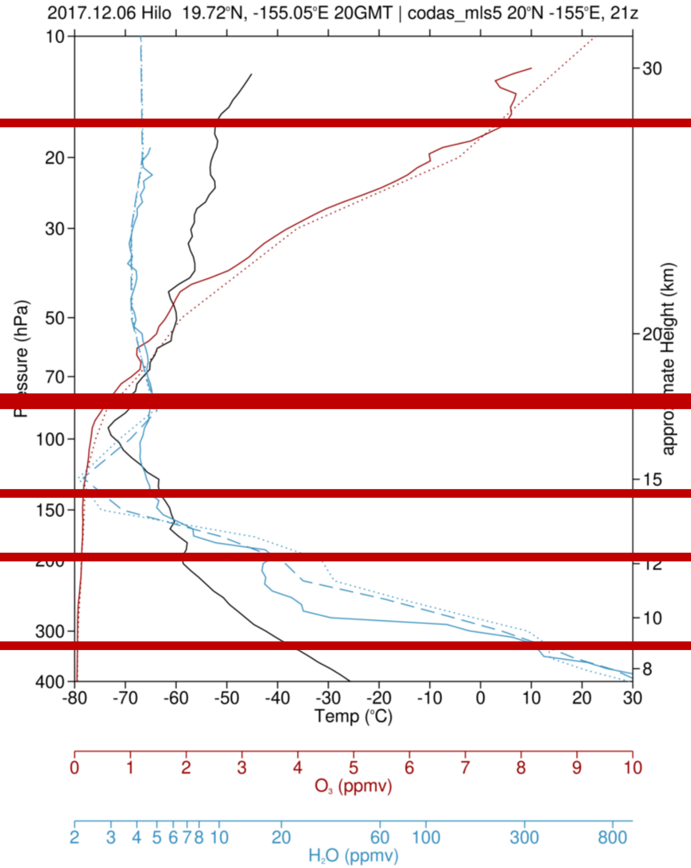
Comparisons against independent observations
Example: FPH at Hilo, December 6, 2017

