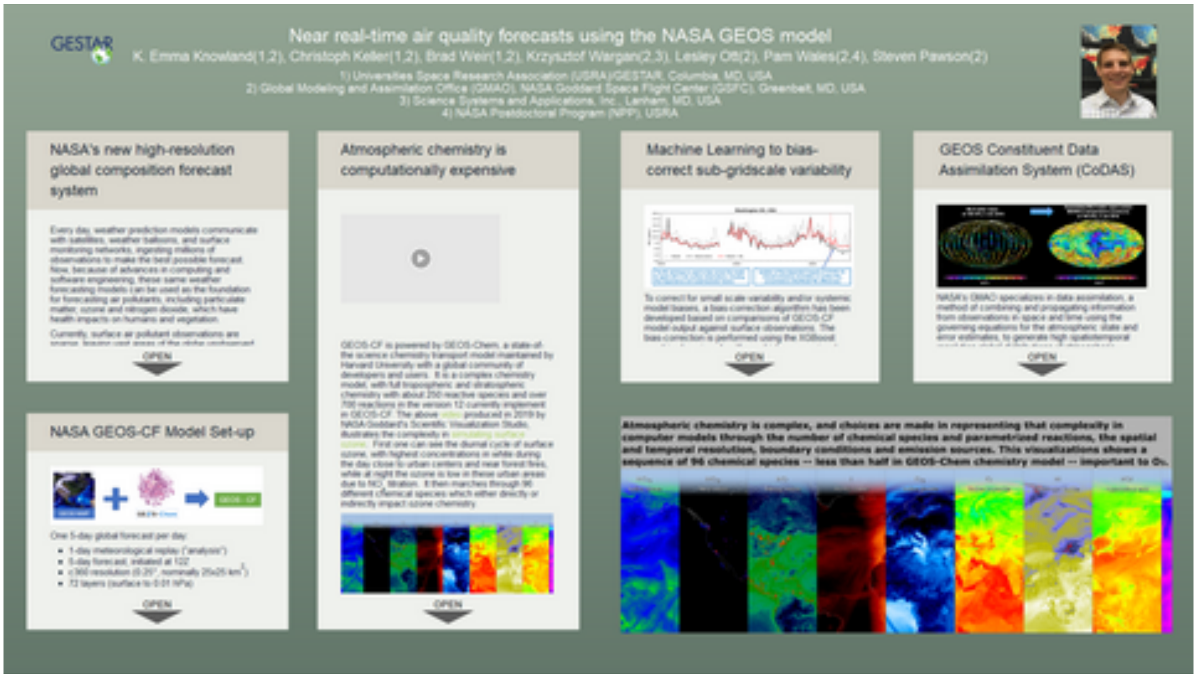
Near real-time air quality forecasts using the NASA GEOS model



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NASA'S NEW HIGH-RESOLUTION GLOBAL COMPOSITION FORECAST SYSTEM

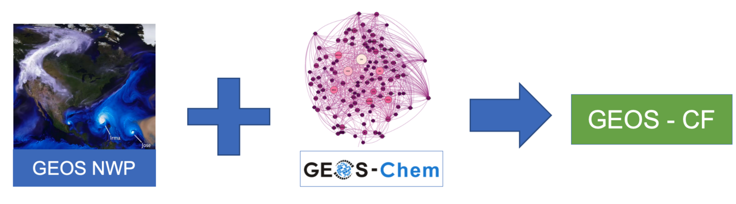
Every day, weather prediction models communicate with satellites, weather balloons, and surface monitoring networks, ingesting millions of observations to make the best possible forecast. Now, because of advances in computing and software engineering, these same weather forecasting models can be used as the foundation for forecasting air pollutants, including particulate matter, ozone and nitrogen dioxide, which have health impacts on humans and vegetation.

