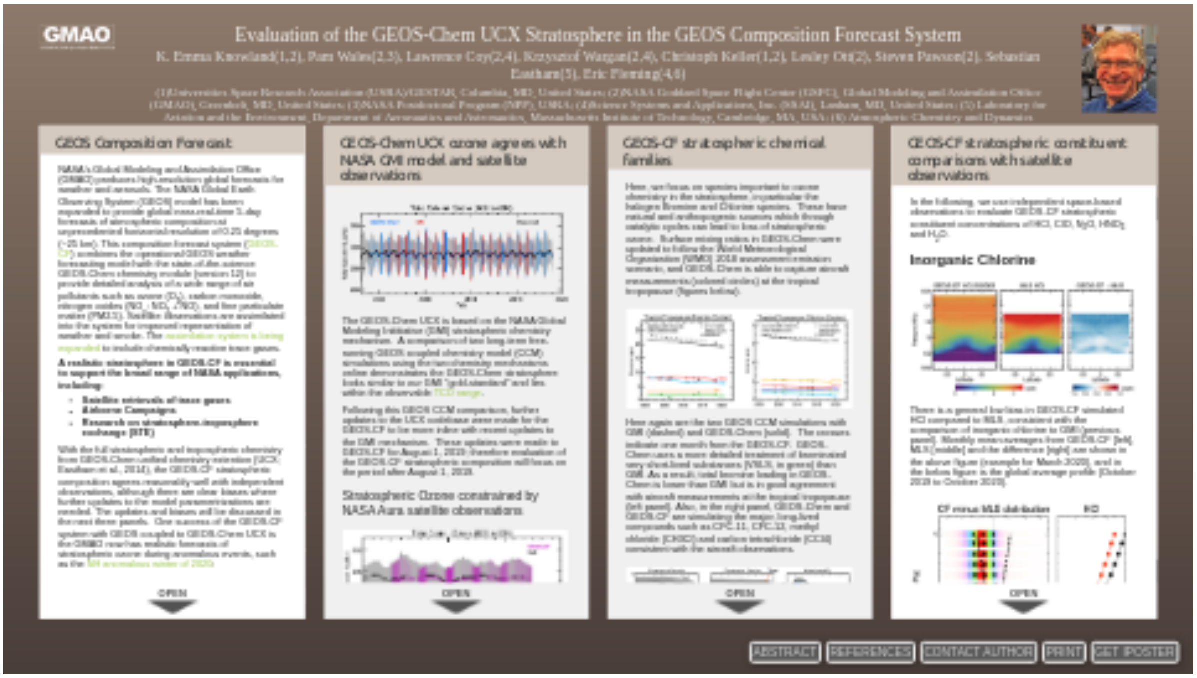
Evaluation of the GEOS-Chem UCX Stratosphere in the GEOS Composition Forecast System



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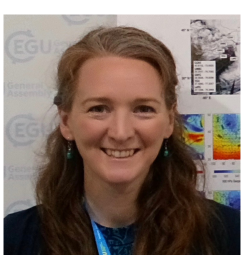


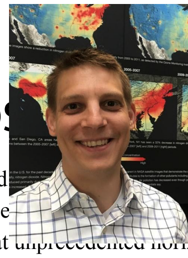

GEOS COMPOS OF

NASA's Global Modeling and (C h- asts for weather and aerosols. The NASA Global Earth Obse S) nc ear-real-time 5-day forecasts of atmospheric composition at unprecedented horizontal resolution of 0.25 degrees (~25 km). This composition forecast system (GEOS-CF (https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/)) combines the operational GEOS weather forecasting model with the state-of-

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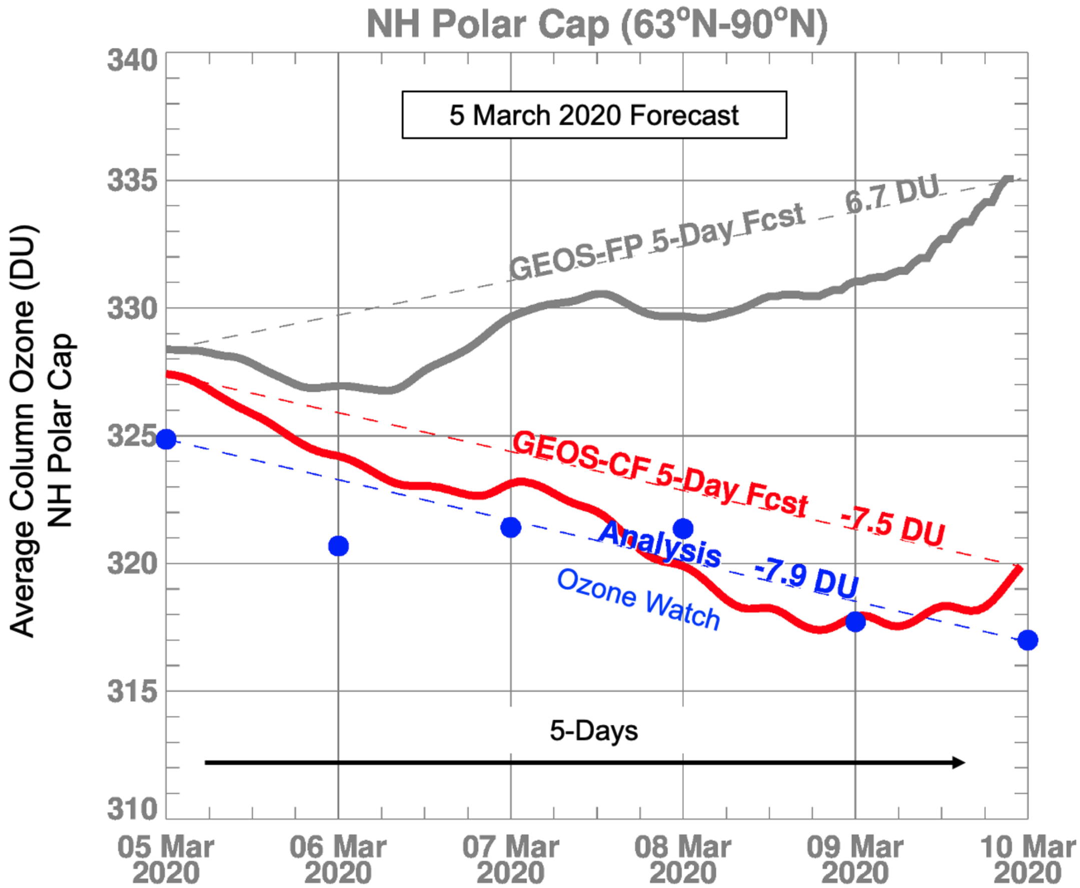
module (version 12) to provide detailed analysis of a wide range of air pollutants such as ozone (O_3), carbon monoxide, nitrogen oxides (NO_x: NO_2 + NO), and fine particulate matter (PM2.5). Satellite observations are assimilated into the system for improved representation of weather and smoke. The assimilation system is being expanded (http://agu2020fallmeeting-agu.ipostersessions.com /Default.aspx?s=DF-E8-ED-74-02-A2-E1-93-A6-D8-F7-EE-46-58-14-A1) to include chemically reactive trace gases.

A realistic stratosphere in GEOS-CF is essential to support the broad range of NASA applications, including:

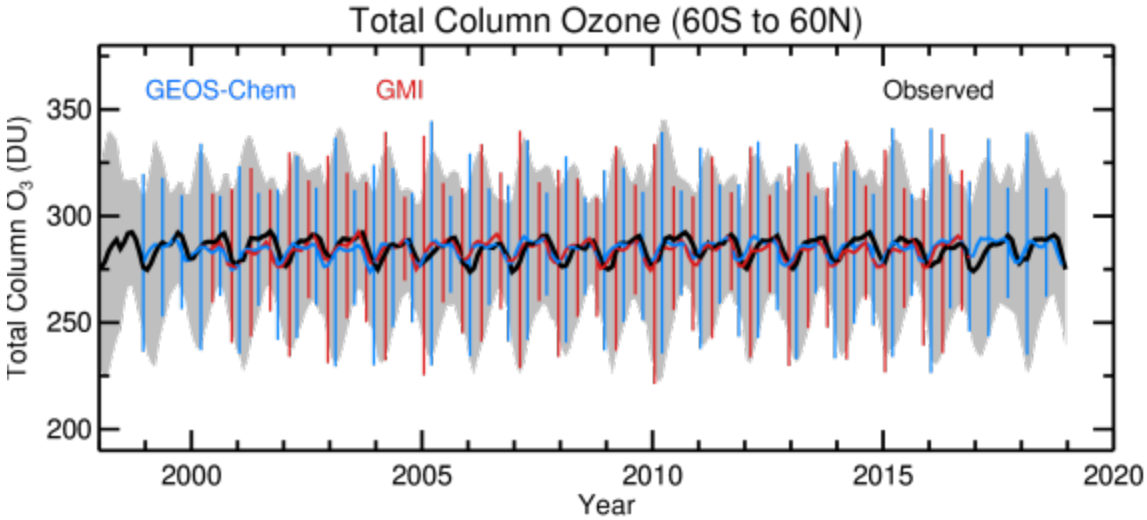
- **Satellite retrievals of trace gases**
- **Airborne Campaigns**
- **Research on stratosphere-troposphere exchange (STE)**

