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

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NASA GMAO global meteorology and chemistry products

GEOS

Bindle et al., 2021 GMD

OMPS (O₃)

www.nasa.gov
NASA GMAO global meteorology and chemistry products

GEOS

- Forecasting
  - GEOS FP
  - GEOS FP-IT

- Reanalysis
  - MERRA-2
    - GEOS-CF
    - M2-SCREAM
    - MERRA2-GMI

https://gmao.gsfc.nasa.gov/GMAO_products/

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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
    - 0.5° latitude x 0.625° 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 3 - Improvements in analyzed O\(_3\) were seen after the assimilation of MLS profiles and OMI TCO compared to SBUV profiles and TCO. Reproduced from Wargan et al. (2017).

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$_2$O, HCl, HNO$_3$, & N$_2$O 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

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
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
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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)
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.
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.

**MERRA2 – SAGE III/ISS solar O$_3$**

2018 mean bias
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-GMI” (a.k.a. M2GMI) is a GMI chemistry simulation constrained by MERRA-2 meteorology

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

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**Figure 4** - Transitions in the assimilated observing system can lead to fictitious changes in the reanalysis constituent behavior which must be addressed for trend analysis. For MERRA-2 O₃ there are three discontinuities in the time series to correct: the introduction of MLS and OMI measurements (October 2004) and two changes related to MLS (June 2015, May 2016). We propose to use a similar methodology as Wargan et al. (2018) to bias correct MERRA-2 using M2-GMI as a transfer function: averaging the monthly differences over latitude bands (yellow dots, bottom row) at every level over a short period of time before ($\Delta_{\text{before}}$) and after ($\Delta_{\text{after}}$) the discontinuity (orange contours). The difference ($\Delta_{\text{before}} - \Delta_{\text{after}}$) is then applied to MERRA-2 following the discontinuity as a bias-correction factor, resulting in a time series without any noticeable discontinuities (purple contour). 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
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
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

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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)
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].

M2-SCREAM is wetter
SAGE Experiment is wetter
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

M2-SCREAM is wetter
SAGE Experiment is wetter
GEOS CoDAS experiments

3. SAGE-only post-Aura: SAGE WV

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

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

CoDAS SAGE III

CoDAS MLS

Control

Dotted: Forecast
Dashed: Analysis

Dash-dot: Chemistry only

Dotted: Forecast
Dashed: Analysis
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.
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.
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- 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!