Currently, surface air pollutant observations are sparse, leaving vast areas of the globe unobserved. Air pollutant concentrations can be inferred from satellite observations; however, overpasses may be infrequent and it is often difficult to infer the 'nose-level' concentrations that air quality managers need. **Global models with state-of-the-science atmospheric chemistry equations help fill in the gaps left by observations and provide insight on future conditions.**

Forecasting air quality has typically been performed at the local-scale, either for an individual city, state or country. Simulating the emission, transport, and chemical evolution of air pollutants globally and at high spatial resolution requires a powerful supercomputer, such as the one at NASA Goddard Space Flight Center, in Greenbelt, Maryland. Here, NASA's Global Modeling and Assimilation Office is using its weather forecasting model "GEOS" to develop **a global, high-resolution atmospheric composition forecast system "GEOS-CF" capable of providing air quality forecasts in near-real time.** This model uses a complex atmospheric chemistry model "GEOS-Chem" and is run on NASA's Center for Climate Simulation supercomputer, using the computing power equivalent to 3600 personal computers. This forecast has the highest resolution of a global atmospheric composition forecast to-date, providing information at 25 km (16 miles). At each time step, the atmosphere is represented by 75 million data points, with a horizontal resolution 10 times higher than conventional global atmospheric chemistry simulations.

Air quality can vary dramatically by region and time of day. With this new global air quality forecast, we can give the best information to those making decisions regarding human health and agriculture while providing support to NASA flight campaigns, instrument teams, and satellite missions.

NASA GEOS-CF MODEL SET-UP



One 5-day global forecast per day:

- 1-day meteorological replay ("analysis")
- 5-day forecast, initiated at 12Z
- c360 resolution (0.25°, nominally 25x25 km^2)
- 72 layers (surface to 0.01 hPa)

Chemistry (e.g., O_3, NO_x, CO, VOCs, PM) and Meteorology on same resolution.

Data distributed via OpenDAP (https://opendap.nccs.nasa.gov/dods/gmao/geos-cf) and NCCS data portal weblink (https://portal.nccs.nasa.gov/datashare/gmao/geos-cf/):

- 15 minute "surface" fields (lowest model layer)
- 1-hour average and instantaneous 2D & 3D chemistry and meteorology fields

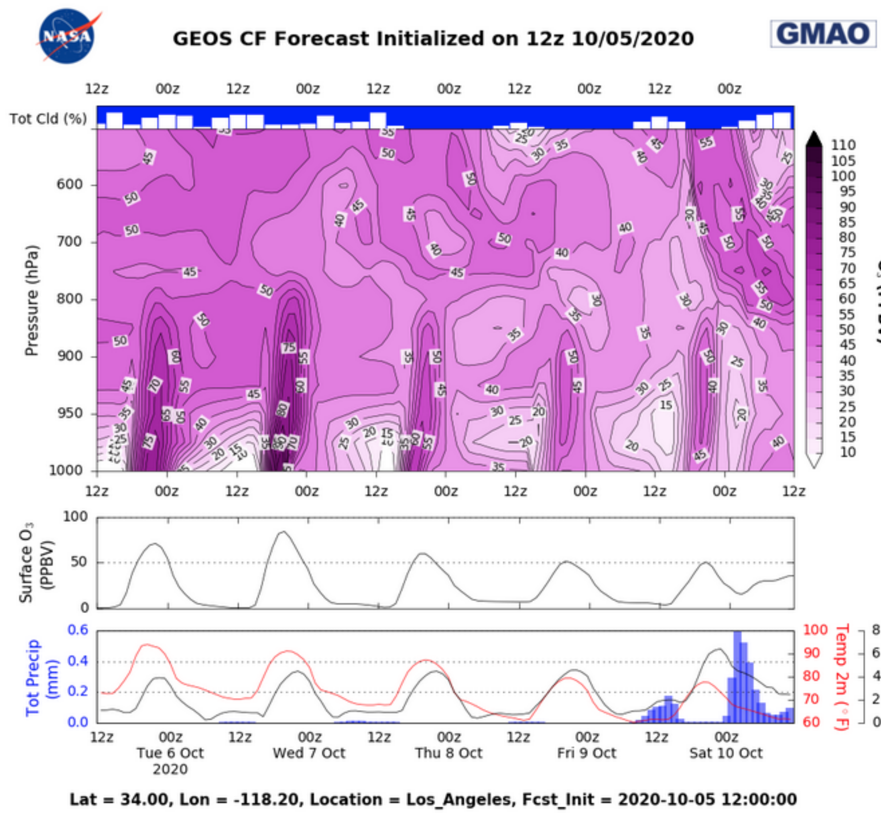
For more information on GEOS-CF products (https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/).

