Air Pollution Forecasts using the NASA GEOS model

K. Emma Knowland

USRA/GESTAR

NASA Global Modeling and Assimilation Office (GMAO)

In collaboration with:

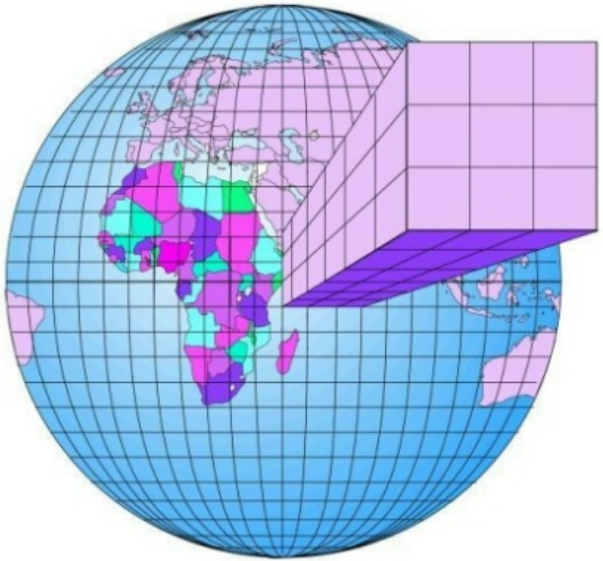
GMAO: Christoph Keller, Pamela Wales, Larry Coy, Kris Wargan, Lesley Ott, Steven Pawson

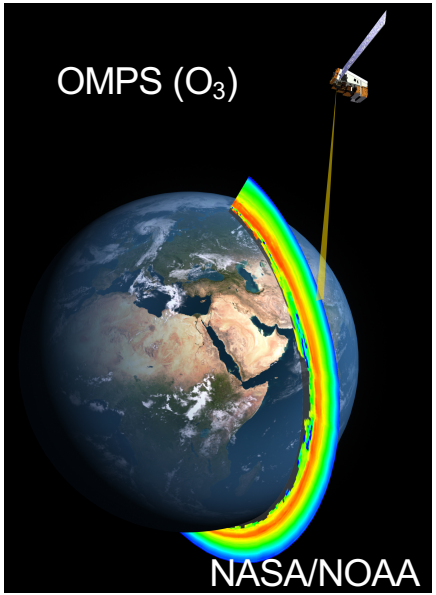
Atmospheric Chemistry and Dynamics Lab: Bryan Duncan, Sarah Strode, Junhua Liu, Julie Nicely, Dan Anderson, Eric Fleming

10 March 2021

NASA GMAO global meteorology and chemistry products

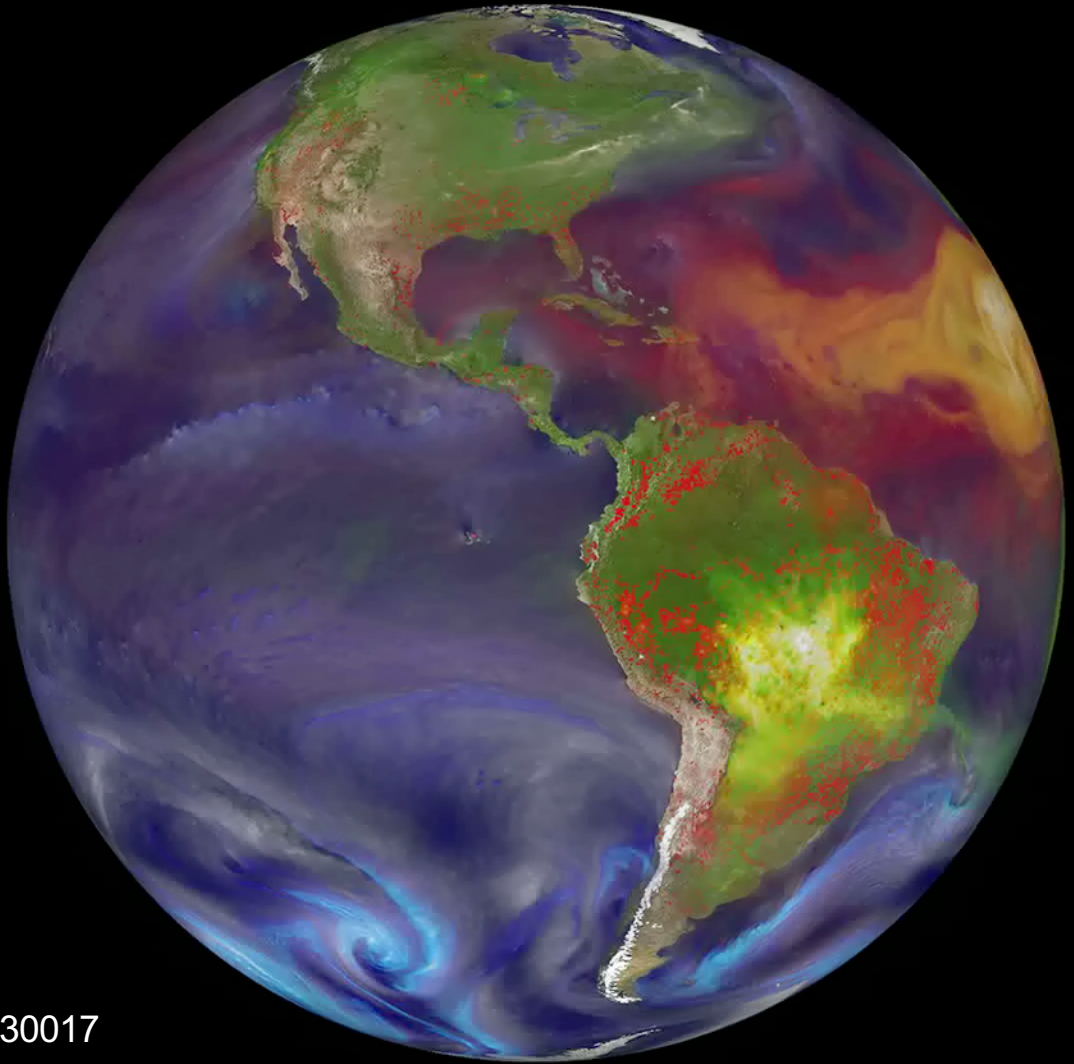
GEOS





www.nasa.gov

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov



https://svs.gsfc.nasa.gov/30017

NASA GMAO global meteorology and chemistry products

GEOS

Forecasting

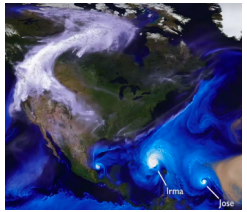
Reanalysis

GEOS FP

GEOS FP-IT

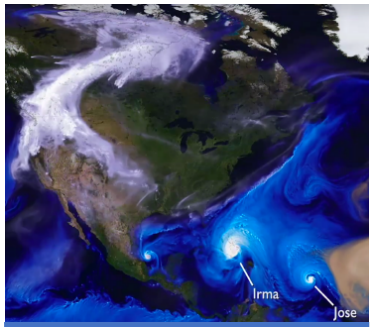
MERRA-2

GEOS-CF



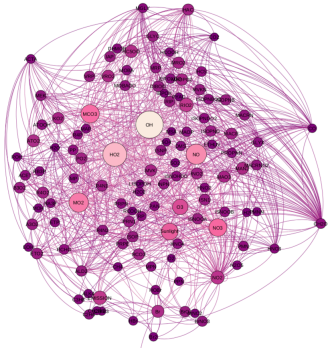
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