With the full stratospheric and tropospheric chemistry from GEOS-Chem unified chemistry extention (UCX; Eastham et al., 2014), the GEOS-CF stratospheric composition agrees reasonably well with independent observations, although there are clear biases where further updates to the model paramertrizations are needed. The updates and biases will be discussed in the next three panels. One success of the GEOS-CF system with GEOS coupled to GEOS-Chem UCX is the GMAO now has realistic forecasts of stratospheric ozone during anomalous events, such as the NH anomalous winter of 2020 (http://agu2020fallmeeting-agu.ipostersessions.com/Default.aspx?s=6E-50-CA-59-43-D2-B1-84-DB-E8-D9-C0-96-B7-4F-48):



Sample 5-day forecast trajectories for GEOS-CF and GEOS-FP for NH polar cap ozone compared to a daily ozone observation-based Ozone Watch (https://ozonewatch.gsfc.nasa.gov/)"Analysis" product. The tendecy for higher ozone is apparent in GEOS-FP.

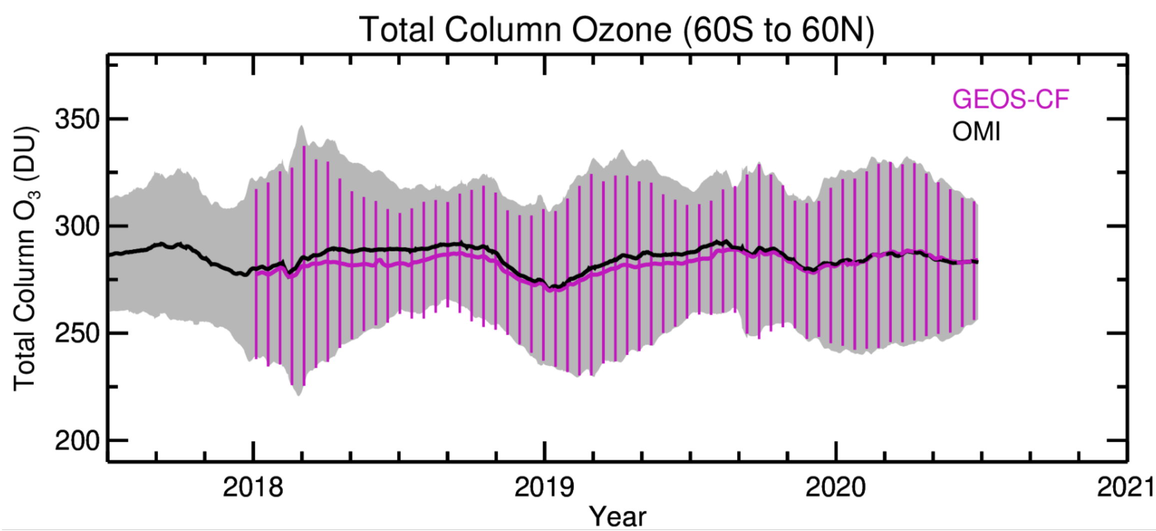
GEOS-CHEM UCX OZONE AGREES WITH NASA GMI MODEL AND SATELLITE OBSERVATIONS



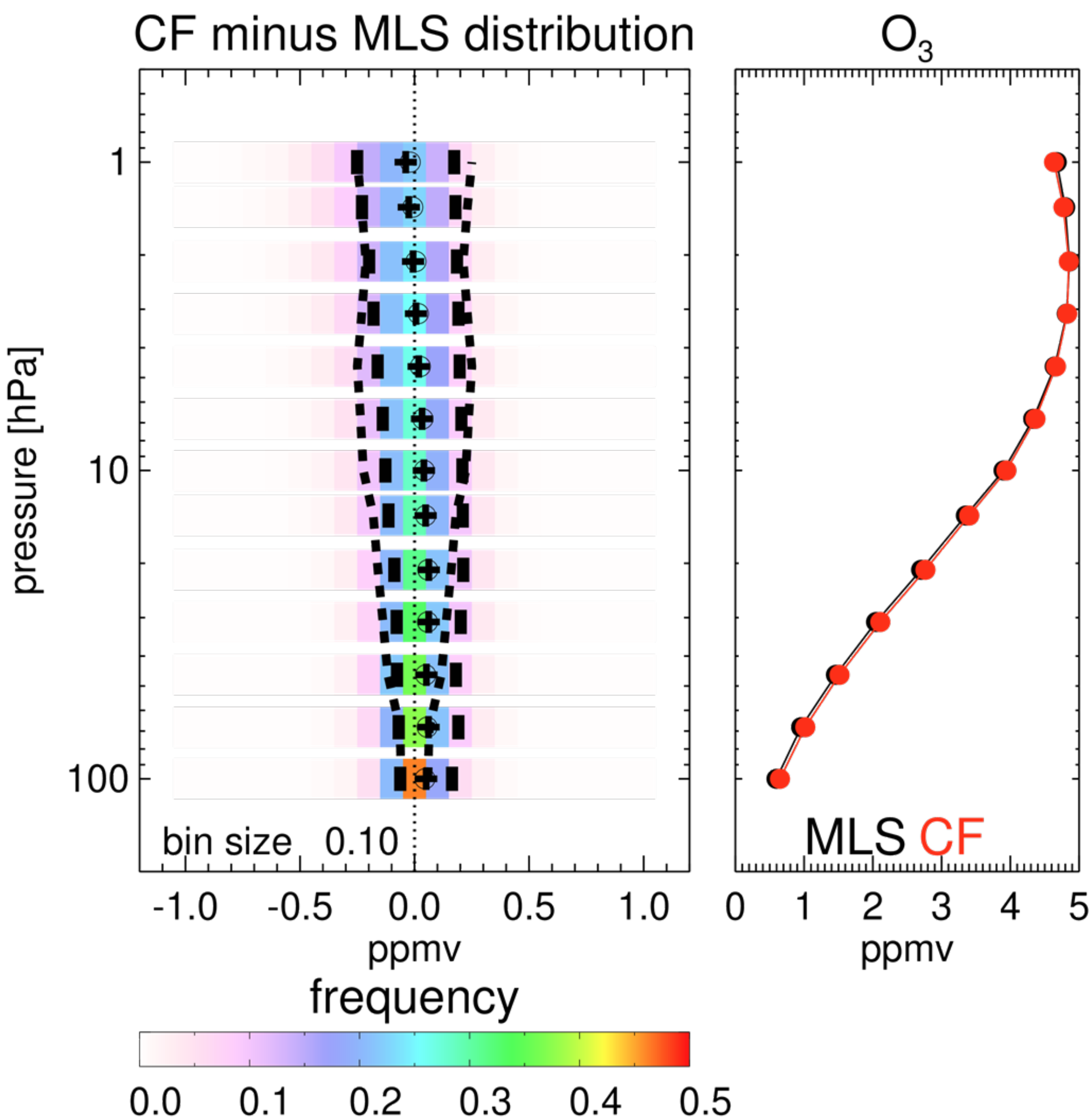
The GEOS-Chem UCX is based on the NASA Global Modeling Inititiative (GMI) stratospheric chemistry mechanism. A comparison of two long-term free-running GEOS coupled chemistry model (CCM) simulations using the two chemistry mechanisms online demonstrates the GEOS-Chem stratosphere looks similar to our GMI "gold-standard" and lies within the observable TCO range (https://acd-ext.gsfc.nasa.gov/Data_services/merged/index.html).

Following this GEOS CCM comparison, further updates to the UCX codebase were made for the GEOS-CF to be more inline with recent updates to the GMI mechanism. These updates were made to GEOS-CF for August 1, 2019; therefore evaluation of the GEOS-CF stratospheric composition will focus on the period after August 1, 2019.