CoDAS SAGE III



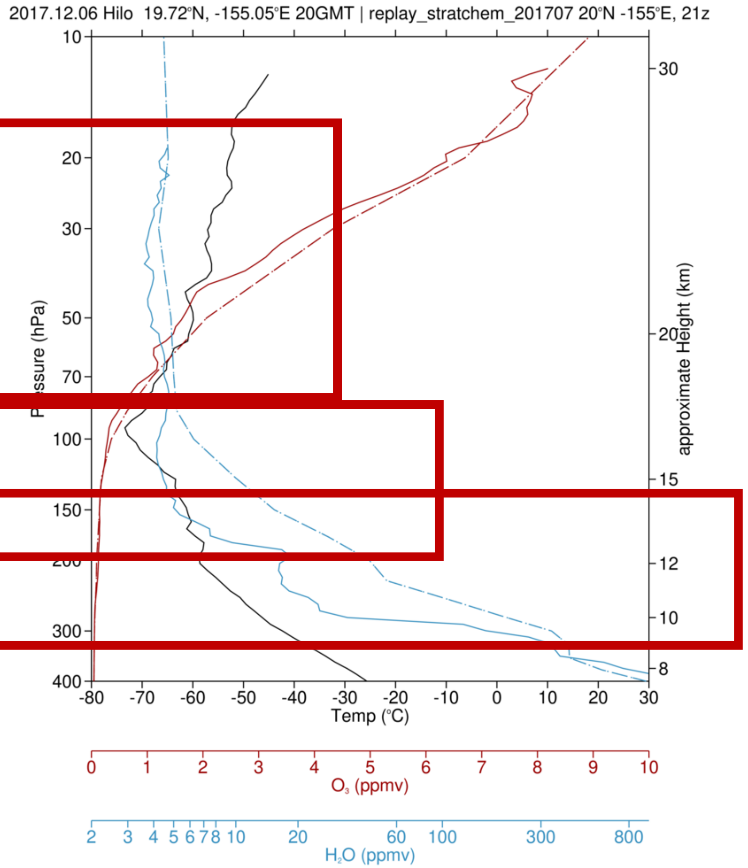
Dotted: Forecast
Dashed: Analysis

CoDAS MLS



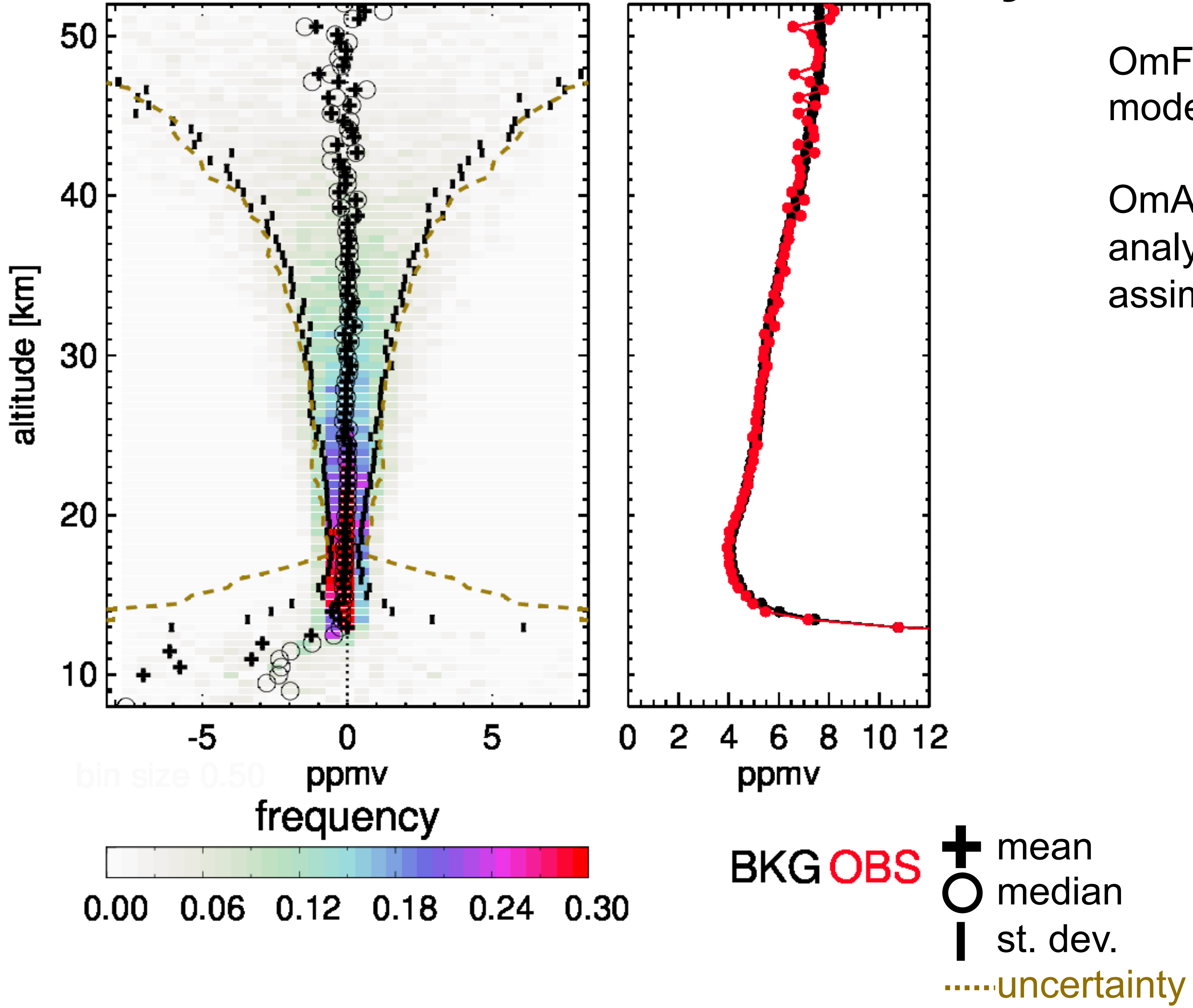
Dotted: Forecast
Dashed: Analysis

Control