GEOS Composition Forecast

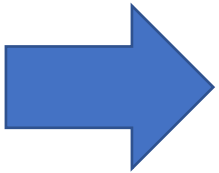


GEOS NWP





GEOS-Chem



GEOS - CF

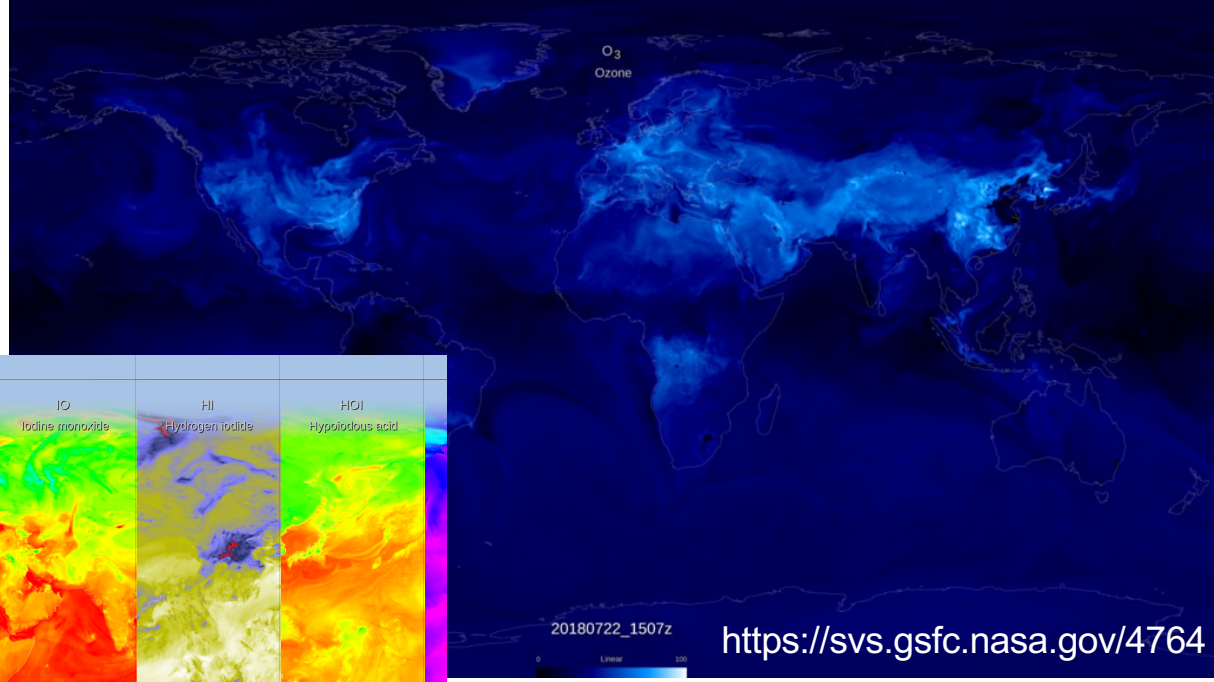
Summary of major GMAO products

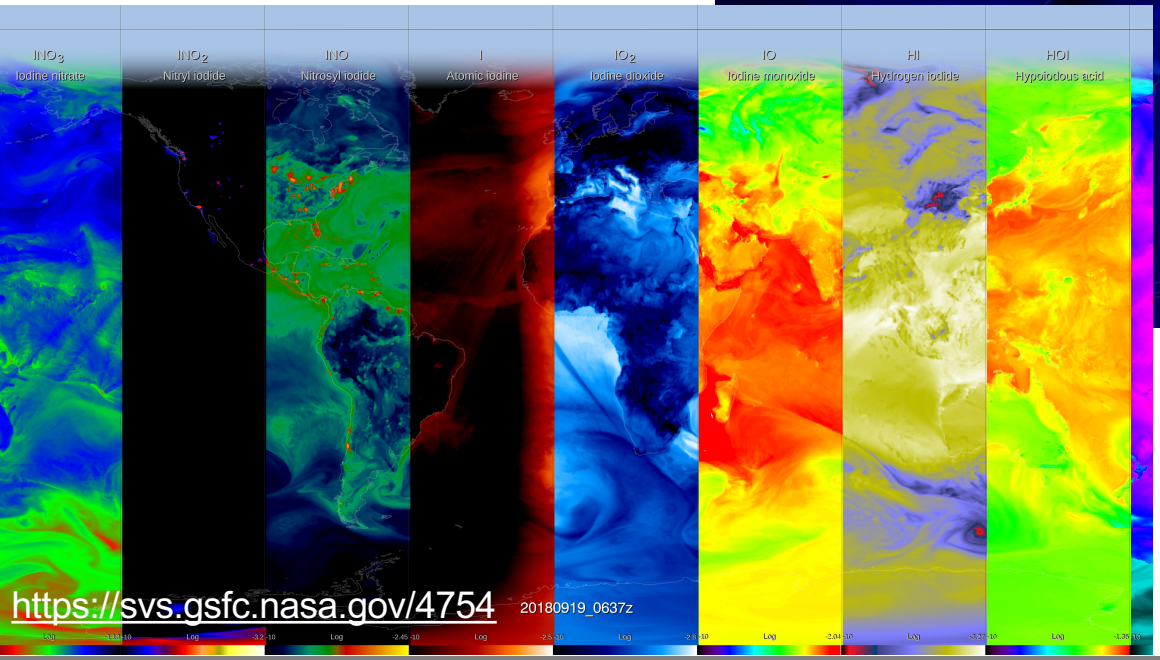
System	Focus	Customers/Applications
GEOS-FP "weather prediction"	Impacts of NASA observations on NWP: forefront resolution and complexity	NASA Field Missions (weather, aerosols) Multiple Agencies: NOAA/FAA; NOAA field stations; NRL
GEOS-CF "air quality"	Pioneering global system for atmospheric composition using multiple NASA assets	Health/Air Quality studies (via NASA Applied Sciences) Multiple agencies: NIH, US Army Public Health Center, NOAA
GEOS-S2S "seasonal prediction"	Ensembles of coupled Earth System predictions, emphasizing NASA observations	National ensembles (NMME, SubX), drought/sea-ice prediction Multiple Agencies and international linkages
MERRA-2 "reanalysis"	Stable product for climate studies, emphasizing NASA data	Only current national reanalysis: USGCRP/NCA applications Interagency use: DoE, DoT, NOAA, …
GEOS-FPIT "mission support"	Stable, well validated, low-latency product for use by NASA instrument teams	More than 20 NASA Instrument Teams
GEOS-Nature Run "mission planning"	Complex Earth System simulations at fine resolution with obs. simulators	Planning for new space-based missions NOAA and broad community; DoE/Smithsonian; NSF

GMAO's current products that are documented both technically and through robust file specifications, well validated, and released to the broad community for research and applications

GEOS-Chem

- 250 Chemical Species
- 725 Chemical Reactions

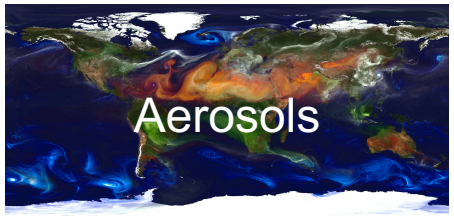


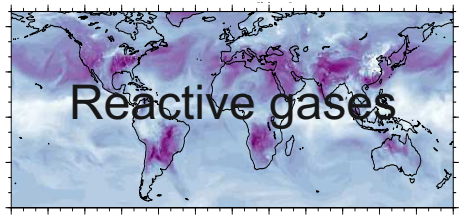


GEOS-Chem v12

- Tropospheric and Stratospheric chemistry

Aerosol and Gas Phase Chemistry





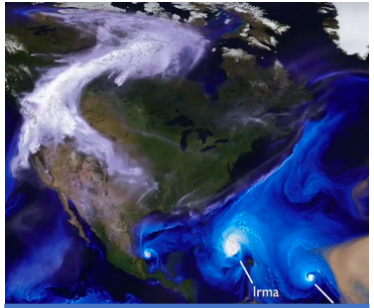
- Particulate matter:
  - Carbon
  - Sea salt
  - Dust
  - Sulfate
  - (Nitrate)
  - (Secondary Organics)

GOCART

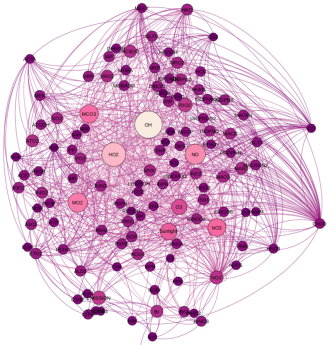
- Ozone (O_3)
- Nitrogen dioxide (NO_2)
- Carbon monoxide (CO)
- Volatile organic compounds (VOCs):
  - Formaldehyde
  - Benzene / Toluene
  - And many more!

GEOS-Chem

Daily composition forecast



GEOS FP-IT

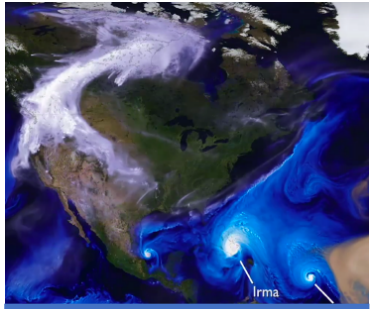


GEOS - Chem

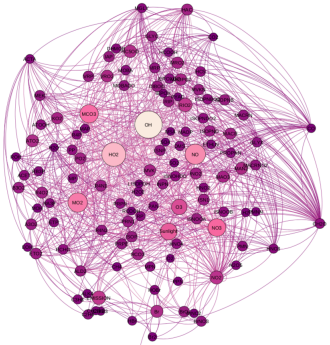
GEOS - CF

One **5-day forecast** per day

Daily composition forecast



GEOS FP-IT



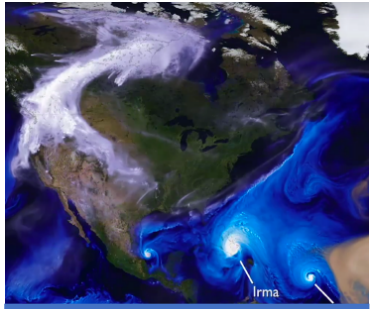
GEOS - Chem

GEOS - CF

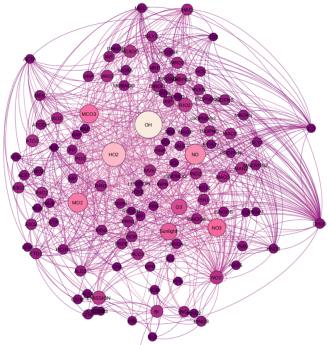
One **5-day forecast** per day

- 1-day meteorological replay "analysis"
- 5-day forecast

Daily composition forecast



GEOS FP-IT



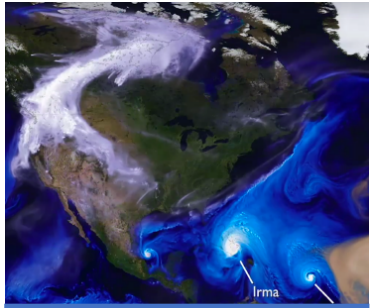
GEOS - Chem

GEOS - CF

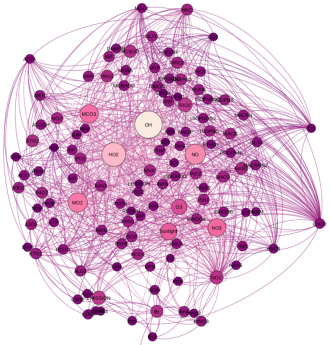
One **5-day forecast** per day

- 1-day replay
- 5-day forecast
- c360 (0.25°, **~25x25 km²**) resolution, 72 model layers