Stratospheric Ozone constrained by NASA Aura satellite observations

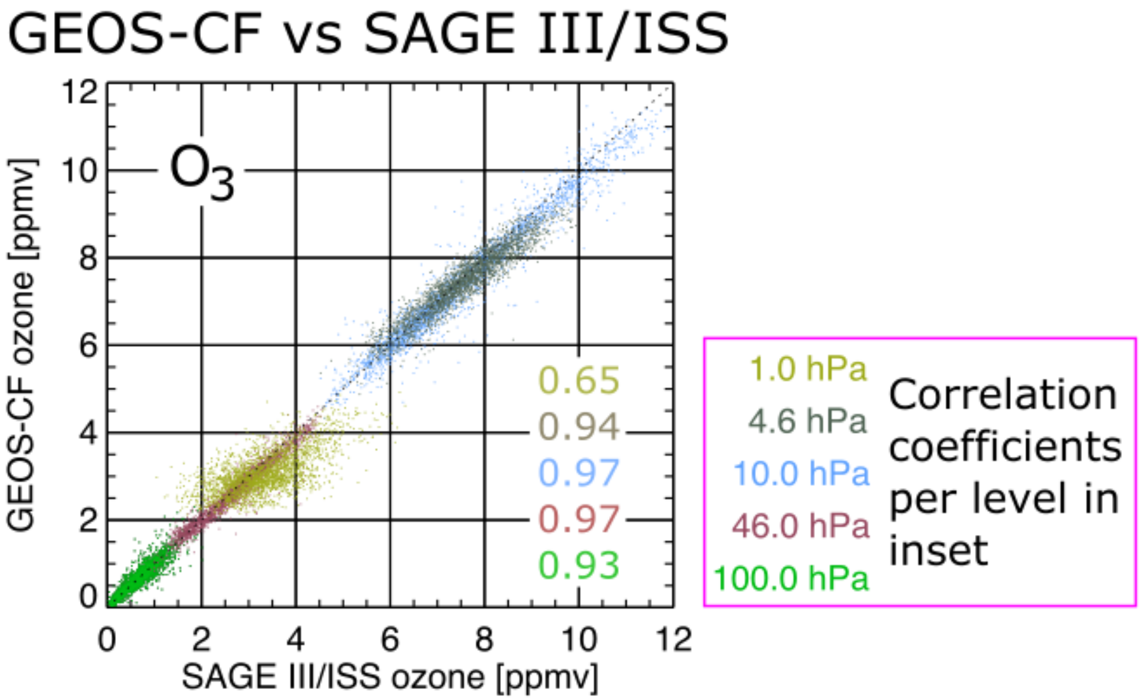


While there is no direct data assimilation in the current GEOS-CF system, there is near-real time information constraining parts of the system. The GEOS-CF stratospheric ozone is weakly nudged towards the GEOS Forward Processing (FP) assimilated ozone product, with the intention to keep stratospheric ozone in line with observations while still allowing GEOS-Chem to simulate over 700 reactions in the troposphere and stratosphere. The GEOS-CF total column ozone (TCO) agrees well with OMI, especially after August 2019 (figure above) and MLS (figure below) because measurements from these instruments -- both aboard NASA's Aura satellite -- are assimilated into GEOS-FP.



In these profile comparison figures, left-hand side shows the pdf of the differences of GEOS-CF minus MLS for MLS data, mean difference (open circle), median difference (cross), 1σ standard deviation (long dash), and approximate instrument 1σ uncertainty from the MLS quality document tables (short dash). The right-hand side shows the mean concentrations at 13 MLS pressure levels. For O_3, we used MLS data within half an hour of the synoptic times (0, 6, 12, 18 UTC) for October 2019 to October 2020.

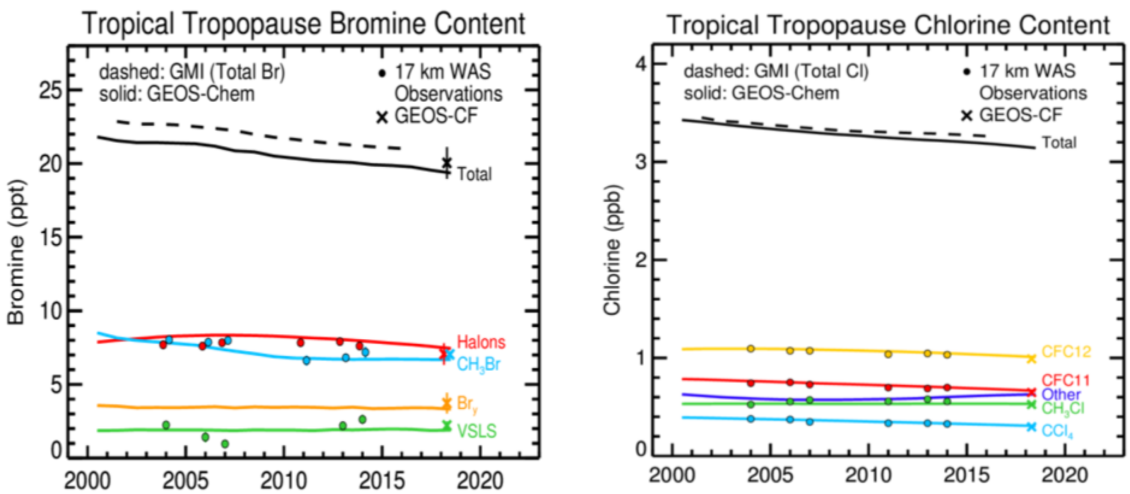
Validation with independant SAGE III/ISS profiles



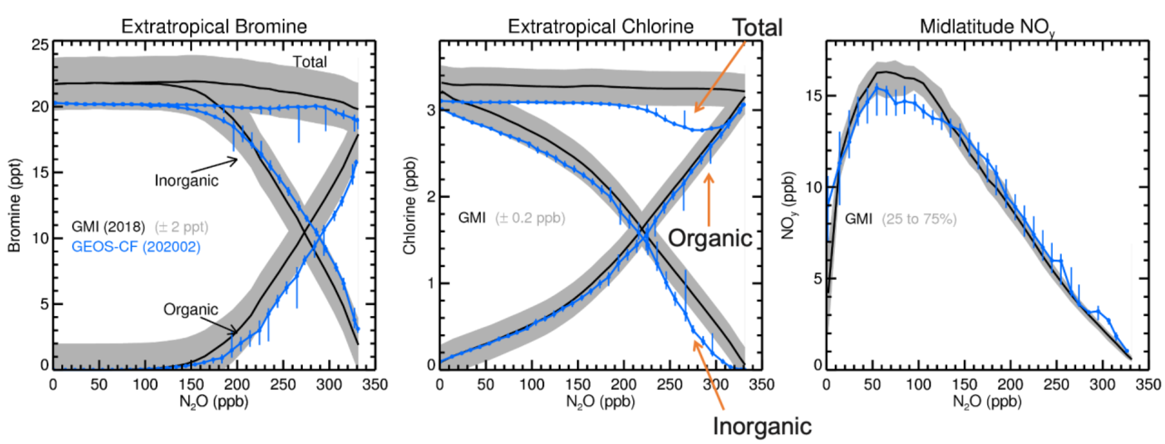
When compared to independent observations, such as SAGE III/ISS solar occultation ozone profiles for Oct 2019 - Aug 2020, stratospheric ozone correlates well (100 to 4.6 hPa; $r \geqq 0.93$); however at higher altitudes, near 1 hPa, the correlation is reduced with SAGE reporting higher values than simulated by GEOS-CF. This may be a result of the SAGE III/ISS observations occuring near twilight and within 1.5 hours of the model times in a region where chemical time scales are short; MLS ozone is slightly higher than GEOS-CF at 1 hPa (above) but still agrees very well.

GEOS-CF STRATOSPHERIC CHEMICAL FAMILIES

Here, we focus on species important to ozone chemistry in the stratosphere, in particular the halogen Bromine and Chlorine species. These have natural and anthropogenic sources which through catalytic cycles can lead to loss of stratospheric ozone. Surface mixing ratios in GEOS-Chem were updated to follow the World Meteorological Organization (WMO) 2018 assessment emission scenario, and GEOS-Chem is able to capture aircraft measurements (colored circles) at the tropical tropopause (figures below).