Dash-dot: Chemistry only

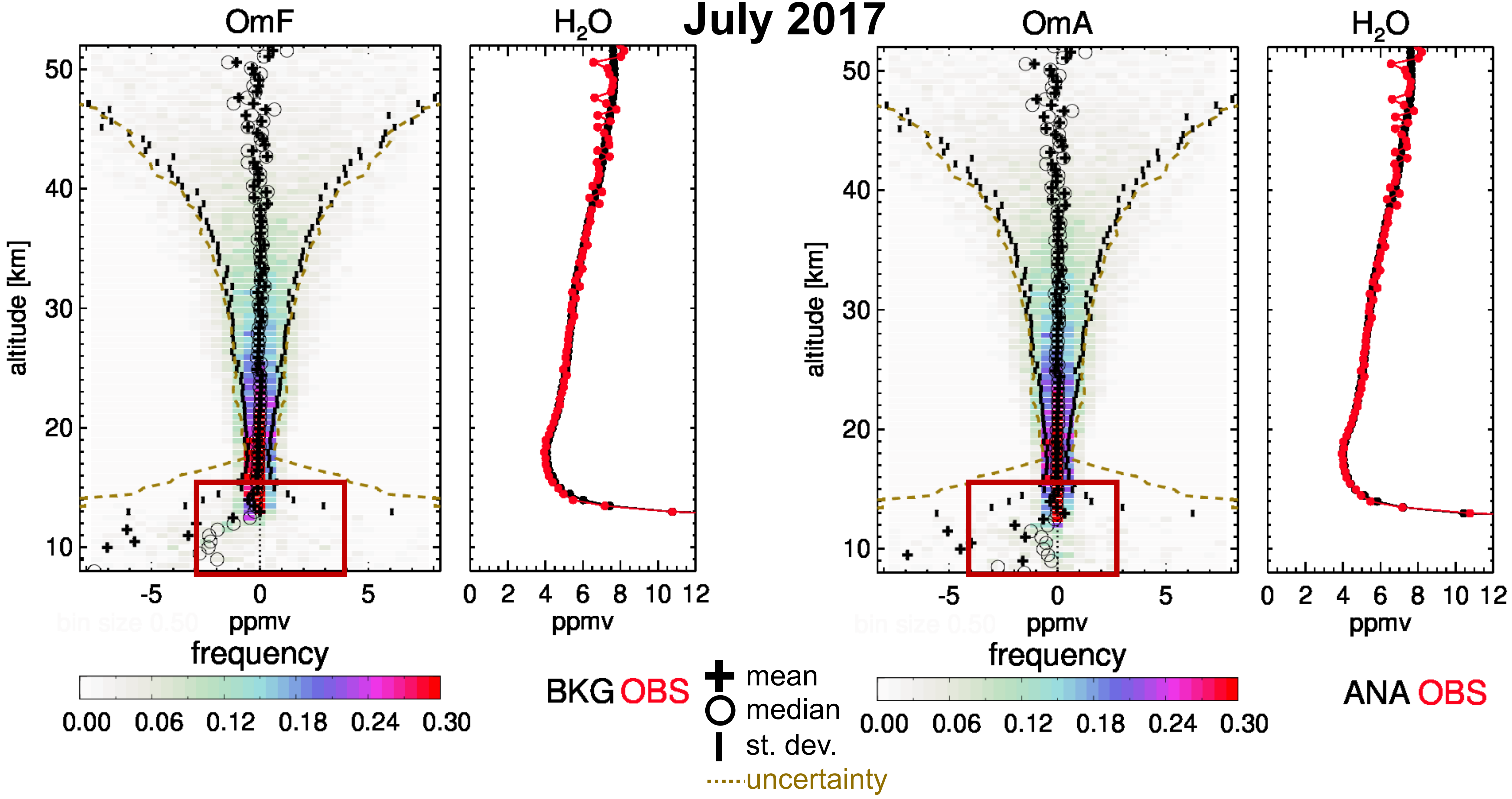
July 2017 CoDAS with SAGE III/ISS



OmF: "O minus F" => Observation minus the model forecast or background "BKG" state