Daily composition forecast



GEOS FP-IT



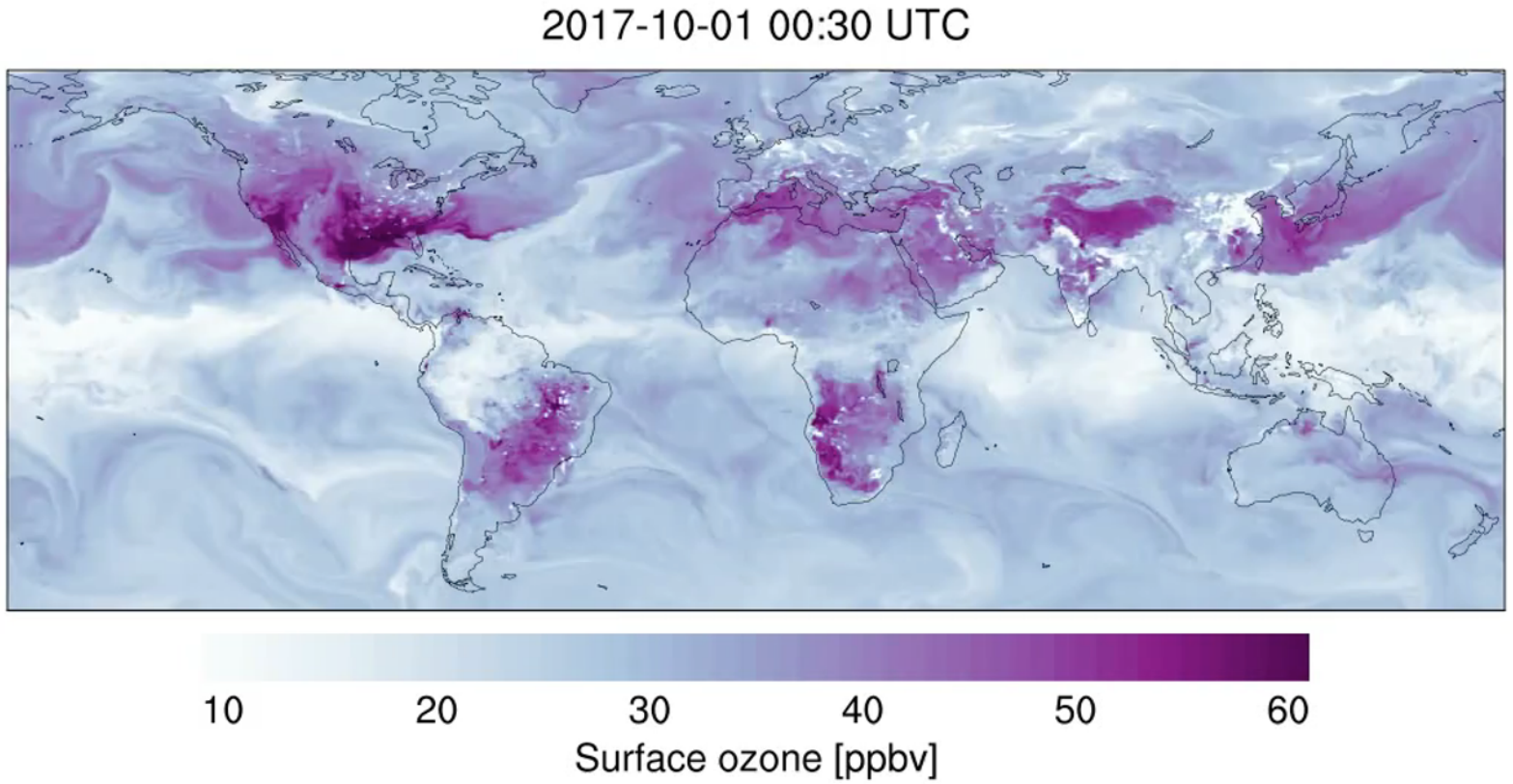
GEOS - Chem

GEOS - CF

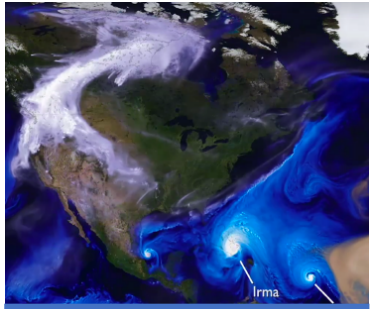
One **5-day forecast** per day

- 1-day replay
- 5-day forecast
- c360 (0.25°, **~25x25 km²**) resolution, 72 model layers
- O_3, NO_x, VOCs, PM ...
- T, U, V, RH ....

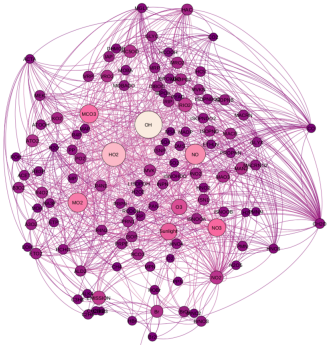
High-Resolution Global Simulation



Daily composition forecast



GEOS FP-IT



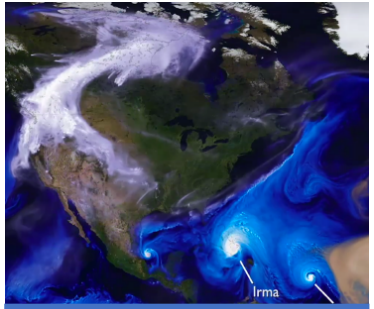
GEOS - Chem

GEOS - CF

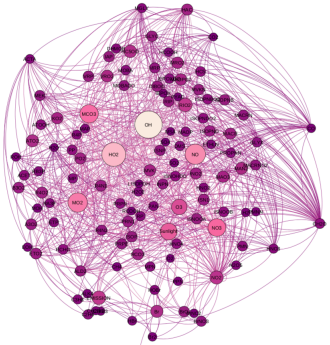
One **5-day forecast** per day

- 1-day replay
- 5-day forecast
- c360 (0.25°, ~25x25 km^2)
- **15 minute** "surface"
- **1-hour** average and instantaneous 2D & 3D

Daily composition forecast



GEOS FP-IT



GEOS - Chem

GEOS - CF

One **5-day forecast** per day

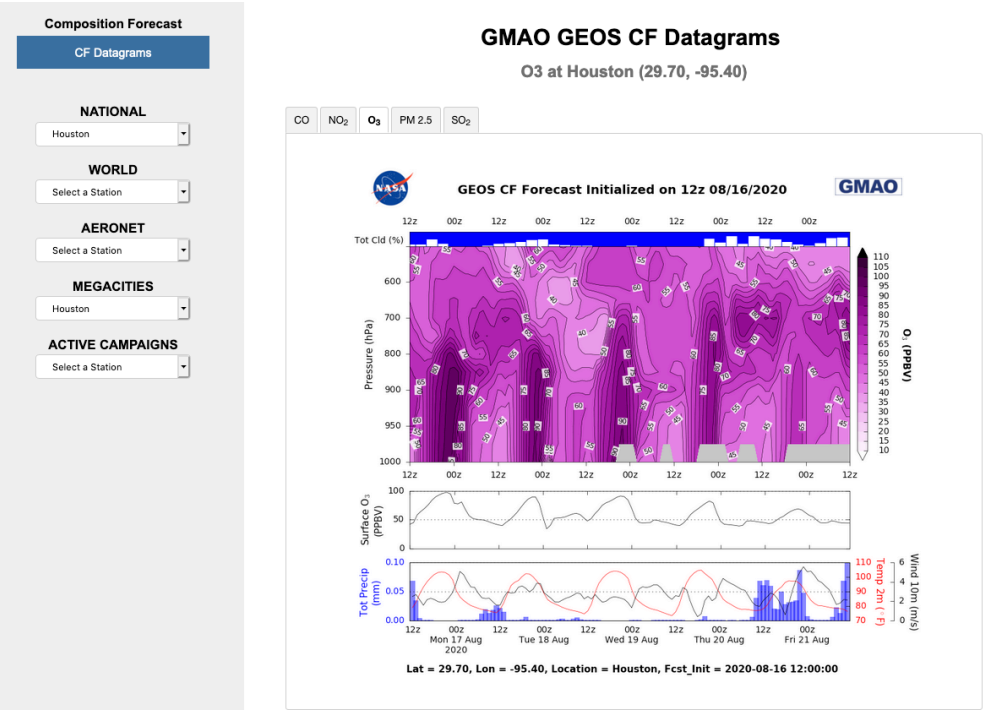
- 1-day replay
- 5-day forecast
- c360 (0.25°, ~25x25 km^2)

- **Available since 1 January 2018**

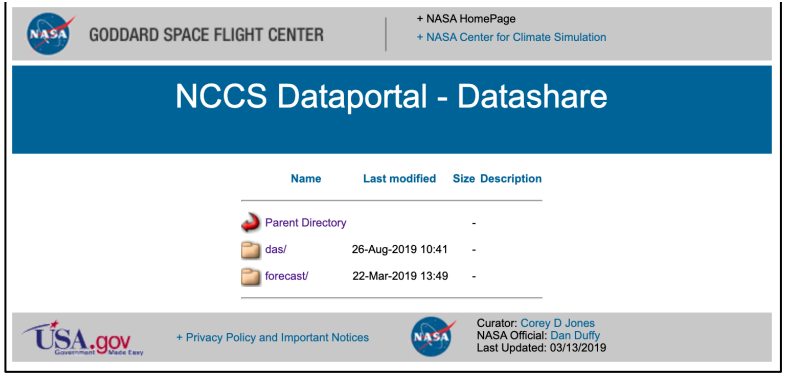
GEOS-CF are available online in near real-time

FLUID is a mobile-friendly website

https://fluid.nccs.nasa.gov/cf/



https://portal.nccs.nasa.gov/datashare/gmao/geos-cf/v1/



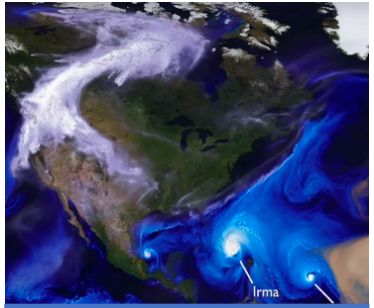
https://opendap.nccs.nasa.gov/dods/gmao/geos-cf/

GrADS Data Server - info for /gmao/geos-cf/assim/chm_tavg_1hr_g1440x721_v1 : dds das

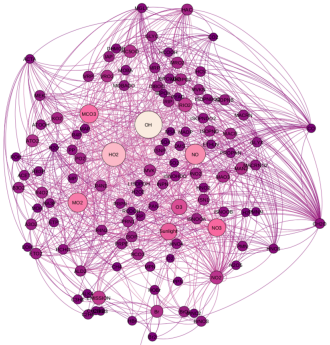
OPeNDAP/DODS Data URL: https://opendap.nccs.nasa.gov/dods/gmao/geos-cf/assim/chm_tavg_1hr_g1440x721_v1

Description:	GEOS CF (Composition Forecast)	
Documentation:	(none provided)	
Longitude:	-180.00000000000°E to 179.75000000000°E	(1440 points, avg. res. 0.25°)
Latitude:	-90.00000000000°N to 90.00000000000°N	(721 points, avg. res. 0.25°)
Altitude:	72.00000000000 to 72.00000000000	(1 points)
Time:	00:30Z01JAN2018 to 11:30Z31OCT2019	(16044 points, avg. res. 0.042 days)
Variables:	**(total of 52)**	
xyle	xylene (c8h10, mw = 106.16 g mol-1) volume mixing ratio dry air	
dst2	dust aerosol, reff = 1.4 microns (mw = 29.00 g mol-1) volume mixing ratio dry air	
hno4	peroxynitric acid (hno4, mw = 79.00 g mol-1) volume mixing ratio dry air	
pm25su_rh35_gcc	sulfate_particulate_matter_with_diameter_below_2.5_um_rh_35	

Daily composition forecast



GEOS FP-IT



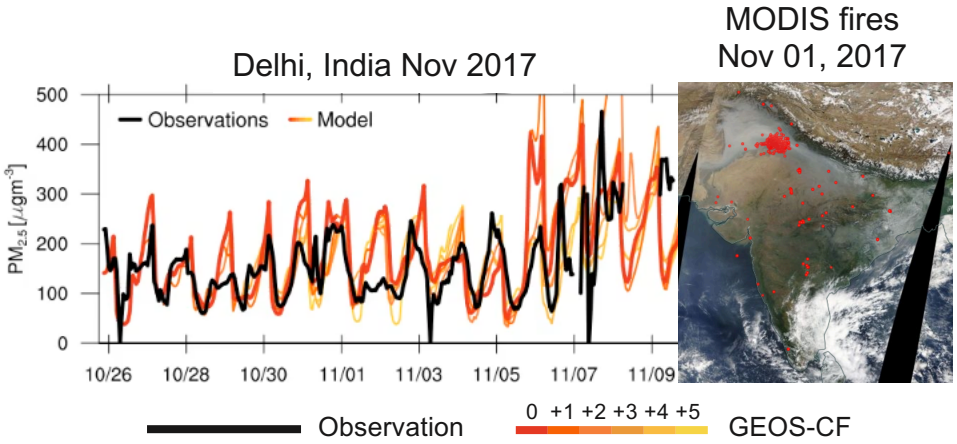
GEOS - Chem

GEOS - CF

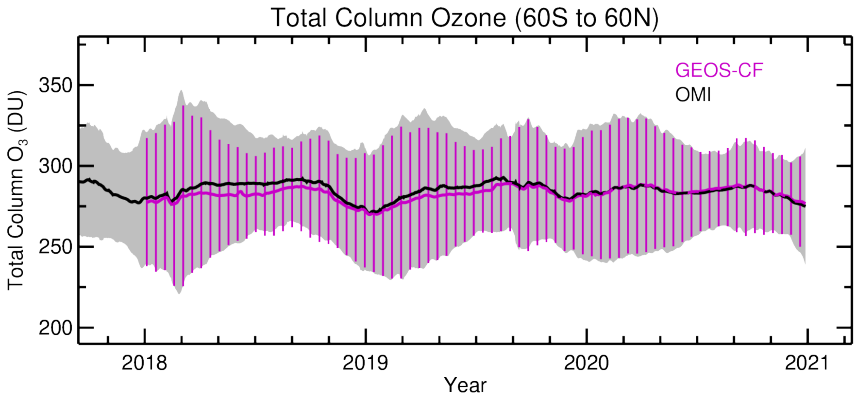
- Currently **no <u>direct</u> data assimilation of constituents** in GEOS-CF