Here again are the two GEOS CCM simulations with GMI (dashed) and GEOS-Chem (solid). The crosses indicate one month from the GEOS-CF. GEOS-Chem uses a more detailed treatment of brominated very short-lived substances (VSLS, in green) than GMI. As a result, total bromine loading in GEOS-Chem is lower than GMI but is in good agreement with aircraft measurements at the tropical tropopause (left panel). Also, in the right panel, GEOS-Chem and GEOS-CF are simulating the major, long-lived compounds such as CFC-11, CFC-12, methyl chloride (CH3Cl) and carbon tetrachloride (CCl4) consistent with the aircraft observations.

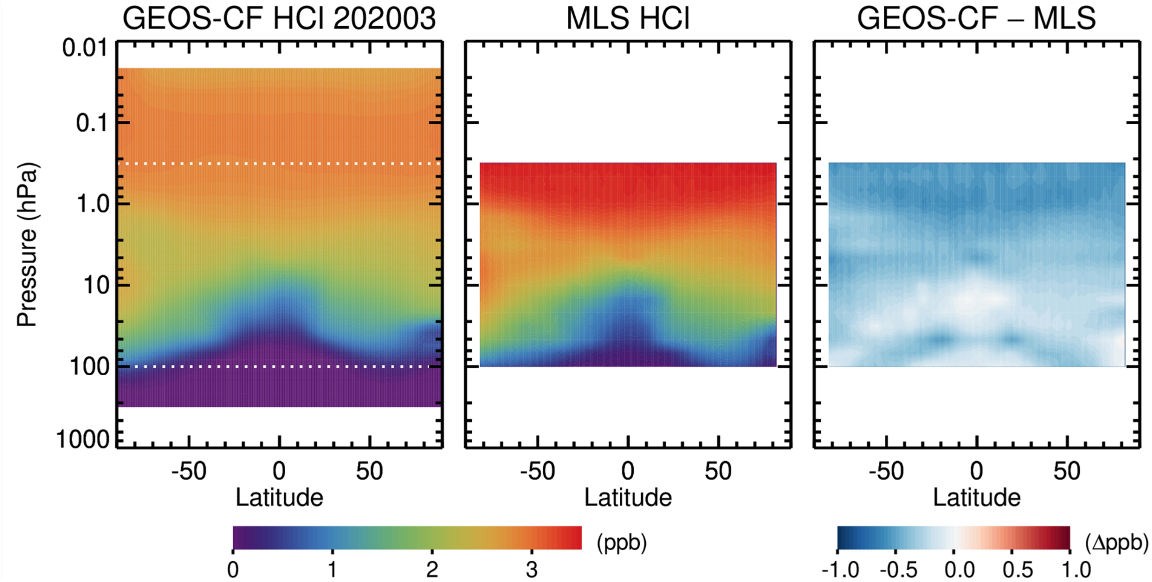


Using GMI as the base, we can identify where there may still be room for improvement in the GEOS-CF, demonstrated with February 2020 as an example. As discussed above, total bromine is lower in GEOS-CF than GMI [left]. The representation of chlorinated organic source gases [middle] is well represented in GEOS-CF with respect to GMI, but there is a pronounced low bias in the Inorganic Chlorine species (Cl_y) at high N_2O concentrations, which indicates that the low bias is mainly in lower stratosphere where N_2O values are high. As for the nitrogen oxide family "NO_y" [right], GEOS-CF is in good agreement with GMI simulations, but there is low bias at lower values of N_2O, higher in the stratosphere. We use space-based observations to investigate these model biases further (next panel).

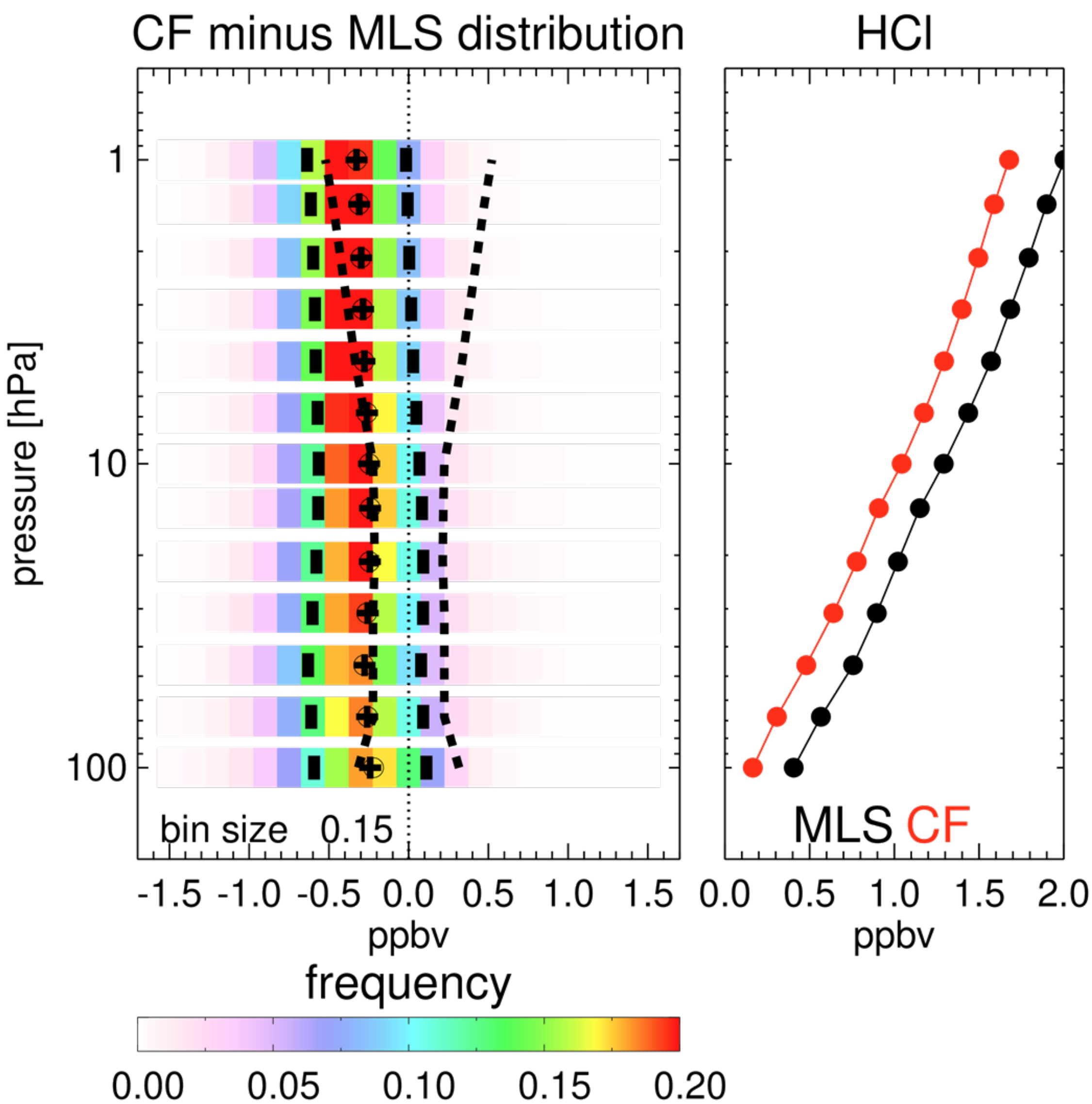
GEOS-CF STRATOSPHERIC CONSTITUENT COMPARISONS WITH SATELLITE OBSERVATIONS

In the following, we use independent space-based observations to evaluate GEOS-CF stratospheric constituent concentrations of HCl, ClO, N_2O, HNO_3 and H_2O.

Inorganic Chlorine



There is a general low bias in GEOS-CF simulated HCl compared to MLS, consistent with the comparison of inorganic chlorine to GMI (previous panel). Monthly mean averages from GEOS-CF [left], MLS [middle] and the difference [right] are shown in the above figure (example for March 2020), and in the below figure is the global average profile (October 2019 to October 2020).