Forecast prepopulated and on-demand imagery available on https://fluid.nccs.nasa.gov/cf/ (https://fluid.nccs.nasa.gov/cf/)

GMAO GEOS CF Datagrams

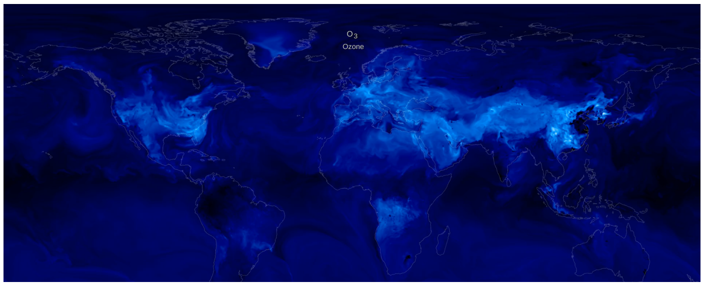
O3 at Los Angeles (34.00, -118.20)

CO | NO_2 | O_3 | PM 2.5 | SO_2

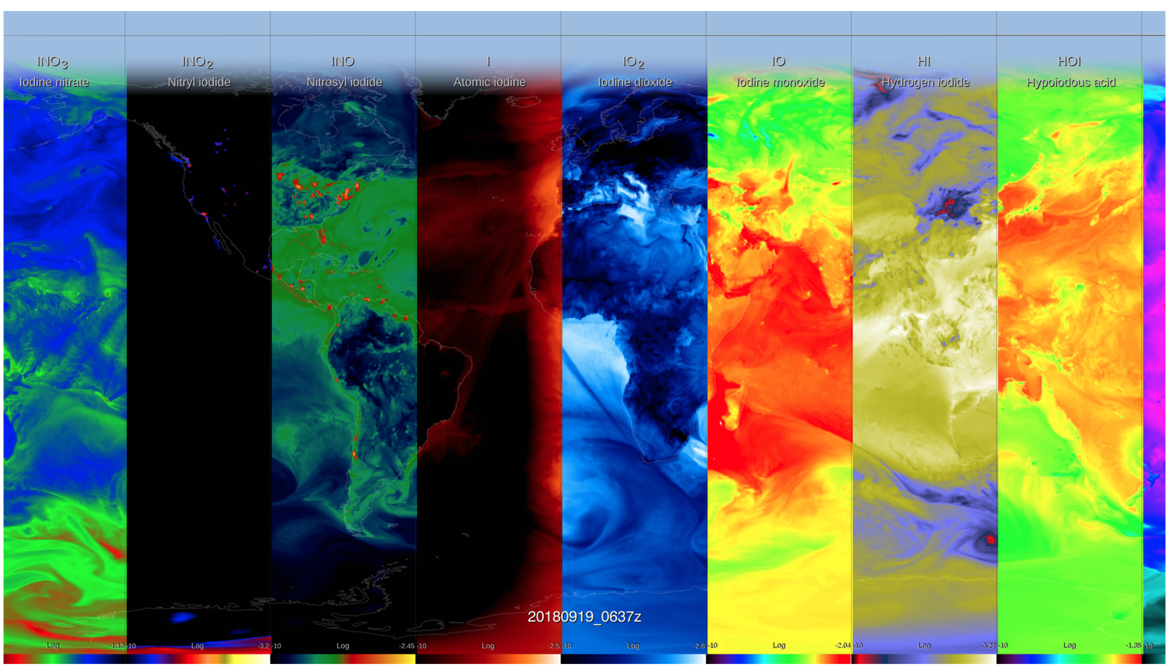


(https://fluid.nccs.nasa.gov/gram/cf_o3/34.0x-118.2/)

ATMOSPHERIC CHEMISTRY IS COMPUTATIONALLY EXPENSIVE



GEOS-CF is powered by GEOS-Chem, a state-of-the science chemistry transport model maintained by Harvard University with a global community of developers and users. It is a complex chemistry model, with full tropospheric and stratospheric chemistry with about 250 reactive species and over 700 reactions in the version 12 currently implement in GEOS-CF. The above video (https://svs.gsfc.nasa.gov/4754) produced in 2019 by NASA Goddard's Scientific Visualization Studio, illustrates the complexity in simulating surface ozone (https://svs.gsfc.nasa.gov/4764). First one can see the diurnal cycle of surface ozone, with highest concentrations in white during the day close to urban centers and near forest fires, while at night the ozone is low in these urban areas due to NO_x titration. It then marches through 96 different chemical species which either directly or indirectly impact ozone chemistry.