Near-real time updates from satellite data

- Biomass burning emissions from near-real time QFED v2.5

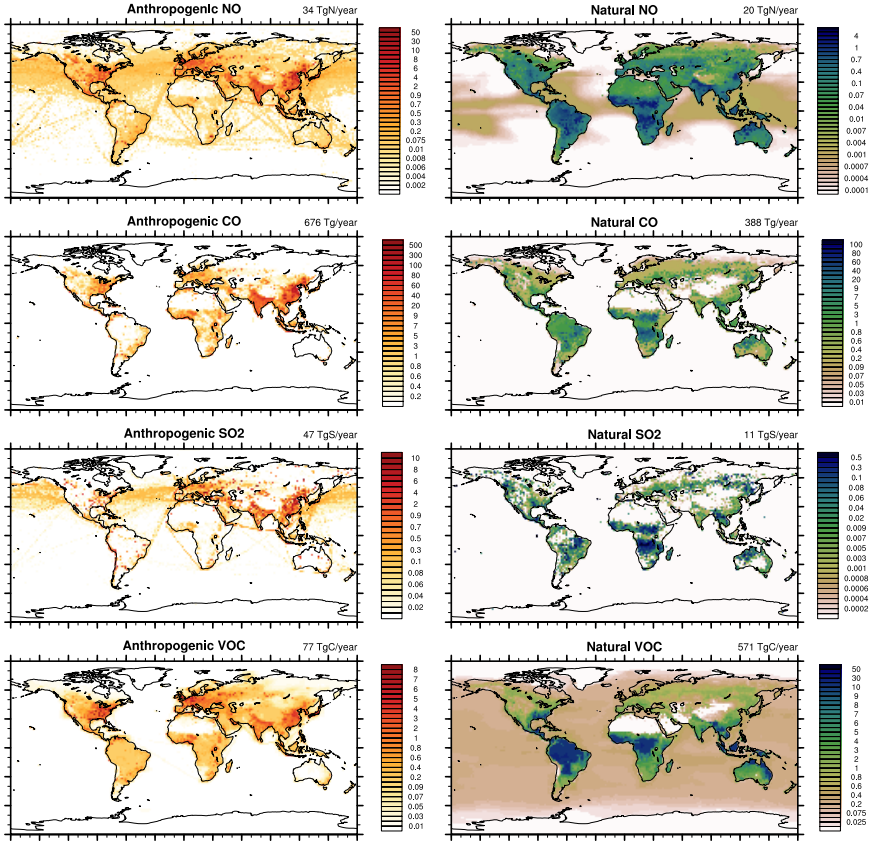


- GEOS-CF Stratospheric O_3 is weakly nudged to the GEOS FP assimilated O_3



k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

GEOS-Chem emissions



Anthropogenic: HTAP, RETRO, DICE (Africa), AEIC (aircraft)

Biomass burning: QFED NRT

Biogenic: Megan 2.1

Lightning: online (Murray et al., 2012)

Soil NOx: online (Hudman et al. 2012)

Dust: online (Zender et al. 2003)

Sea salt: online (Jaegle et al., 2011)

Ocean: online: sea salt, DMS, acetone, acetaldehyde, HOI, I_2

Prescribed: CFCs, VSLS, CH_4, CO_2

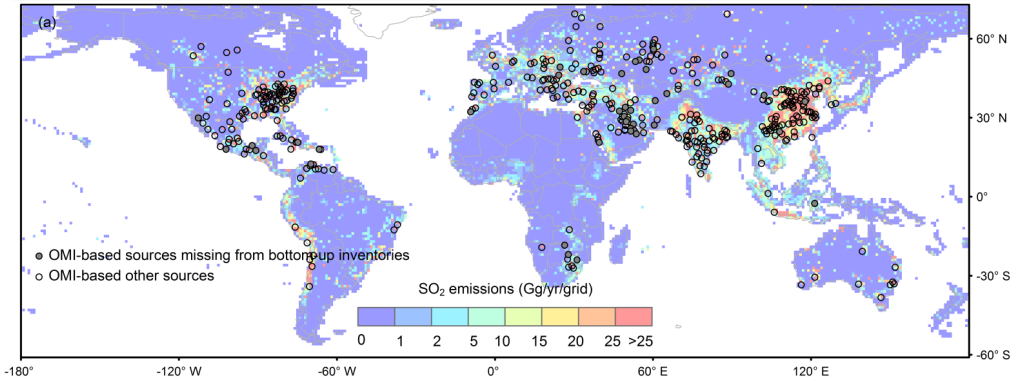
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Year-to-year emissions changes

Emissions:

- Annual gridded scale factors based on satellite data are applied to the emissions of CO (Oda et al., 2017) and SO_2 (Liu et al., 2018).
- "Business-as-usual" assumed for 2020 and 2021

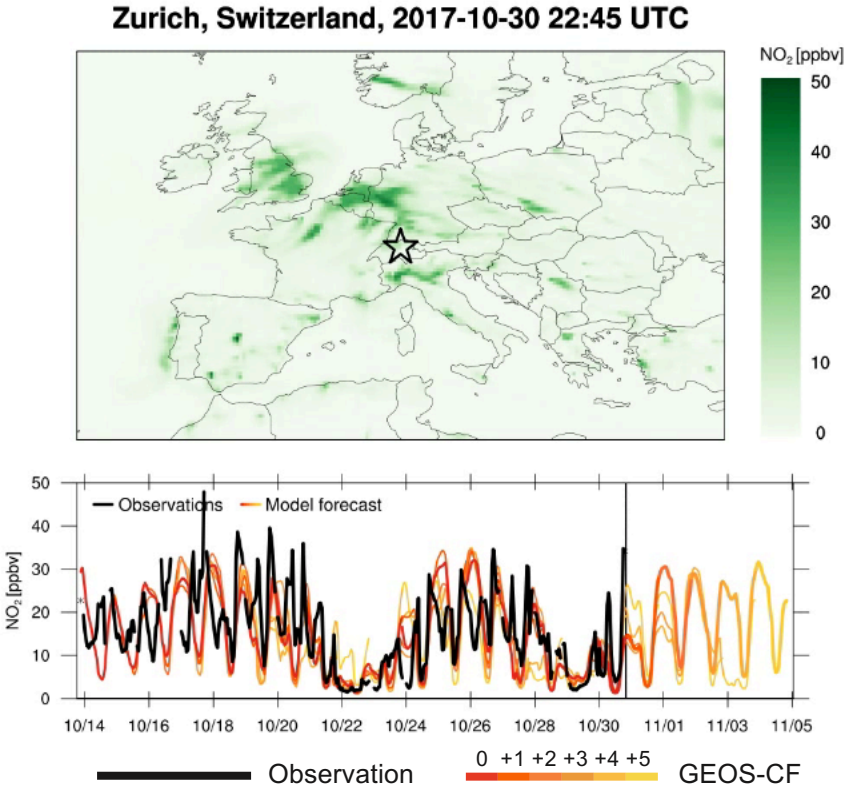
SO_2 emissions in the OMI-HTAP inventory



A new emission inventory, OMI-HTAP, combines OMI-based SO_2 emissions for large sources and the bottom-up inventory, HTAP, for smaller sources.

Liu, F., et al., *Atmos. Chem. Phys., 18*, 2018

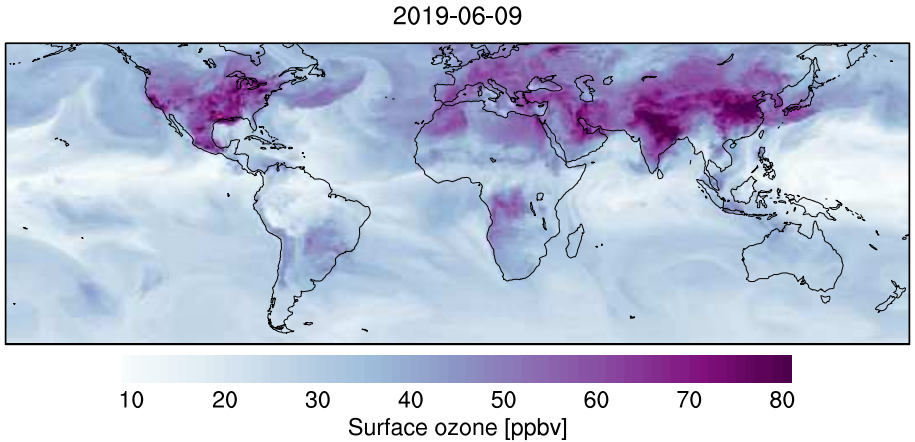
Daily variations of emissions



- Scale factors applied to emissions for diurnal and weekly variations
- These are clearly beneficial for surface NO_2 analyses and forecasts
- Shown for Zurich - weather and diurnal/weekly signals are prominent
- Surface observations obtained through emerging connection to OpenAQ (openaq.org)

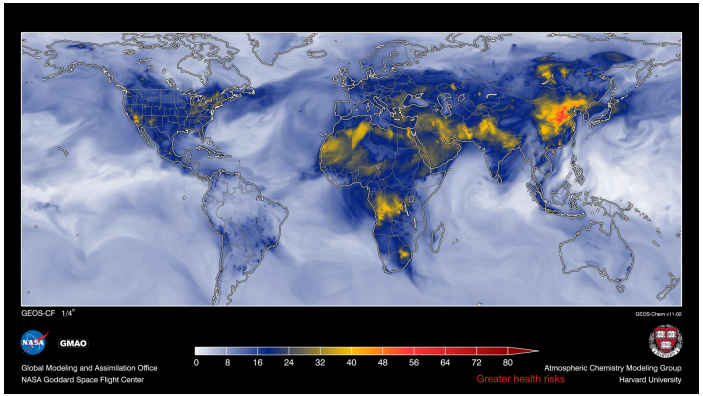
Air quality and health applications

➢ How good is the model?