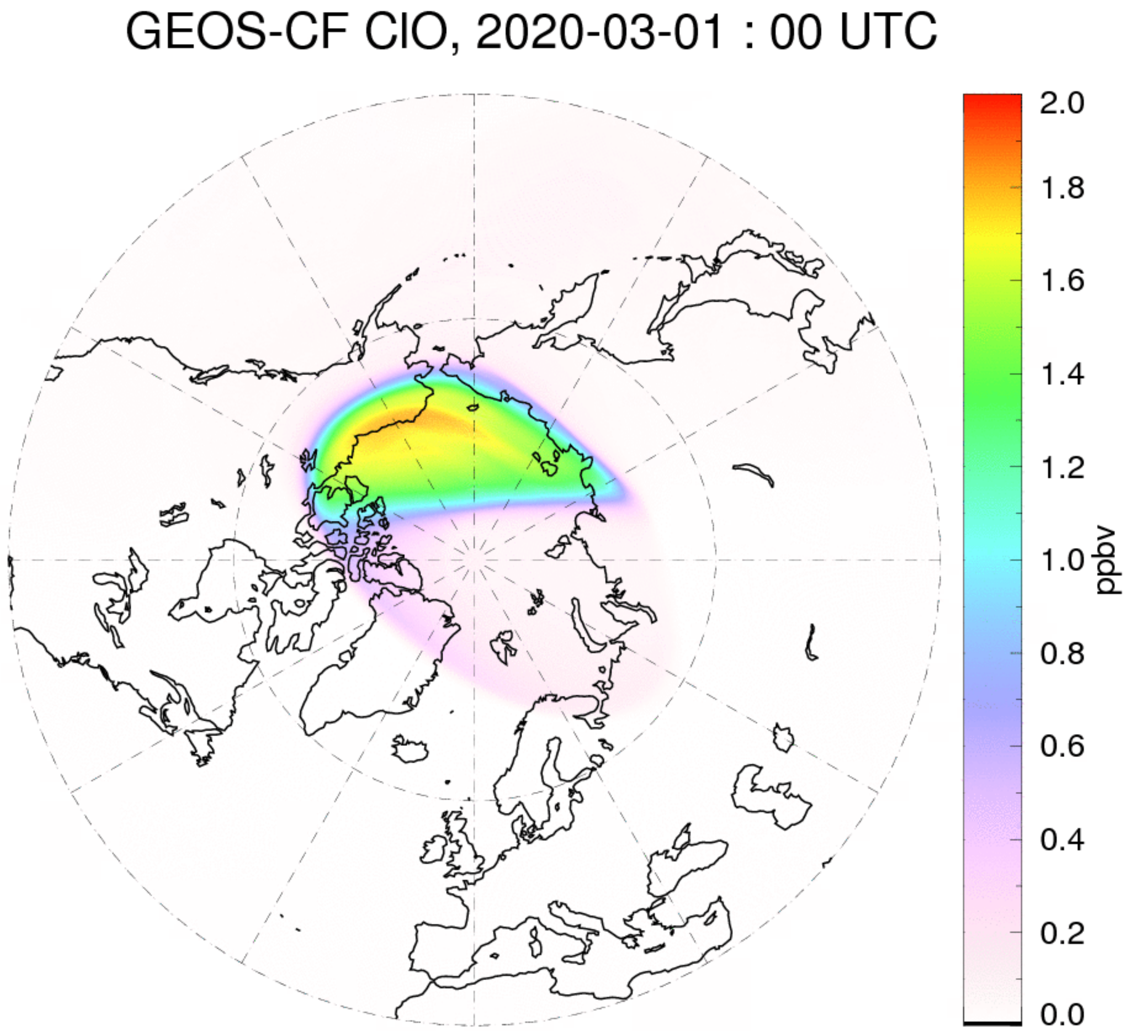
In these profile comparison figures with MLS, left-hand side shows the pdf of the differences of GEOS-CF minus MLS for MLS data, mean difference (open circle), median difference (cross), 1σ standard deviation (long dash), and approximate instrument 1σ uncertainty from the MLS quality document tables (short dash). Only the MLS data within half an hour of 12 UTC is used from the 13 month period from October 2019 through October 2020.

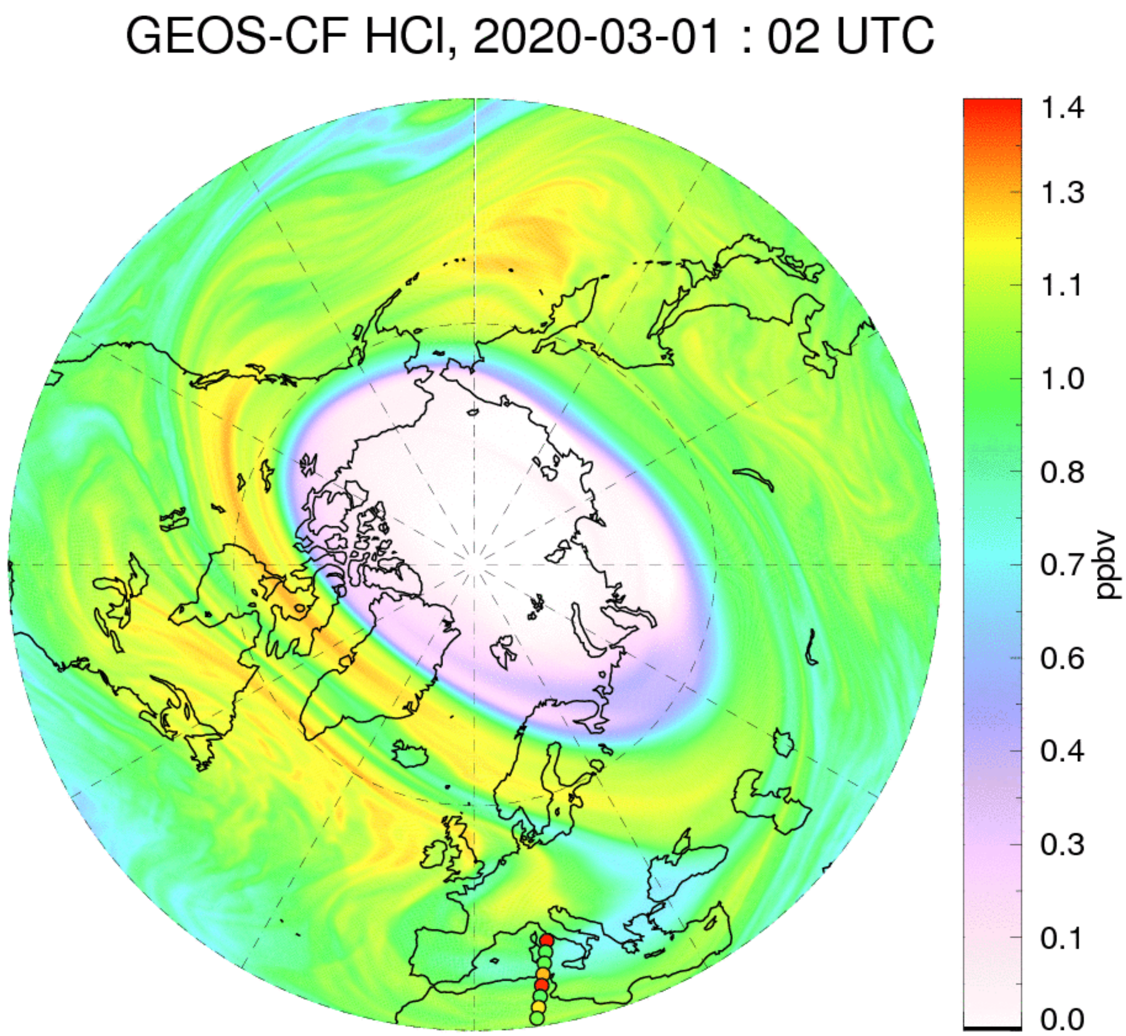
Case study with anomalous NH Polar Vortex Winter/Spring 2020

During the Northern Hemisphere Winter and early Spring of 2020, there was anomalously low stratospheric ozone within the polar vortex. In the following animations, we highlight the ClO and HCl concentrations at 45 hPa and HCl at 68 hPa from GEOS-CF (map) with the MLS overpass (circles) during the first three days of March.