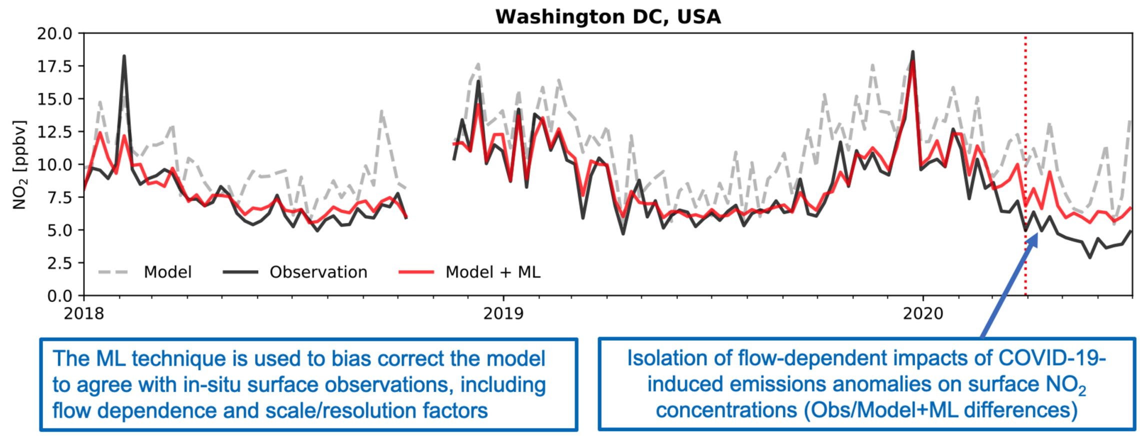


The GEOS-CF is run at the highest horizontal resolution of a global composition forecast system that we are aware of, at 0.25

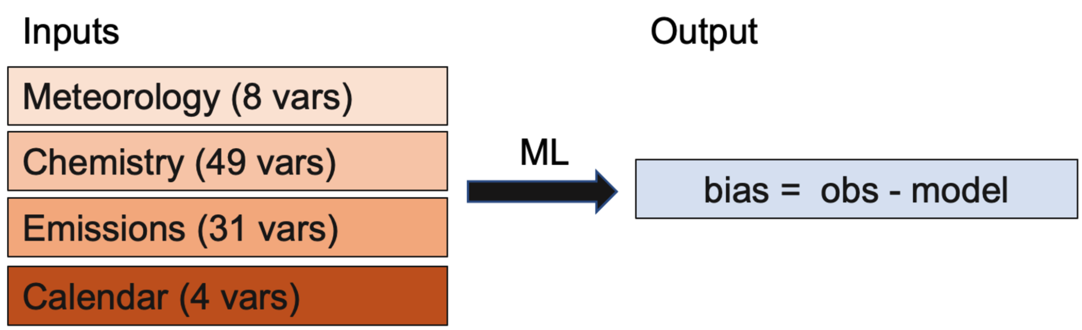
degree, and both the chemistry and meteorology forecasts are freely available to the public.

Since the end of each 1-day replay analysis is the start of the next day's simulation, the GEOS-CF also provides a continuous 3D atmospheric composition product since January 1, 2018.