Optimize model predictions

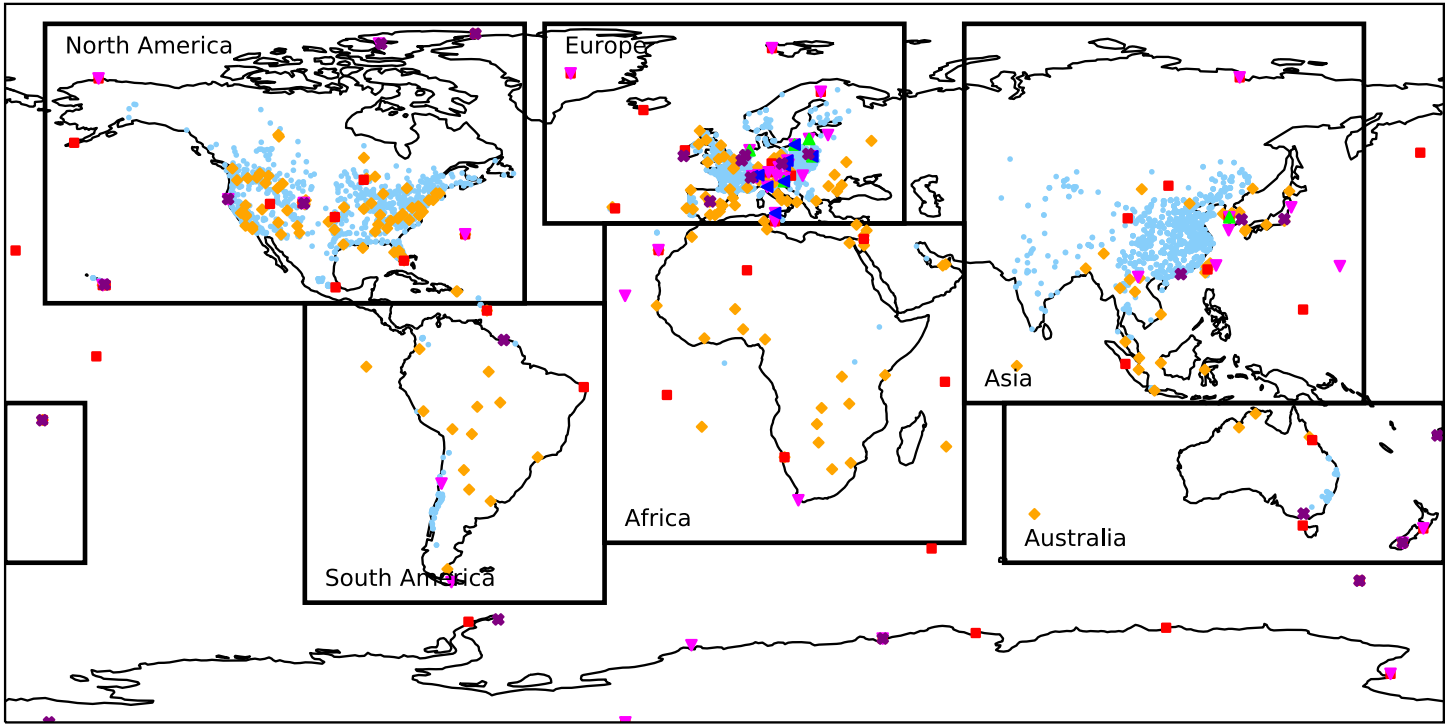
➢ How bad is the air pollution?



Global exposure assessment

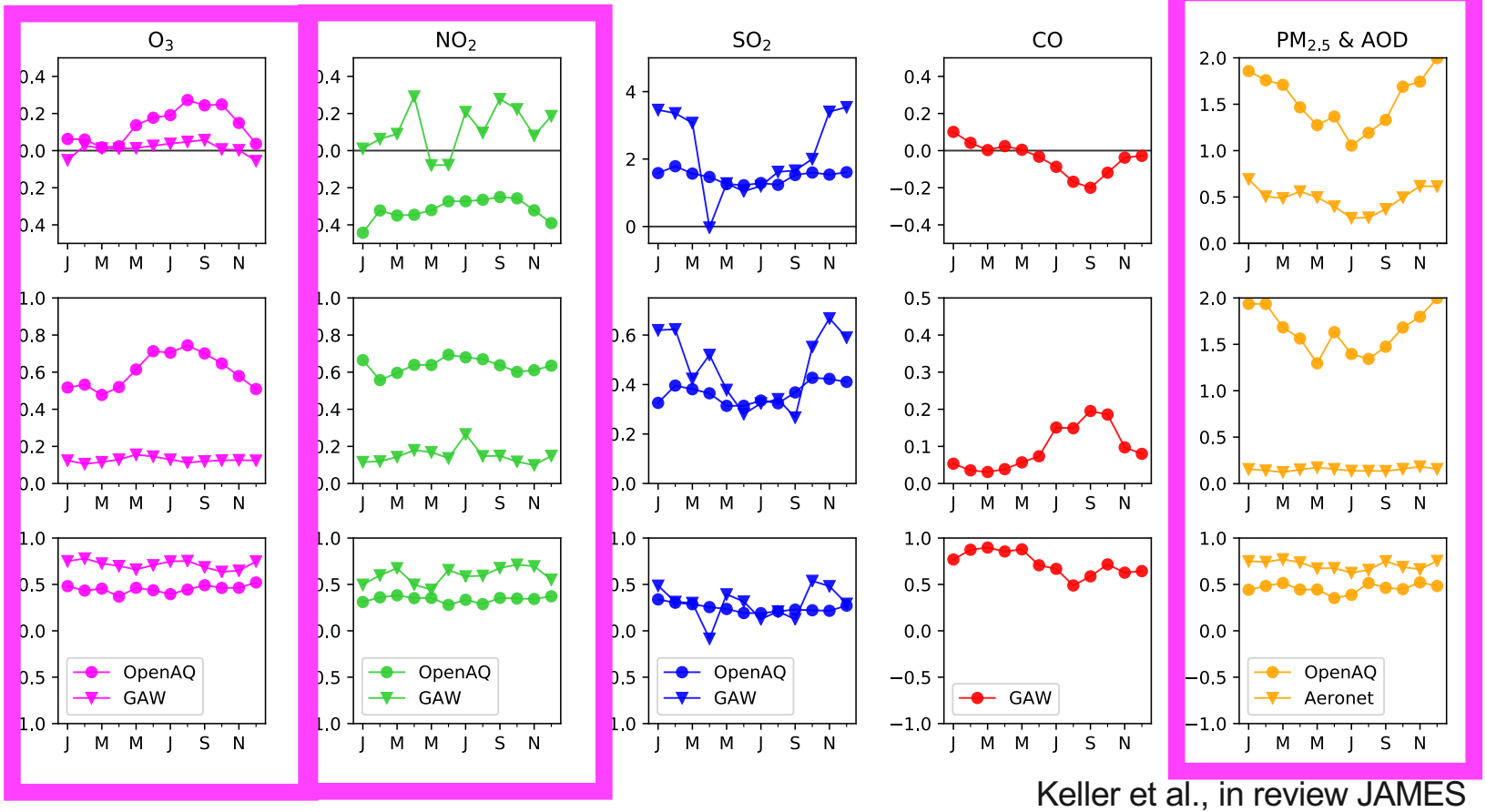
k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Observations for evaluation