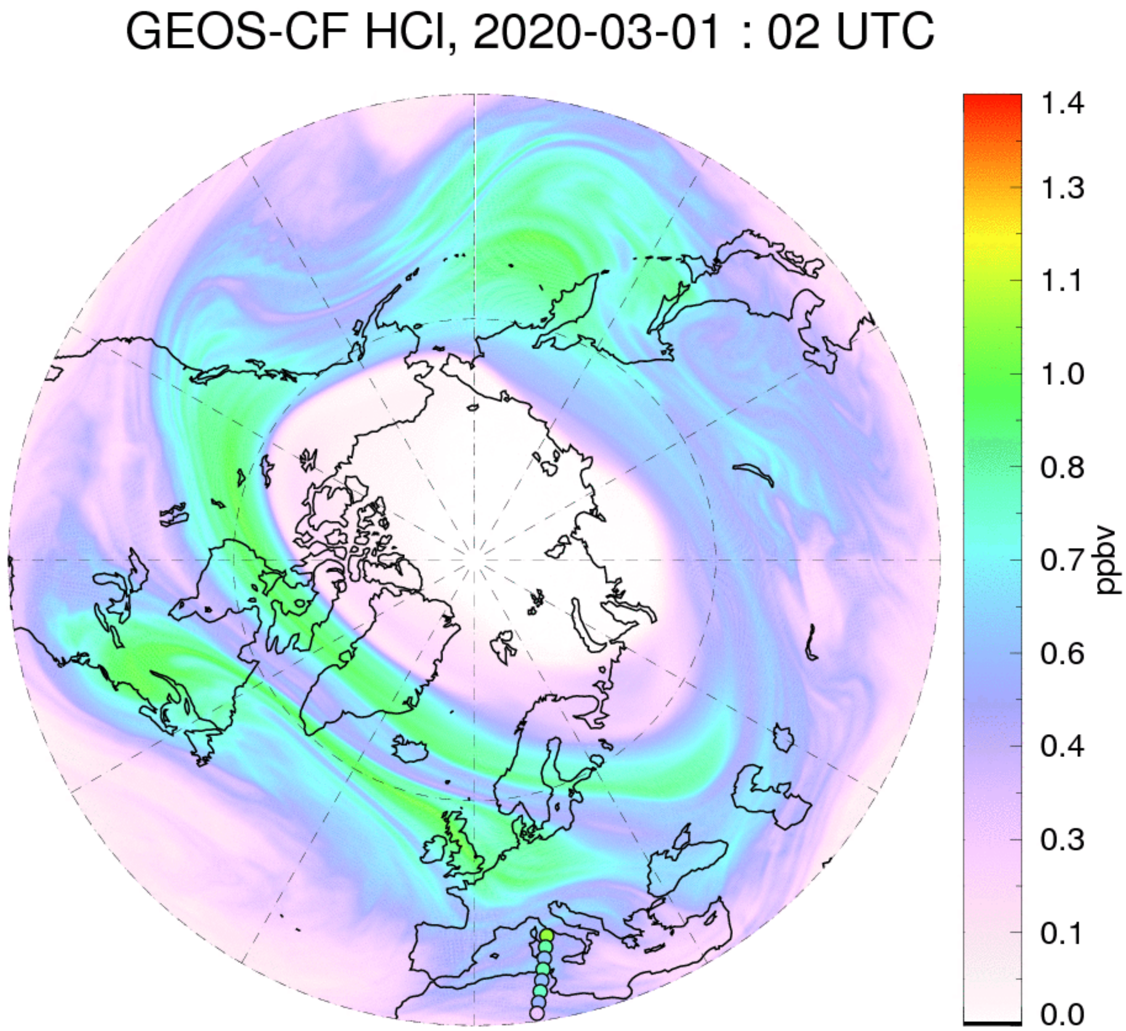
The GEOS-CF simulates the time and location of the vortex and chemistry but does not capture the observed high values of ClO within the vortex and high values of HCl outside of the vortex as seen by MLS.

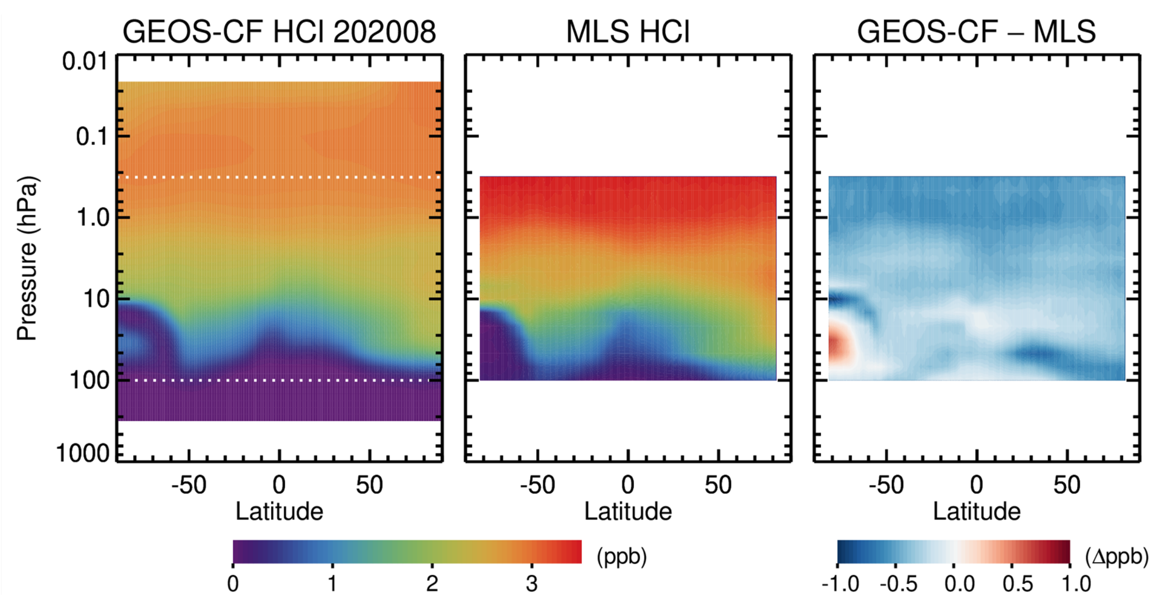
ClO and HCl at 45 hPa:


GEOS-CF ClO, 2020-03-01 : 00 UTC
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
ppbv



HCl at 68 hPa:



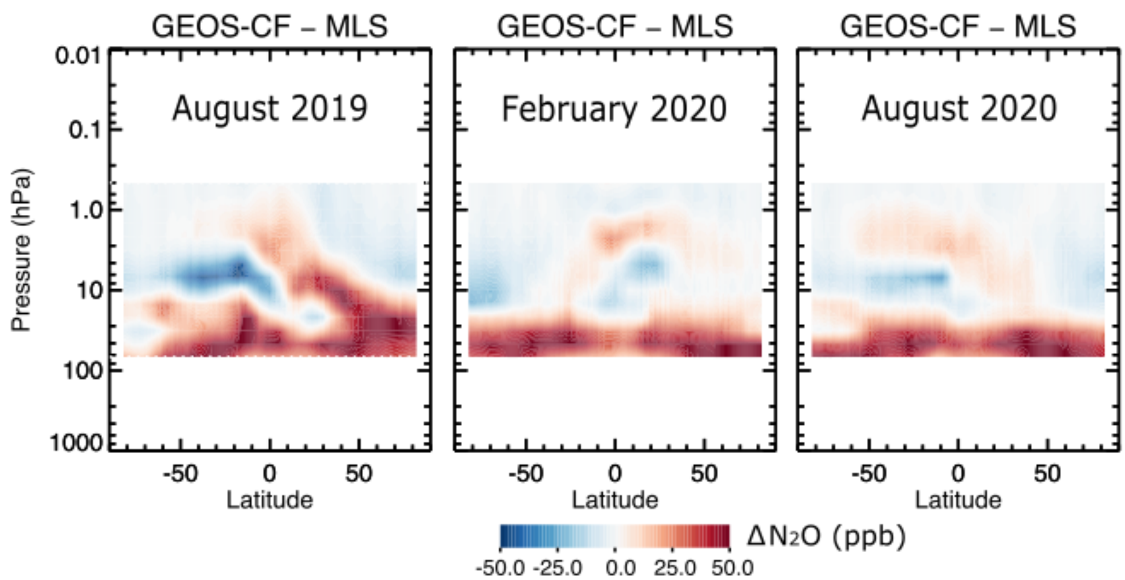


The chlorine activation is under-represented in the SH vortex. During the austral spring, the GEOS-CF exhibits a positive bias in the lower stratosphere within the polar vortex. This positive bias in the southern latitudes was seen in August 2019 (not shown) and appeared again April to August 2020, as highlighted in the above example of August 2020 zonal mean comparison between