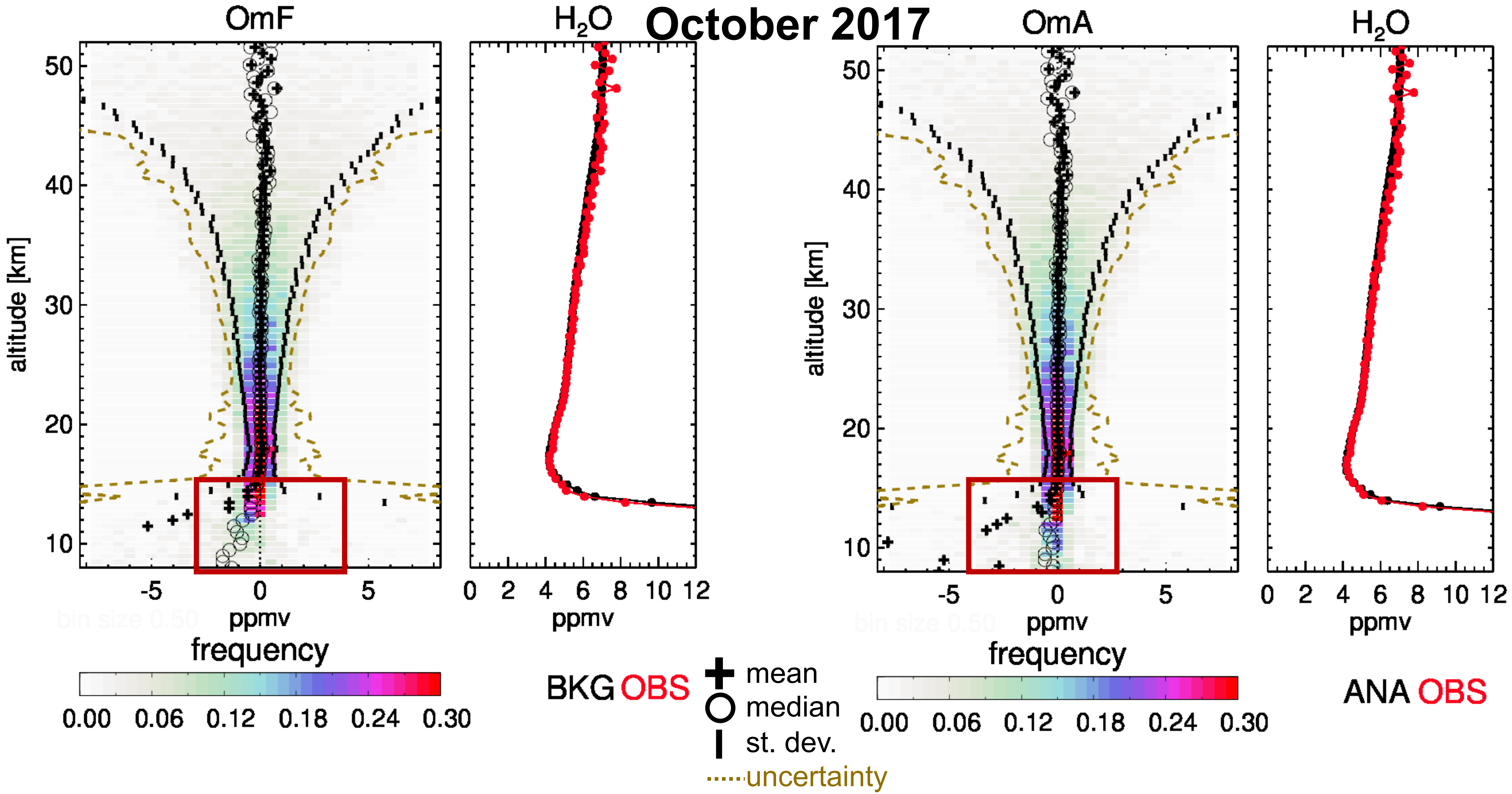
OmA: "O minus A" => Observation minus the analysis, after the observations have been assimilated with the model forecast.