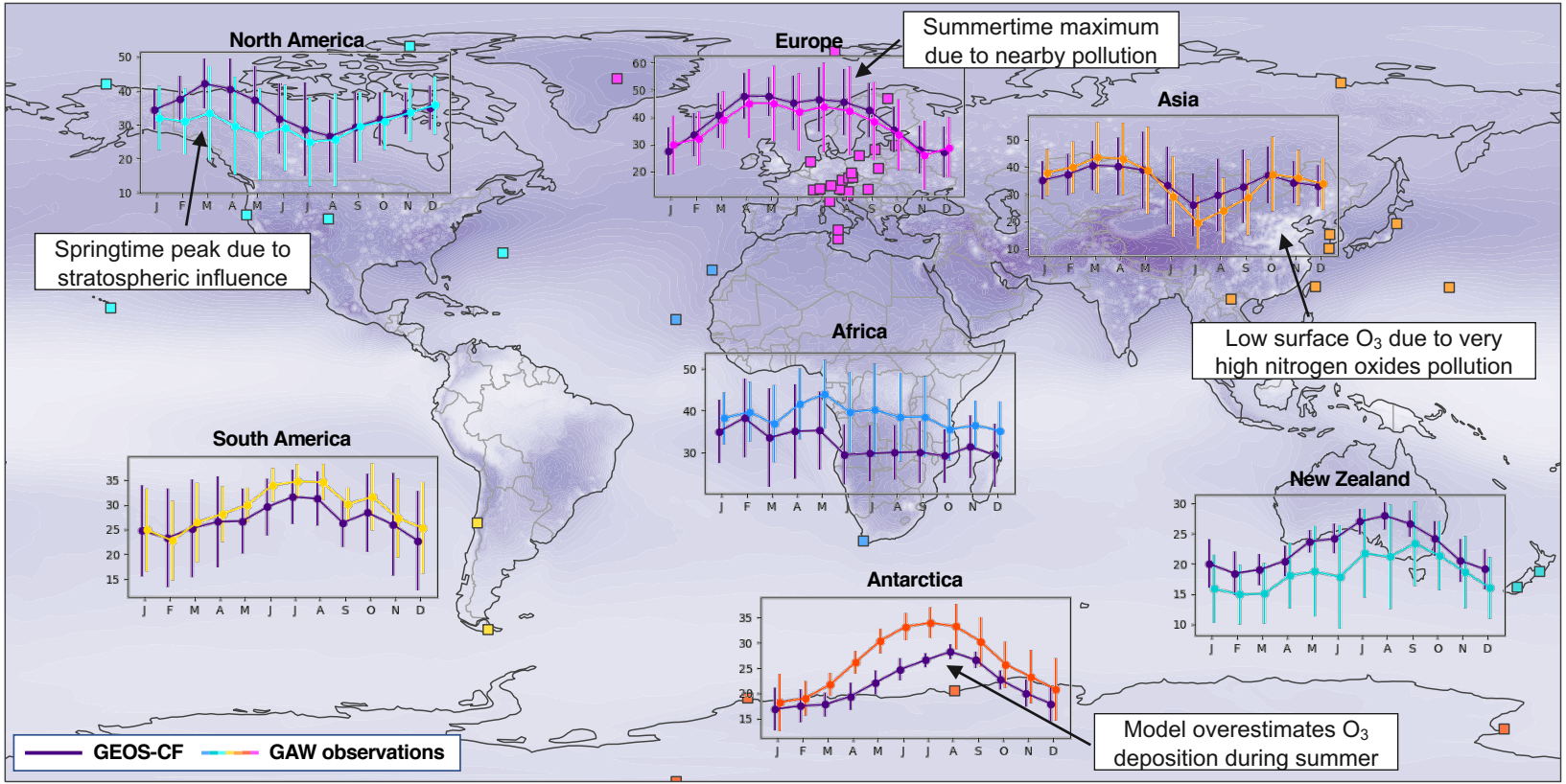
Keller et al., in review JAMES

Global surface comparisons - monthly

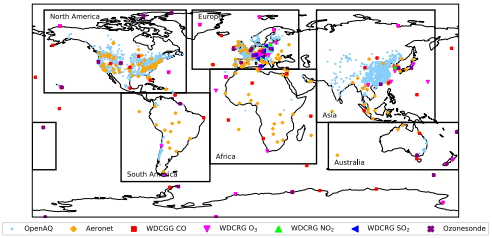


Keller et al., in review JAMES

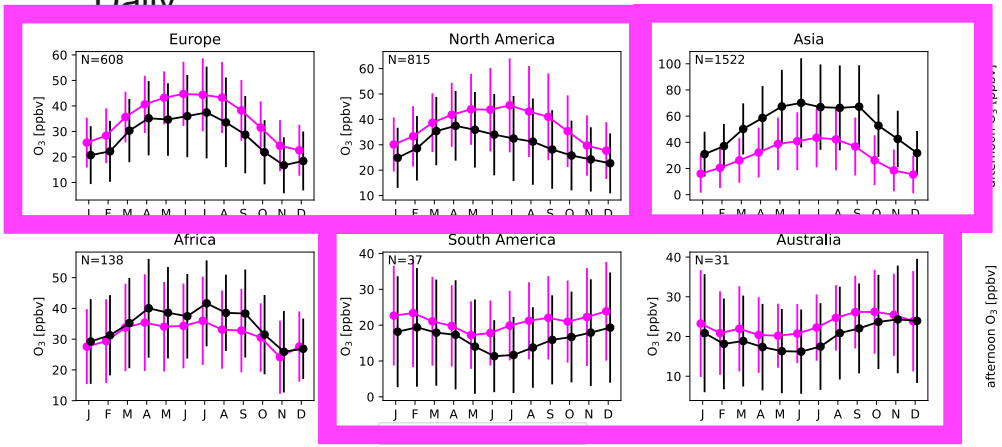
GEOS-CF surface ozone compares well against background observations from the Global Atmospheric Watch (GAW) network



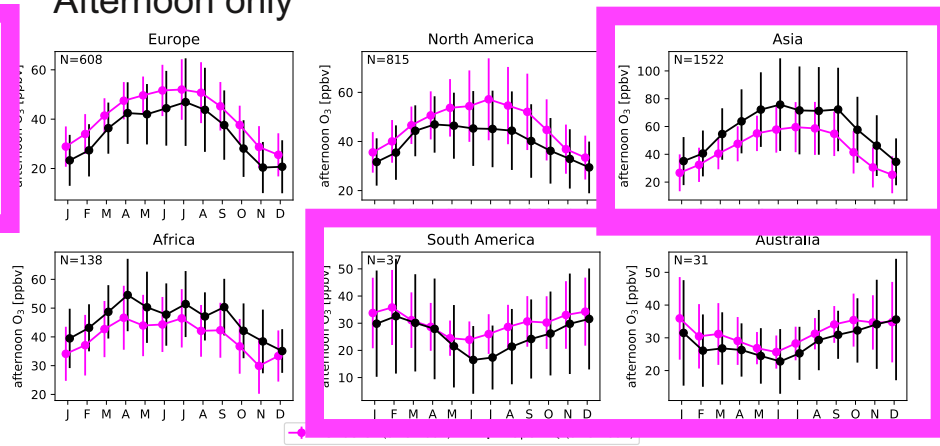
Surface O_3 (OpenAQ sites only)



Daily



Afternoon only

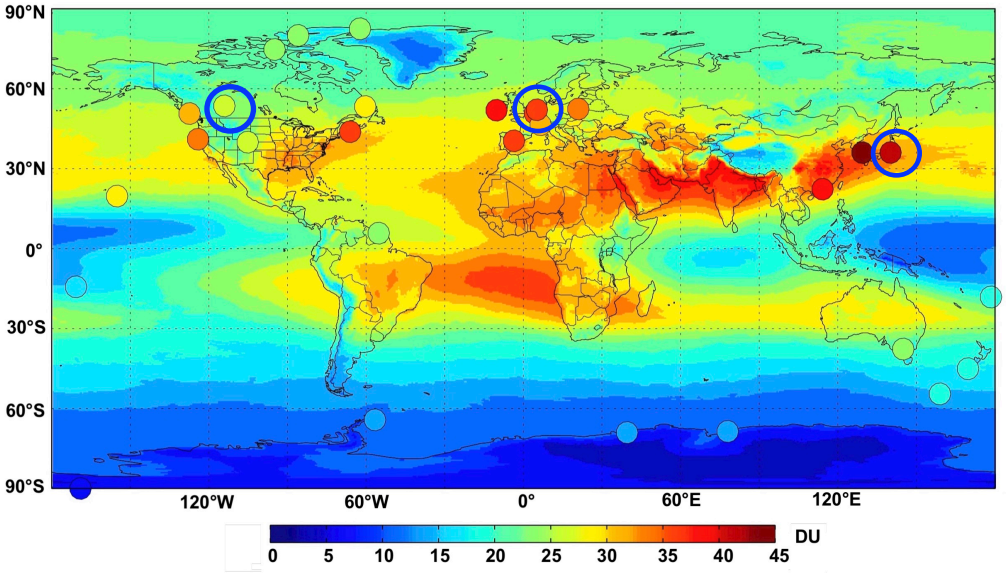


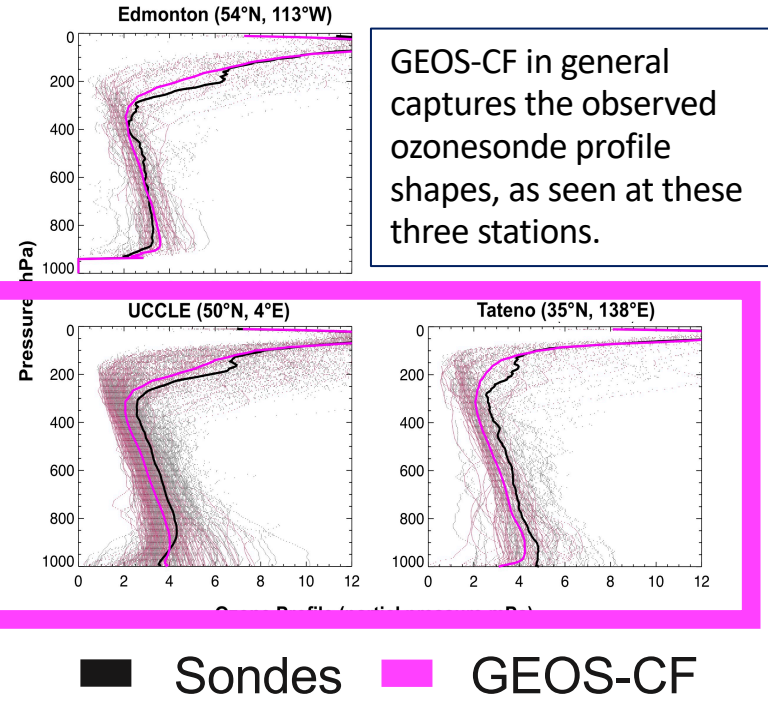
- GEOS-CF captures the overall seasonal cycle in the six regions, but generally overestimates in Europe, North & South America and Australia, while underestimating in Asia and Africa.
- In polluted regions, such as Asia, the bias is reduced when focusing on peak photochemical production period. GEOS-CF still has a bias over US during summer and fall, a known GEOS-Chem issue (Travis et al., 2016;2019; Hu et al., 2018).

Observations GEOS-CF Keller et al., in review JAMES

GEOS-CF captures the observed ozone spatial distribution and profile shapes shown by ozonesondes

2018 Tropospheric O_3 column (TOC): GEOS-CF and sondes





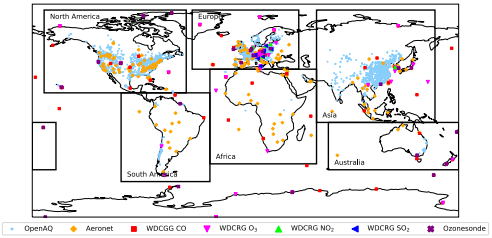
GEOS-CF in general captures the observed ozonesonde profile shapes, as seen at these three stations.

- GEOS-CF captures the overall spatial distribution of ozonesonde TOC, but with underestimates over polluted regions (e.g. sites over eastern US, Europe, east Asia).

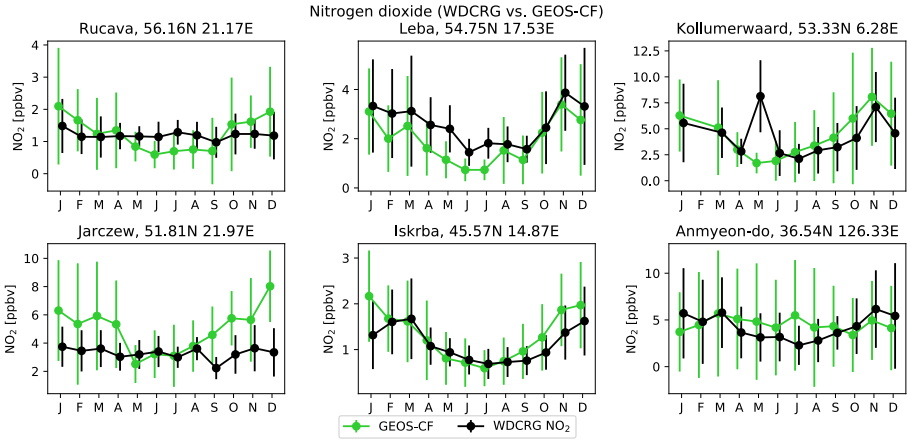
Figures courtesy of Junhua Liu

Thin lines: daily profiles in 2018
Thick lines: annual means

Surface NO_2

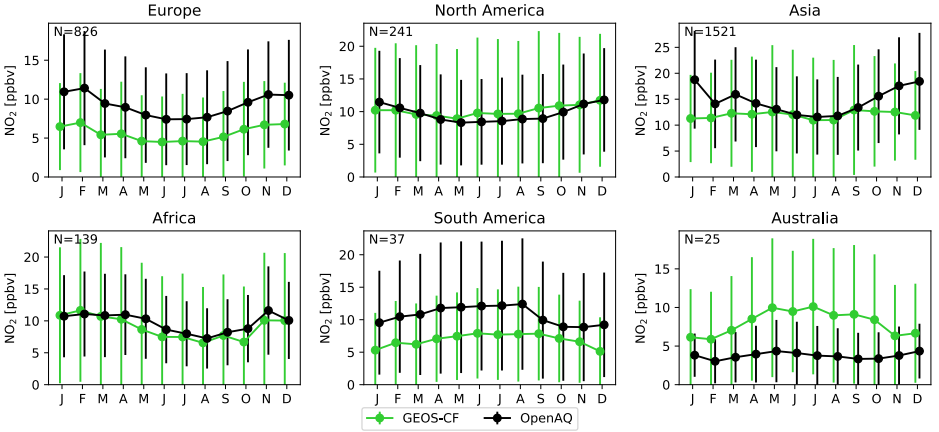


GAW sites (non-mountainous, European sites)



- Generally good agreement with background European surface NO_2.