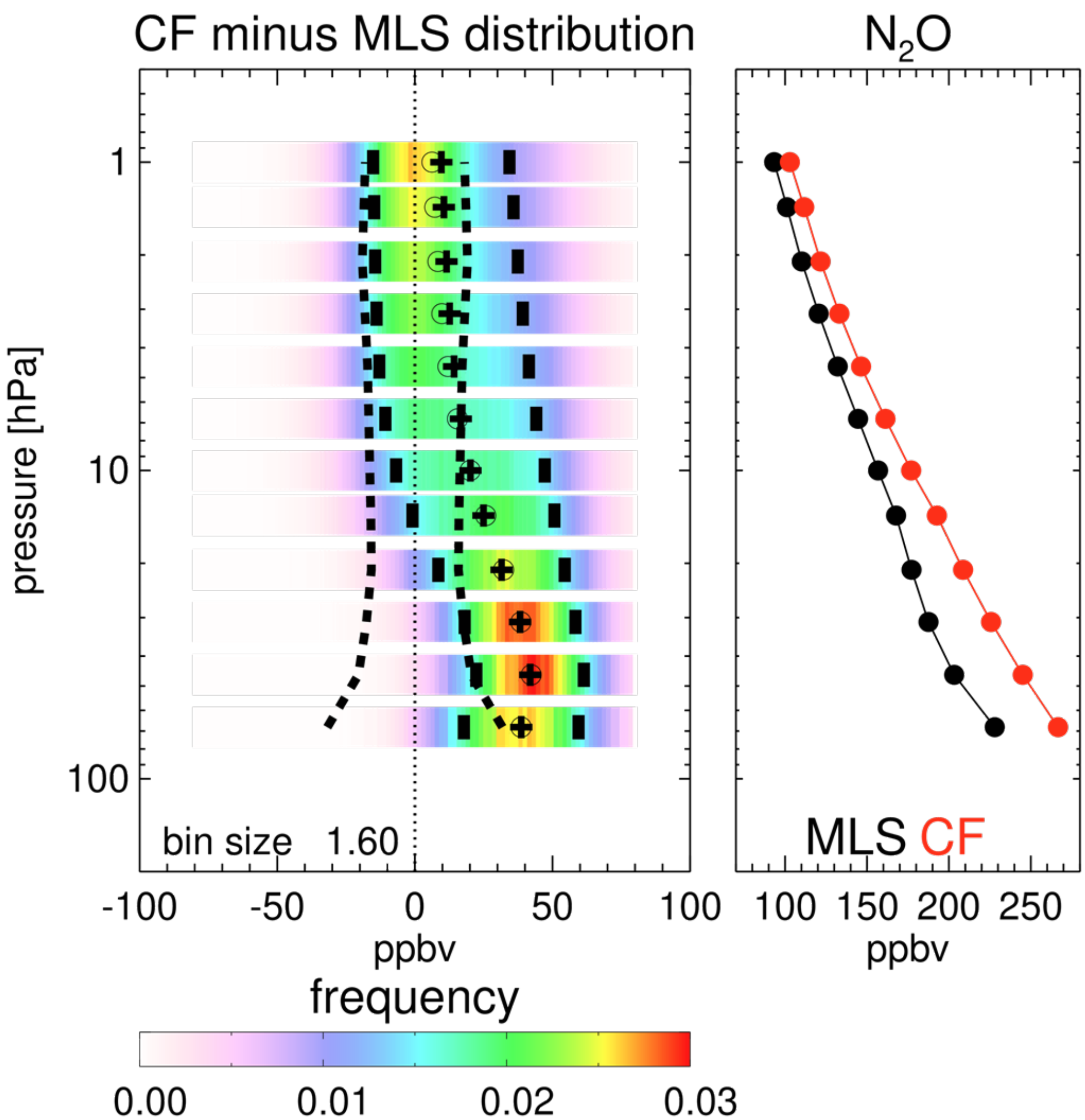
GEOS-CF and MLS HCl.

Nitrogen species

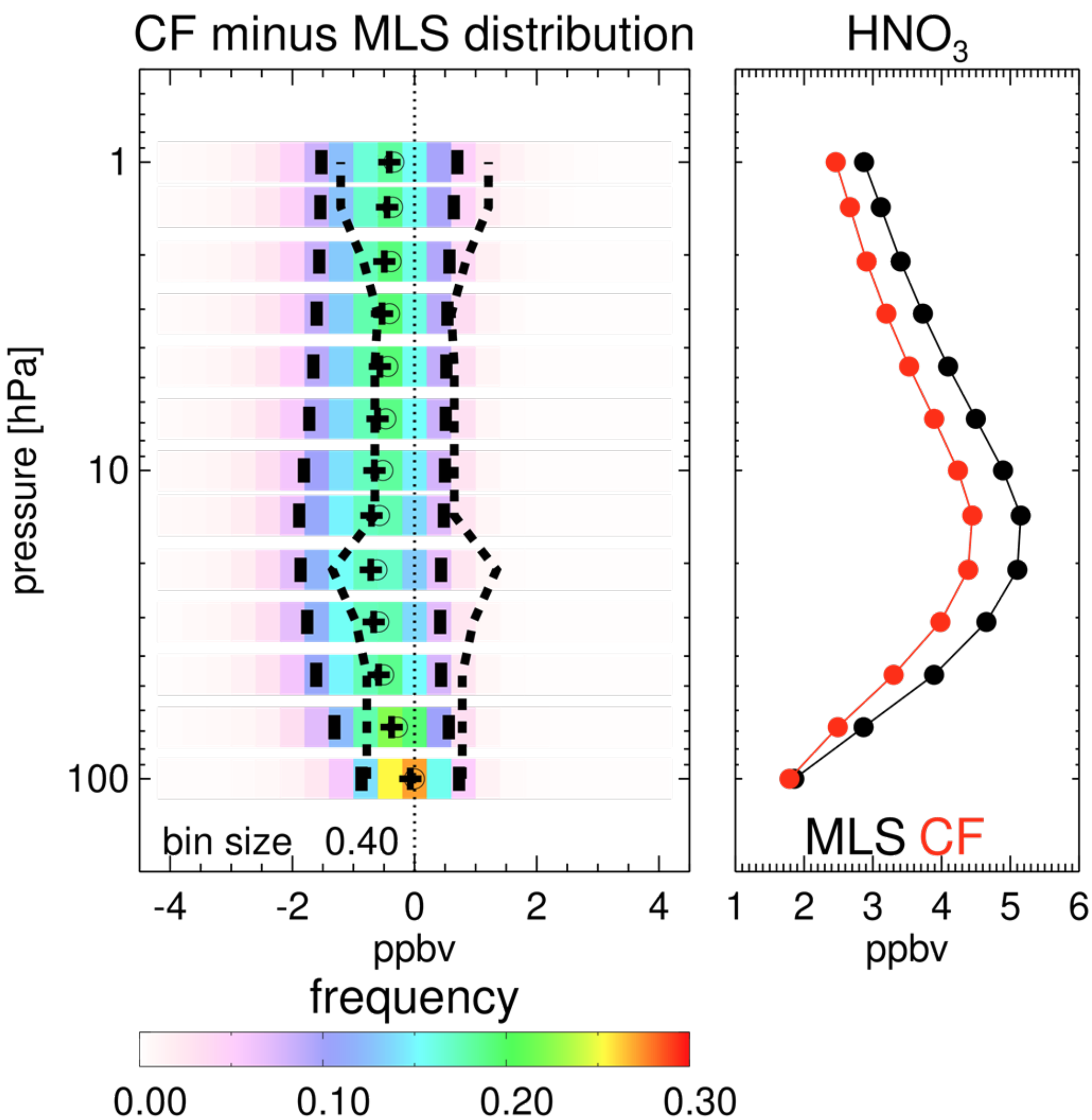
N_2O has tropospheric sources with no significant sinks in the troposphere and lower stratosphere. In the middle stratosphere it dissociates to feed into the NOy family.



As the model continues to spin up, the agreement between GEOS-CF N_2O and MLS N_2O improves (above), however the persistent high bias in the lower stratosphere will be investigated further using ground-based observations to confirm if the sources of N_2O are overrepresented in the model. This difference (color, figure below) is greater than the 1 sigma uncertainty of the MLS instrustment below 10 hPa (short dash lines in the left panel of the figure below).