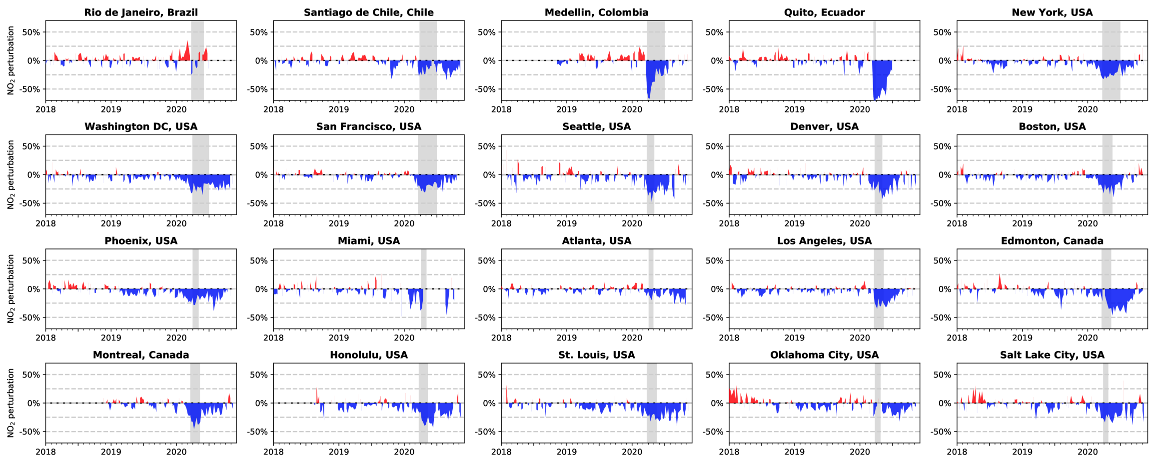
MACHINE LEARNING TO BIAS-CORRECT SUB-GRIDSCALE VARIABILITY



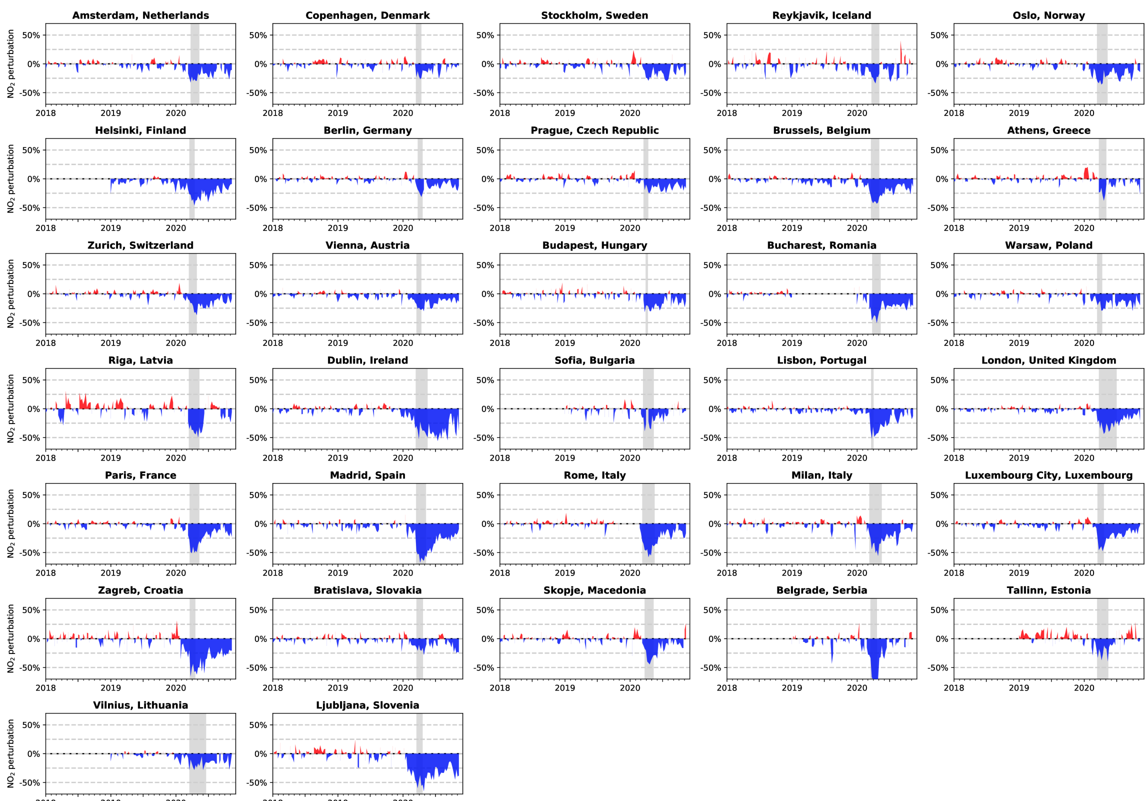
To correct for small scale variability and/or systemic model biases, a bias-correction algorithm has been developed based on comparisons of GEOS-CF model output against surface observations. The bias-correction is performed using the XGBoost machine learning algorithm, which uses as inputs 88 model diagnostics from the GEOS-CF (meteorology, chemistry, and emissions) and 4 inputs related to date and time.