July 2017

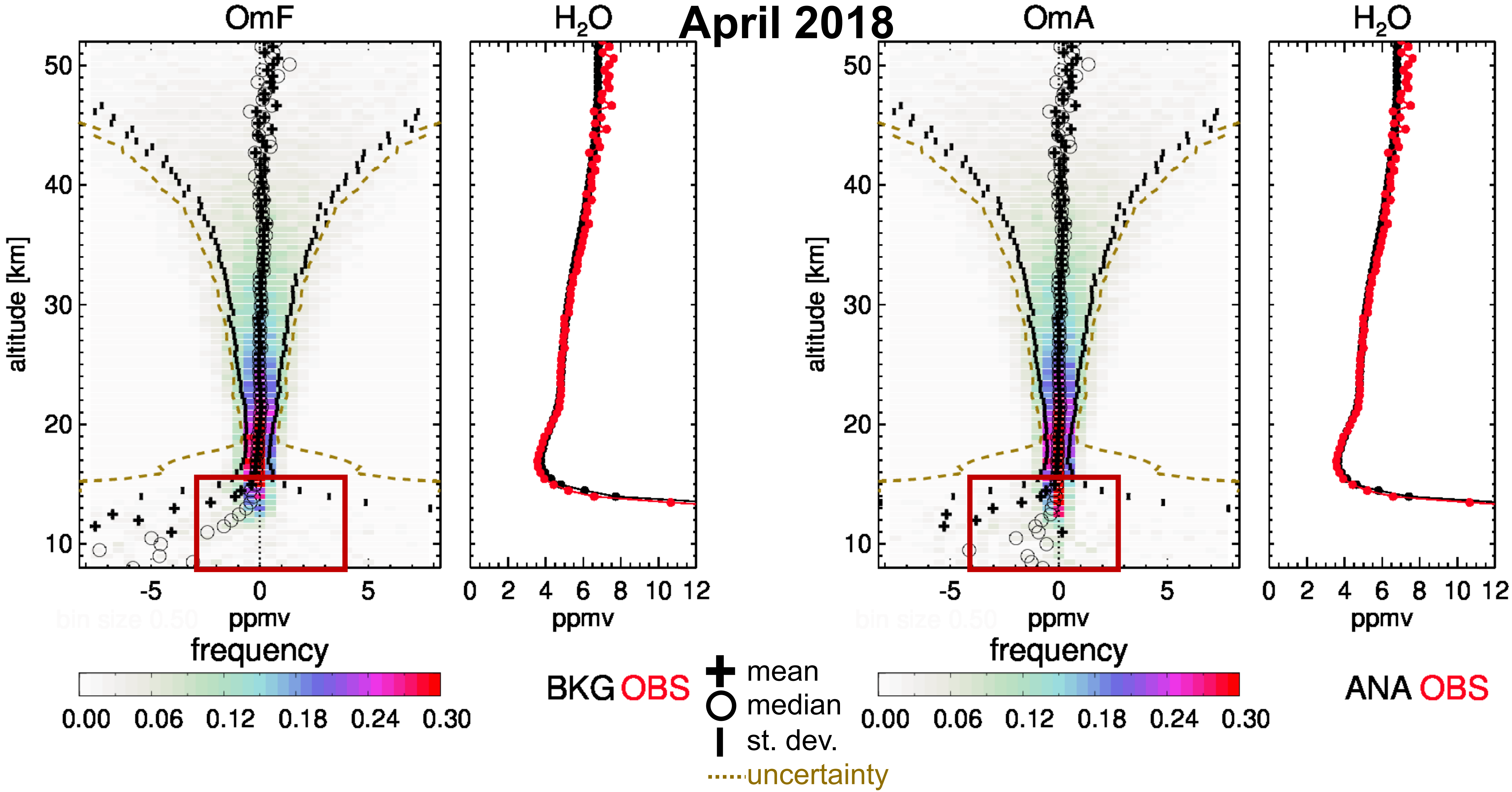


OmF
H$_2$O
OmA
H$_2$O
altitude [km]
50
40
30
20
10
-5
0
5
0 2 4 6 8 10 12
ppmv
frequency
0.00 0.06 0.12 0.18 0.24 0.30
BKG OBS
ANA OBS
mean
median
st. dev.
uncertainty