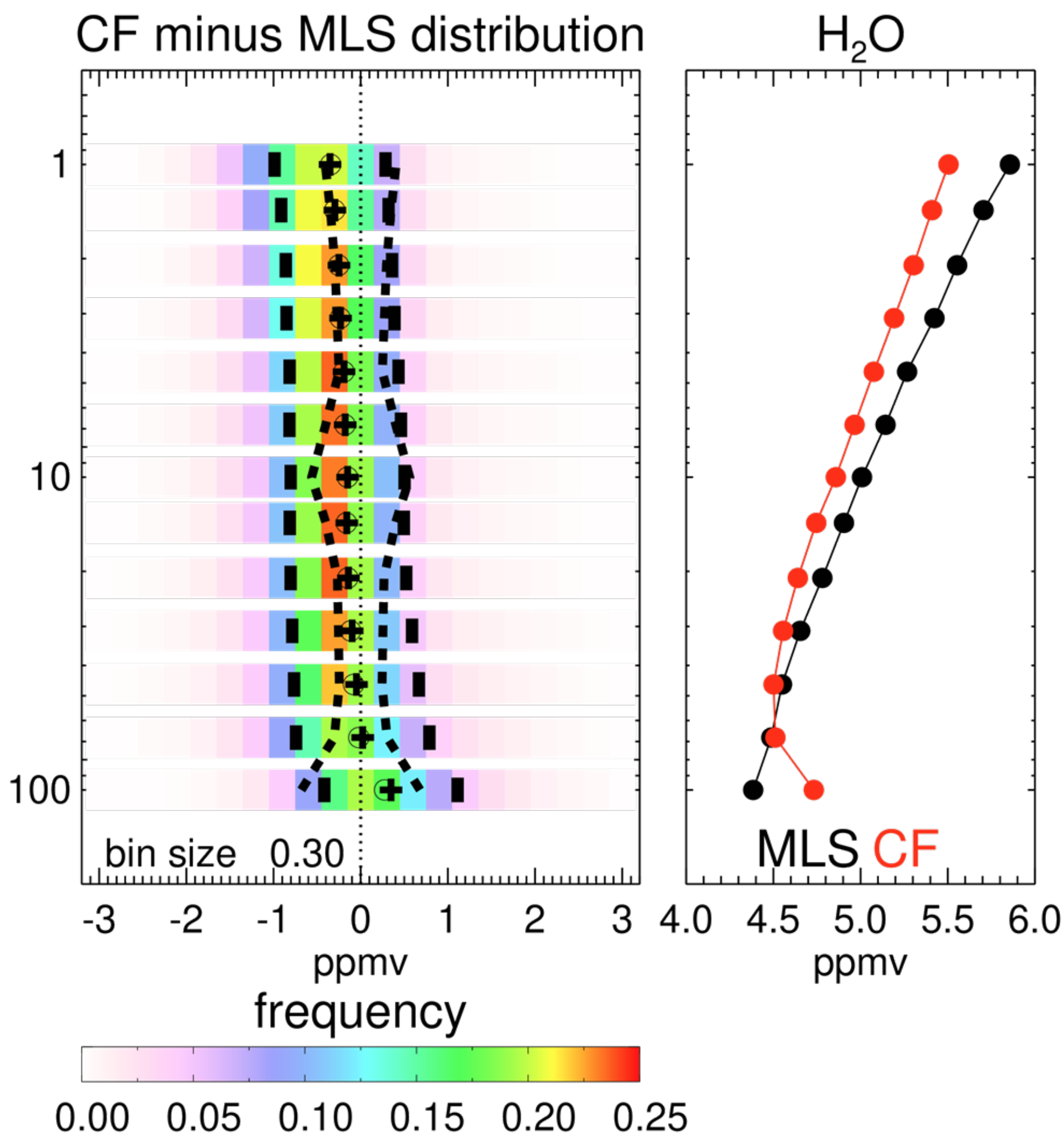


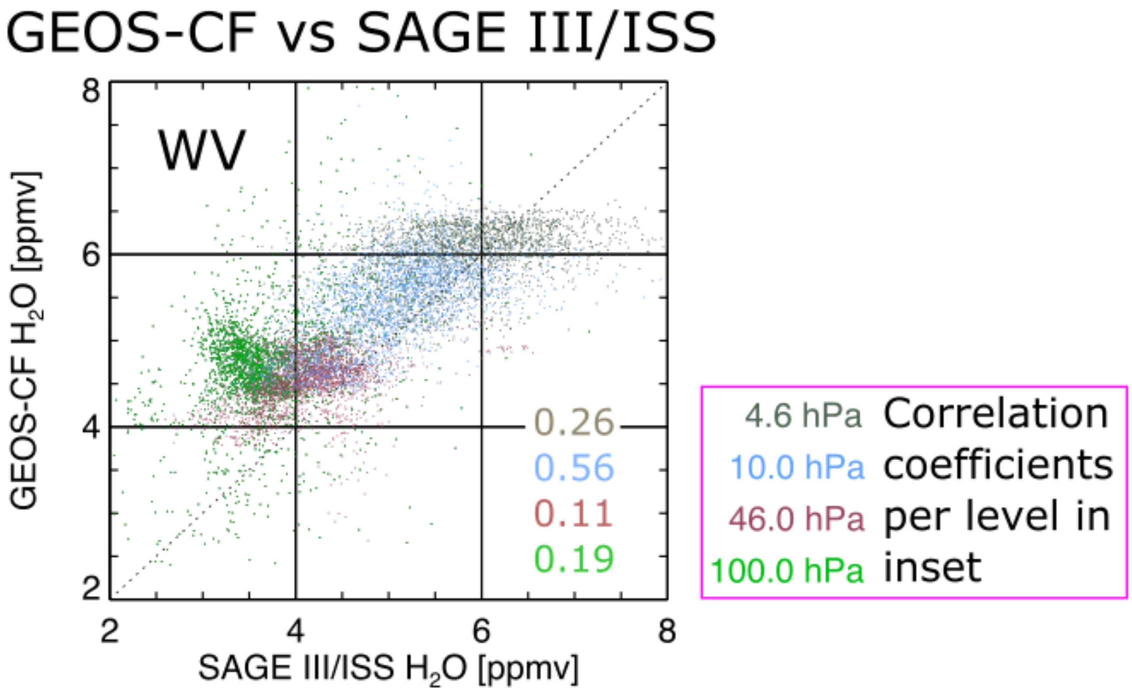
While there is a general low bias in simulated HNO_3 compared to MLS observations, it is within the lower limit of the instrument uncertainty estimate:



Water Vapor

Stratospheric water vapor in reanalysis products are historically poor (Davis et al., 2017). Compared to independant observations from MLS and SAGE III/ISS, GEOS-CF stratospheric water vapor is biased low, although the mean difference is within the MLS instrument's uncertainty estimate. A new GEOS Stratospheric Composition Reanalysis with Aura MLS (GEOS-SCREAM; Wargan et al., 2020) assimilates stratospheric water vapor (http://agu2020fallmeeting-agu.ipostersessions.com /Default.aspx?s=DF-E8-ED-74-02-A2-E1-93-A6-D8-F7-EE-46-58-14-A1) which improves the correlation coefficients of stratospheric water vapor against SAGE III/ISS up to 0.81 at 50 hPa (not shown).


CF minus MLS distribution
H2O
pressure [hPa]
1
10
100
bin size 0.30
-3
-2
-1
0
1
2
3
ppmv
4.0
4.5
5.0
5.5
6.0
ppmv
MLS CF
frequency
0.00
0.05
0.10
0.15
0.20
0.25


GEOS-CF vs SAGE III/ISS
WV
8
6
4
2
2
4
6
8
GEOS-CF H2O [ppmv]
SAGE III/ISS H2O [ppmv]
0.26
0.56
0.11
0.19
4.6 hPa
10.0 hPa
46.0 hPa
100.0 hPa
Correlation coefficients per level in inset

ABSTRACT

The NASA GEOS Composition Forecast (GEOS-CF) system provides 3-dimensional atmospheric composition analyses and forecasts to the public in near-real time at the high spatial resolution of 25 km. While the main focus of this new product is on tropospheric air quality information, the GEOS-Chem chemistry model (v12) used in this system includes the UCX stratospheric chemistry mechanism. Here, we describe the GEOS-CF system and provide comparisons against remote-sensed observations for stratospheric composition, including measurements of HCl, ClO, NO2, and O3. The GEOS-CF nudges the stratospheric ozone towards the GEOS Forward Processing (GEOS FP) assimilated ozone product; as a result the stratospheric ozone analysis in the GEOS-CF agrees well with observations. Additionally, with the inclusion of the GEOS-Chem UCX stratospheric chemistry mechanism in GEOS-CF, 5-day forecasts, especially during the abnormal 2020 NH polar spring, capture the chemical and dynamical changes missed by the GEOS FP system, which tends towards climatology. The GEOS-CF is a new tool for the research community providing near-real time 3-dimensional gridded information on atmospheric composition throughout the troposphere and stratosphere.

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Wargan, K., Weir, B., Manney, G. L., Cohn, S. E., & Livesey, N. J. (2020). The anomalous 2019 Antarctic ozone hole in the GEOS Constituent Data Assimilation System with MLS observations. Journal of Geophysical Research: Atmospheres, 125, e2020JD033335. https://doi.org/10.1029/2020JD033335