The above time series is an example based on the "Global Impact of COVID-19 Restrictions on the Surface Concentrations of Nitrogen Dioxide and Ozone (https://acp.copernicus.org/preprints/acp-2020-685/)" where the machine learning algorithm for each station is trained with 50 % of the observed data in 2018 and 2019 (randomly selected) and the other half was used to validate. In the GEOS-CF model, real-time updates in the emissions are not consider so the bias-correction predicts pollutant concentrations for "business as usual" scenario for 2020; the deviation of observed from the business as usual quantifies the impact of COVID-19 restrictions on surface pollutant concentrations. Below, shows NO_2 changes at cities in North and South America (grey indicates periods of lockdowns):

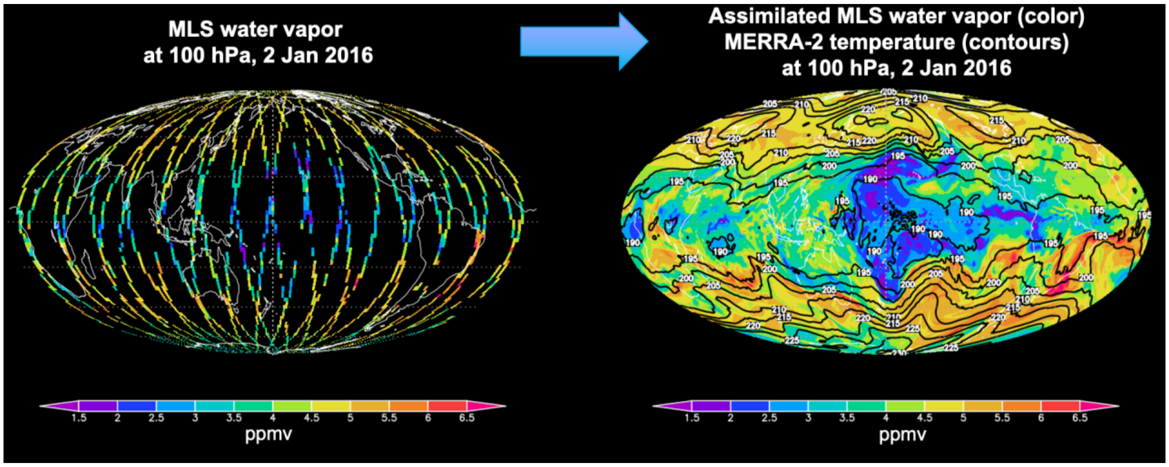


and across Europe:



Many locations experienced a reduction on the order of 25% in NO_2 concentrations. As the world faces a second wave of COVID-19, we will continue to monitor the impacts of activity restrictions on air quality (https://cms.nasa.gov/feature/goddard/2020/nasa-model-reveals-how-much-covid-related-pollution-levels-deviated-from-the-norm).