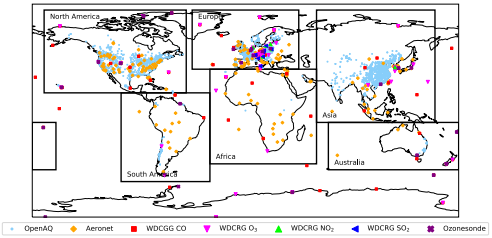
OpenAQ



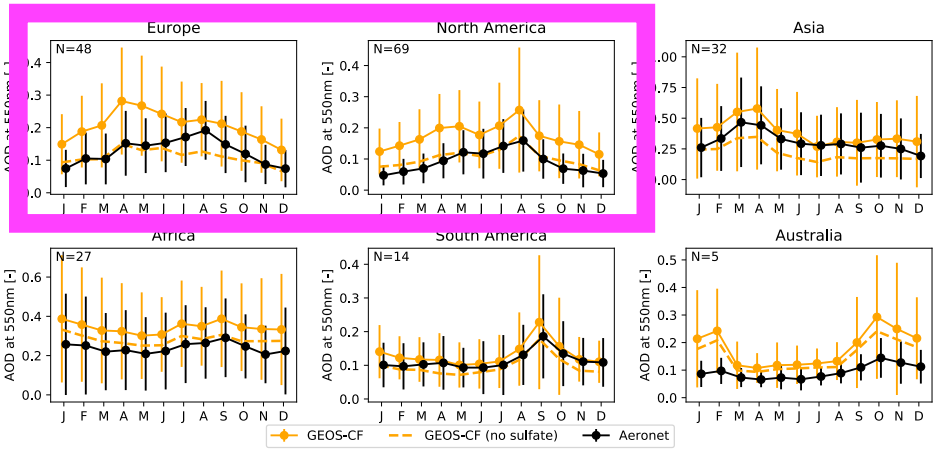
- Excellent agreement over North America, Africa, and summertime Asia.

Observations **GEOS-CF** Keller et al., in review JAMES

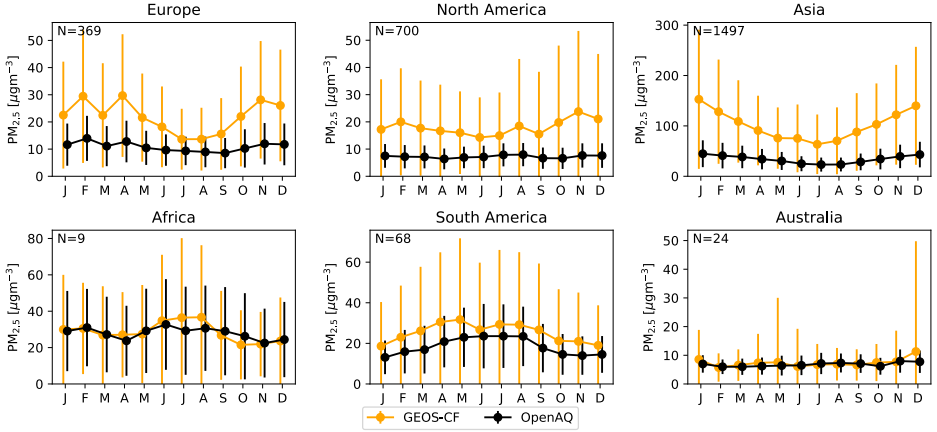
GEOS-CF generally overestimates aerosols (AOD and $PM_{2.5}$)



AOD from Aeronet network



PM2.5 from OpenAQ database

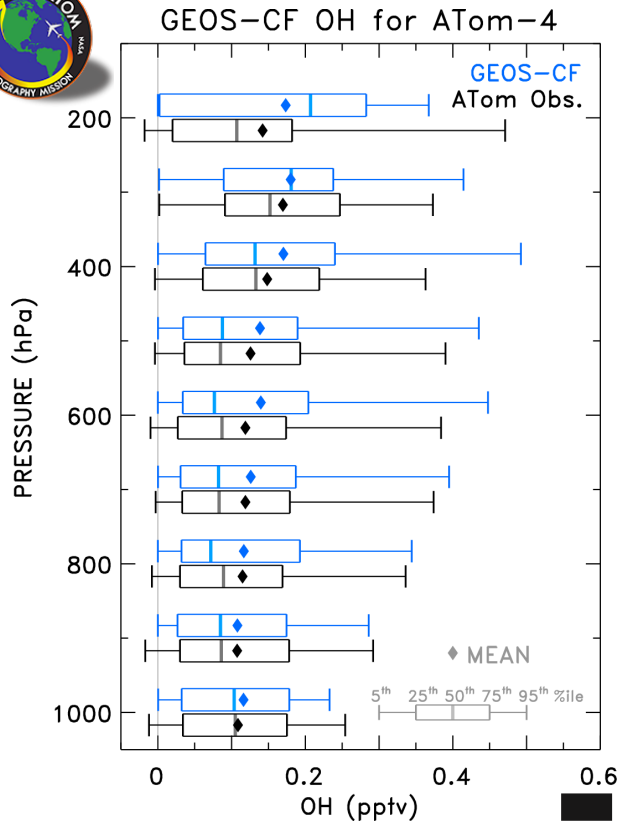


- GEOS-CF overestimates AOD 550 nm at most Aeronet sites. This is likely due to the overestimation of sulfates in the model.
- Similarly, GEOS-CF $PM_{2.5}$ is overestimated in Europe, North America, Asia and South America.

Observations GEOS-CF

Keller et al., in review JAMES

GEOS-CF oxidizing capacity of remote atmosphere compares well to ATom

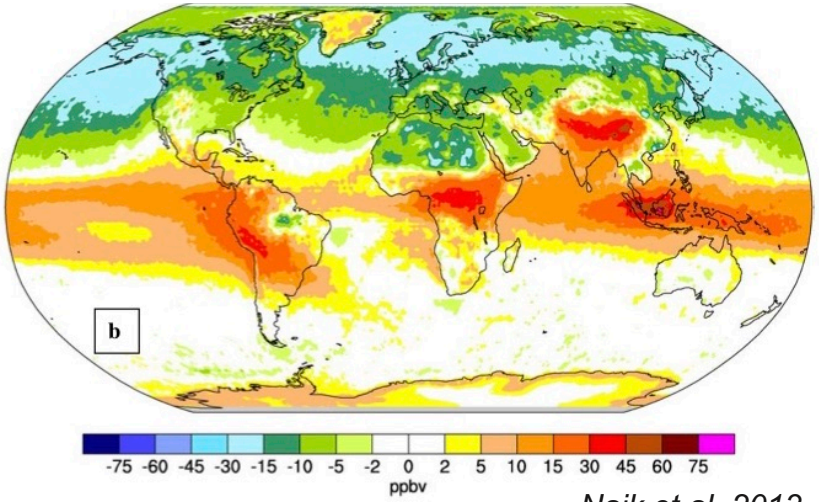


- The hydroxyl radical (OH) is the main tropospheric oxidant, controlling lifetimes of greenhouse gases including methane and initiating formation of secondary pollutants like ozone and aerosols
- OH is difficult to measure; the NASA Atmospheric Tomography Mission (ATom) airborne campaign conducted global-scale *in situ* measurements of OH
- The ATHOS instrument measured OH by laser-induced fluorescence on four deployments of the DC-8 aircraft, primarily over remote Pacific, Atlantic oceans
- GEOS-CF hourly model output was sampled along the flight tracks of the fourth deployment (ATom-4) for April-May 2018.
- Despite OH being difficult to model, distributions of OH compare well between GEOS-CF and observations from the surface to 300 hPa

Figure courtesy of Julie Nicely

GEOS-CF shows significant improvements in CO simulation, especially over NH

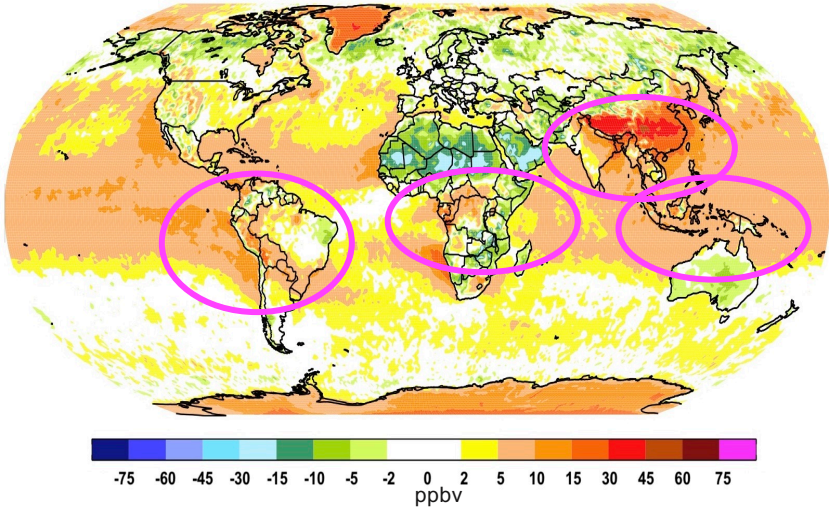
ACCMIP multi-model mean – MOPITT
(500 hPa, 2000-2006)



Naik et al. 2013, ACP

The ACCMIP multi-model mean underestimates the MOPITT CO at 500 hPa in the NH mid-high latitudes (up to 45 ppb), except over northern India and south-central China.