October 2017

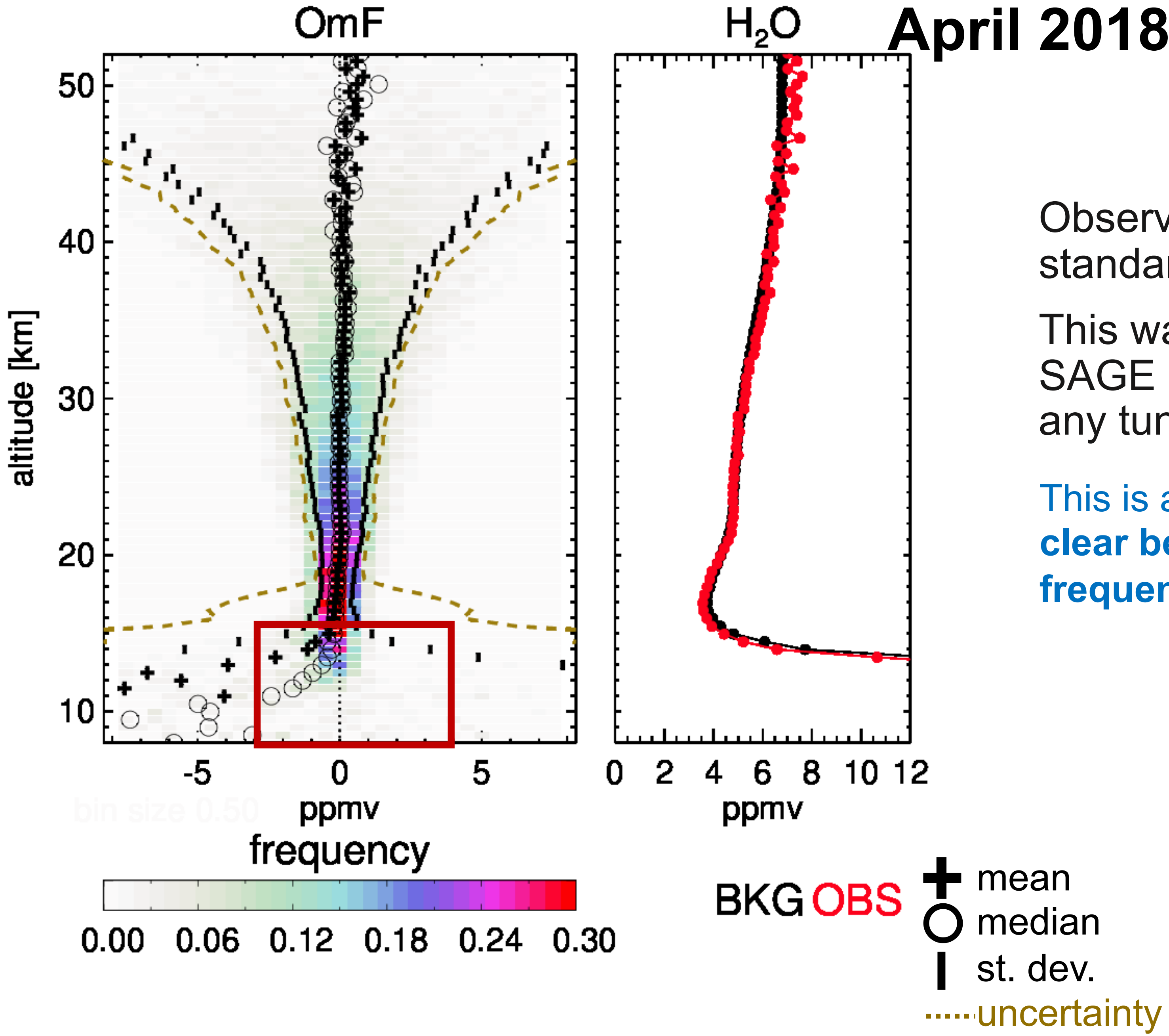


April 2018



OmF
H2O
OmA
H2O
altitude [km]
ppmv
frequency
0.00 0.06 0.12 0.18 0.24 0.30
BKG OBS
ANA OBS
mean
median
st. dev.
uncertainty

April 2018



Next steps

Observation uncertainties are larger than standard deviation of (O-F).

This was a first pass at assimilating the SAGE III/ISS water vapor profiles without any tuning!

This is a very encouraging result. **There is a clear benefit to assimilating the less frequent SAGE III/ISS observations.**

Bridging the SAGE data gap

We will use NASA's uniformly-gridded, global GEOS model and DAS products to bridge the gap between the earlier SAGE missions and the SAGE III/ISS products.

- ➢ A combination of GEOS model and DAS products constrained by satellite retrievals aboard NASA's Aura satellite, has great potential to characterize O_3 and water vapor (WV) distribution, trends, and variability from the SAGE II mission through SAGE III/ISS observations.
  - ✓ Extended the Wargan et al. 2018 study to 2020
  - ❑ Next steps include using SAGE II (and possibly SAGE III/3M) to correct MERRA-2 ozone across discontinuities in the pre-Aura period.
  - ❑ Pam Wales to present at AMS in January 2023
- ➢ The assimilation of SAGE WV and O_3 is now possible in the CoDAS framework to carry-on the trend and climate assessments after the Aura mission.
  - ✓ There is a clear benefit to assimilating the less frequent SAGE III/ISS observations.
  - ❑ Need to tune the system and rerun the experiments
  - ❑ Emma Knowland to present at AGU "GEOS Constituent Data Assimilation beyond Aura MLS: Assimilating NASA SAGE III/ISS profiles of stratospheric water vapor and ozone"

Thank you!

k.e.knowland@nasa.gov