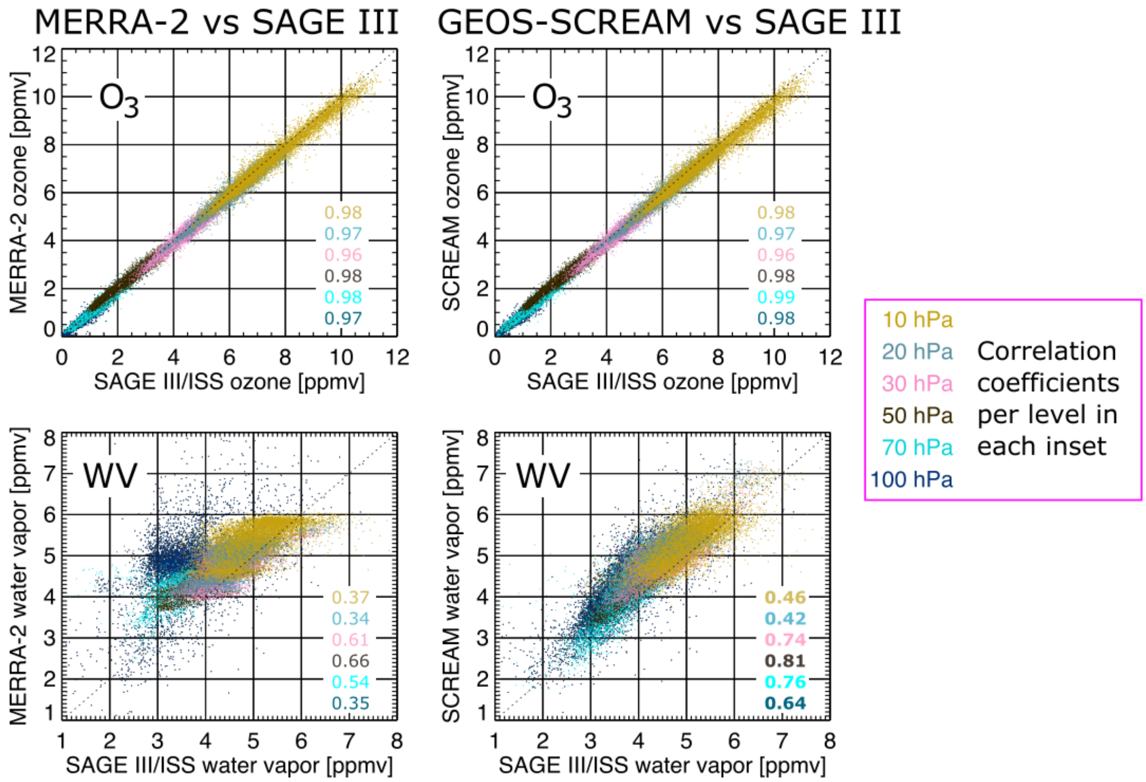
GEOS CONSTITUENT DATA ASSIMILATION SYSTEM (CODAS)



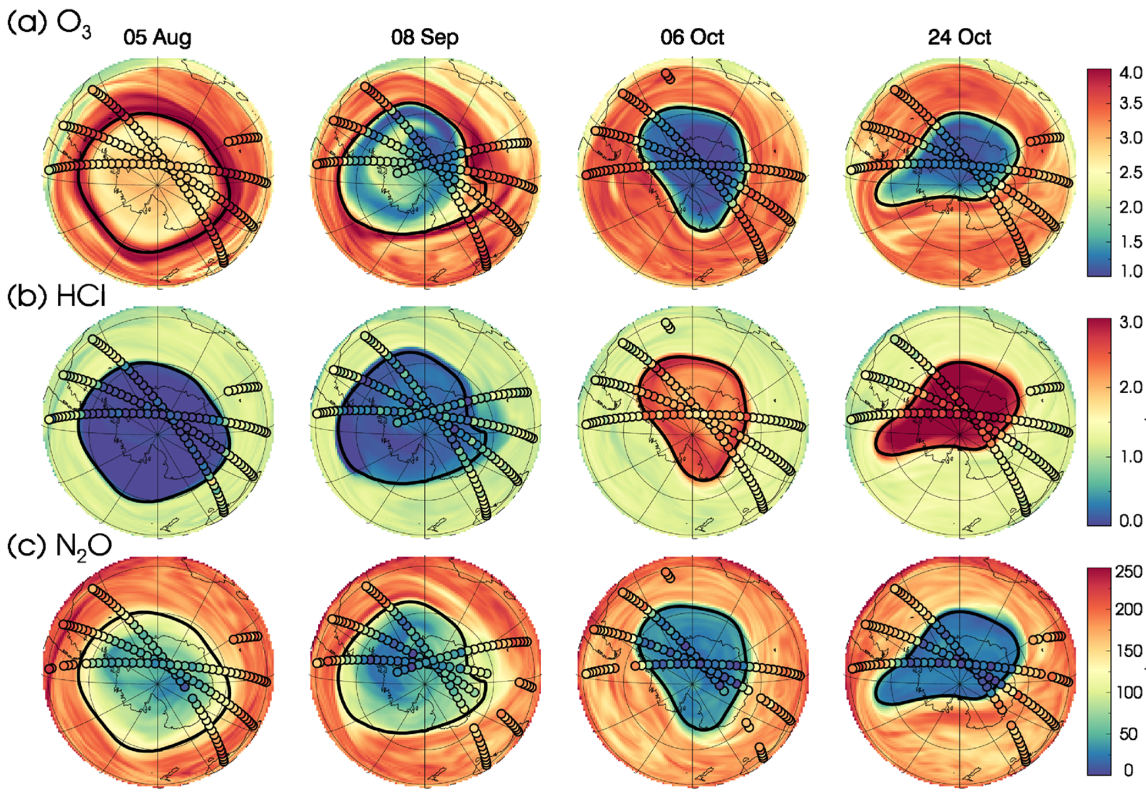
NASA's GMAO specializes in data assimilation, a method of combining and propagating information from observations in space and time using the governing equations for the atmospheric state and error estimates, to generate high spatiotemporal resolution global distributions of atmospheric composition even from relatively sparse data by updating the prior conditions obtained from previous assimilation steps. The advantage of a global data assimilation system is that it is designed to handle the non-uniform sampling of satellite observations.

While there is currently no direct data assimilation of chemical constituents in the GEOS-CF system, stratospheric ozone and biomass burning emissions are constrained by near-real-time satellite-based observations.

Future development in the GEOS-CF system will be to include data assimilation of constituent species. The novel multi-species GEOS Stratospheric Composition REanalysis with Aura MLS (GEOS-SCREAM) product uses the GEOS Constituent Data Assimilation System (CoDAS) capability, constrained by NASA's MERRA-2 reanalysis meteorology with a stratospheric chemistry mechanism "StratChem". The CoDAS framework has the capability to handle new observations of water vapor, ozone, and other chemical species.



It is essential for trend and climate analysis to have consistent well-constrained data products such as reanalyses. MERRA-2 assimilates ozone observations from instruments aboard the Aura satellite but has only simplified parameterized ozone chemistry. (Top) Despite differences in the complexity of stratospheric O_3 chemistry, the analyzed O_3 in both reanalyses have near perfect correlation with co-located 2018 SAGE III/ISS O_3. (Bottom) GEOS-SCREAM is among the first reanalysis products to assimilate stratospheric water vapor; reanalysis products were notoriously poor at capturing this field (Davis et al., 2017). It is the assimilation of MLS v4.2 water vapor in GEOS-SCREAM which has the greatest impact.



Besides assimilating MLS water vapor, GMAO also assimilated MLS HCl and N_2O. This plot reproduced from Wargan et al. (2020) (https://agupubs.onlinelibrary.wiley.com/doi/10.1029/2020JD033335) show some of the assimilated species along with MLS observed mixing ratios (circles) on the 520-K potential temperature surface. Constraining the model chemical species with observations improves the model's representation of stratospheric polar vortex chemistry which is important for monitoring the recovery of the stratospheric antarctic ozone hole.

ABSTRACT

NASA's Global Modeling and Assimilation Office (GMAO) produces high-resolution global forecasts for weather, aerosols, and air quality. The NASA Global Earth Observing System (GEOS) model has been expanded to provide global near-real-time 5-day forecasts of atmospheric composition at unprecedented horizontal resolution of 0.25 degrees (~25 km). This composition forecast system (GEOS-CF) combines the operational GEOS weather forecasting model with the state-of-the-science GEOS-Chem chemistry module (version 12) to provide detailed analysis of a wide range of air pollutants such as ozone, carbon monoxide, nitrogen oxides, 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 to include chemically reactive trace gases. We discuss current capabilities of the GEOS Constituent Data Assimilation System (CoDAS) to improve atmospheric composition modeling and possible future directions, notably incorporating new observations (TROPOMI, geostationary satellites) and machine learning techniques. We show how machine learning techniques can be used to correct for sub-grid-scale variability, which further improves model estimates at a given observation site.

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