GEOS-CF – MOPITT
(500 hPa, 2018-2019)



GEOS-CF shows **significant improvements in CO simulation** except over south-central China:

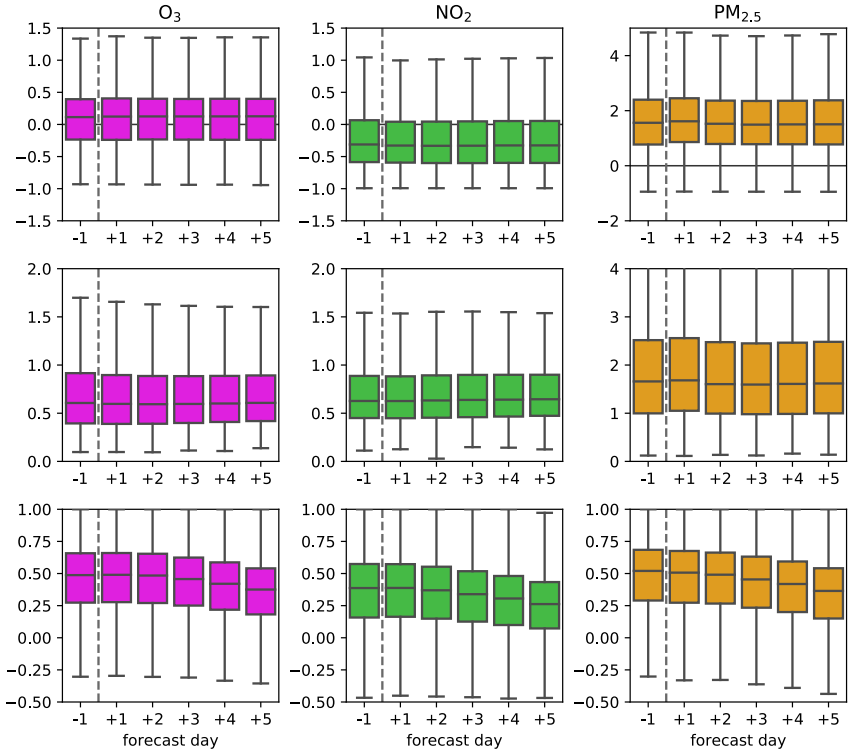
Figures courtesy of Junhua Liu

GEOS CF Forecast skill (GAW and OpenAQ)

Normalized Mean Bias (NMB)

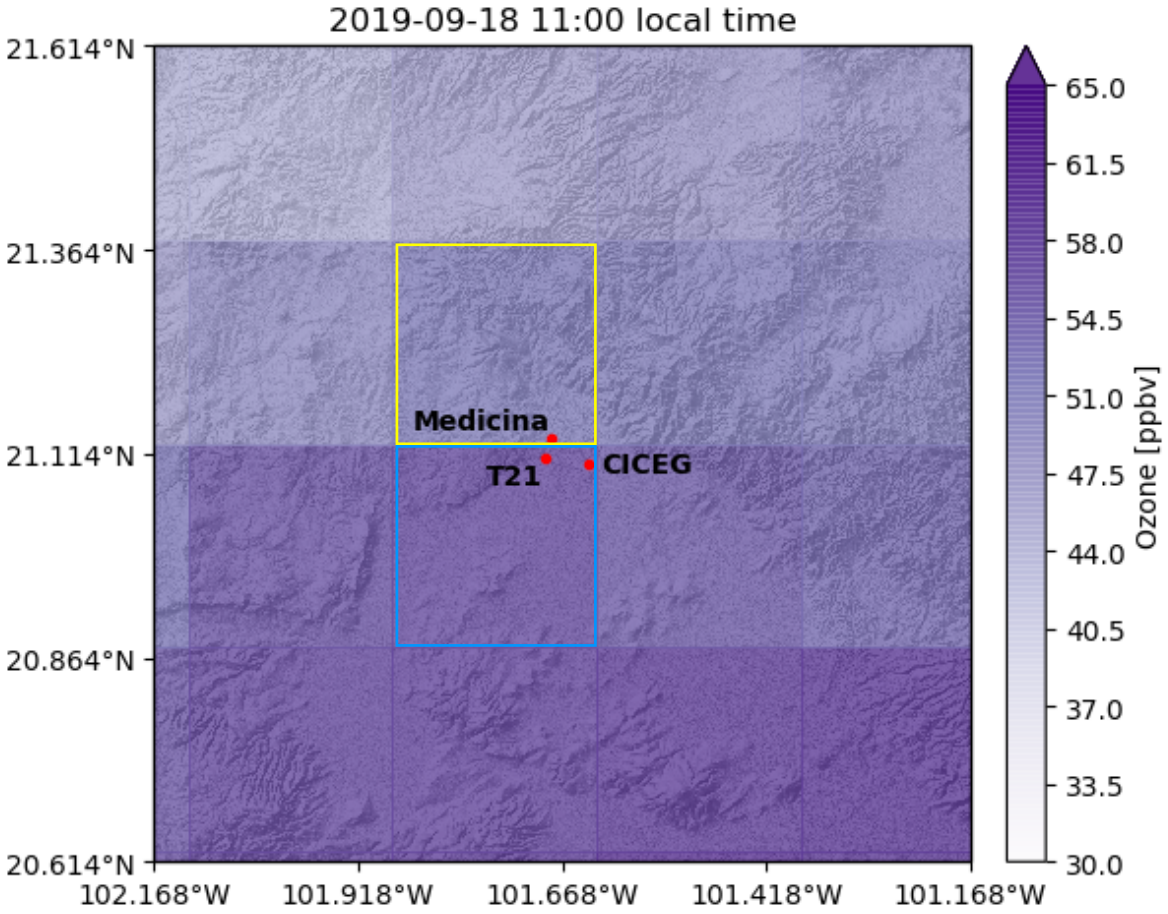
Normalized Root Mean Square Error (NRMSE)

Pearson Correlation Coefficient (R)



- Little variation in the skill scores out to 5 days
- Correlation tends to decrease after day 2 and this is likely due to changes in the meteorological forecast and biomass burning emissions.

Keller et al., in review JAMES

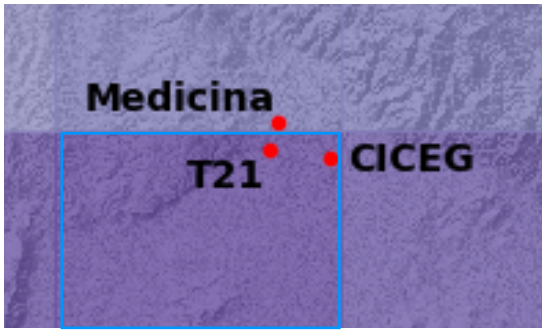


Improve local forecasts using statistical bias correction

3 monitoring stations in Leon, Mexico

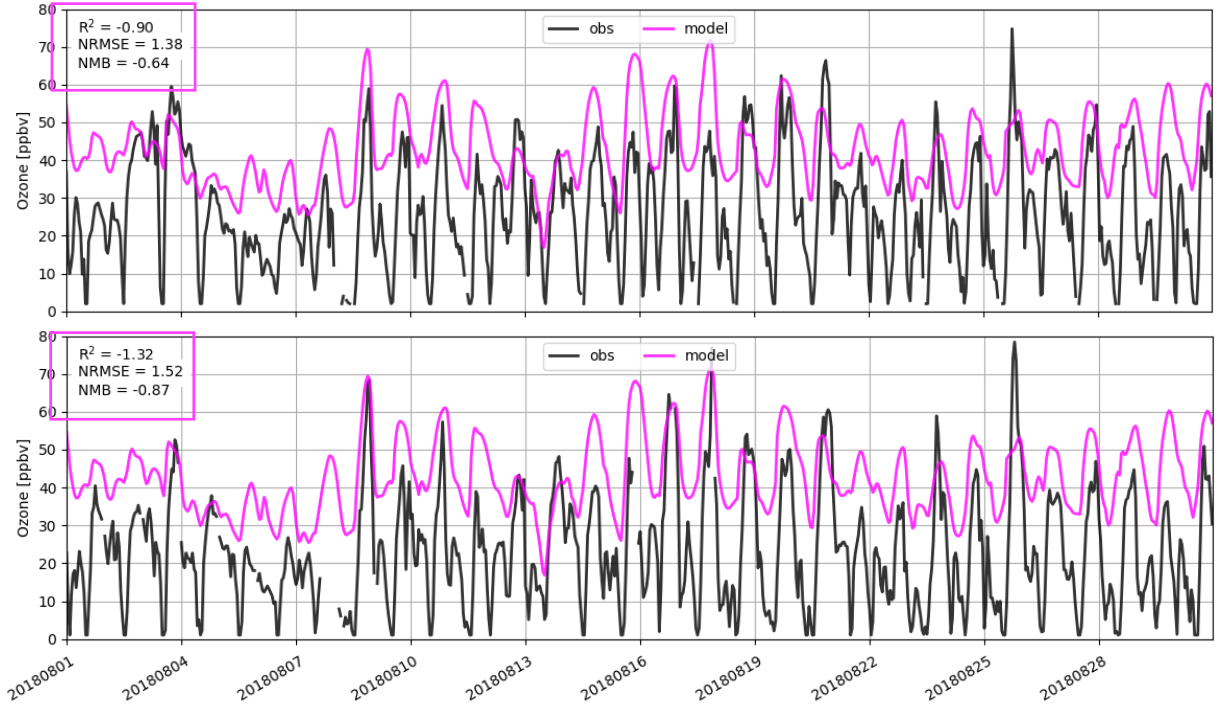
- 1 in one grid box
- 2 share a grid box
- Difficult terrain within each grid box

Improve local forecasts using statistical bias correction



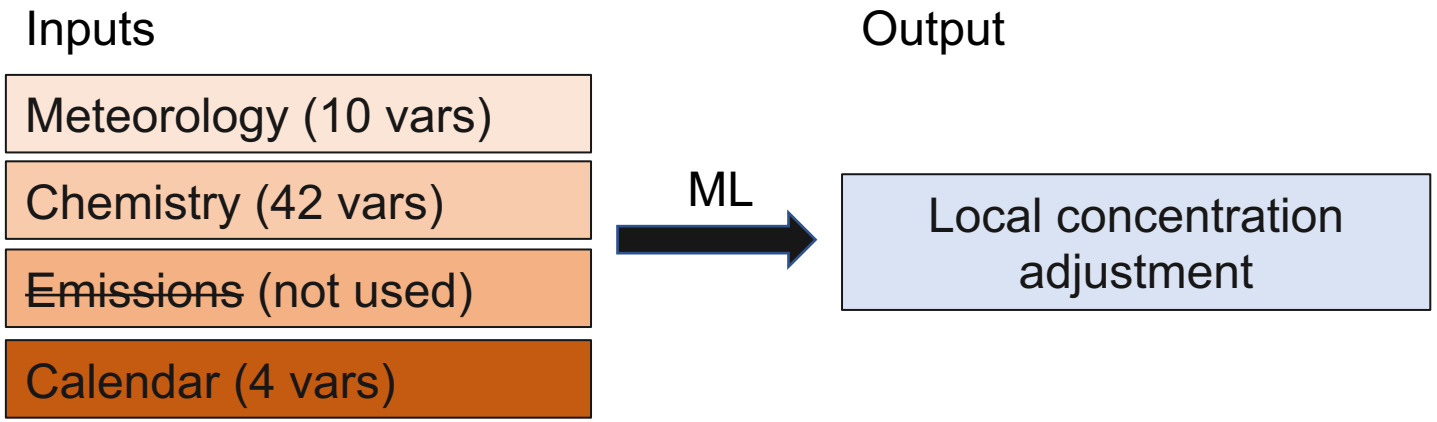
Two observation sites in the same grid box

- GEOS-CF generally over-estimates



Observations Model

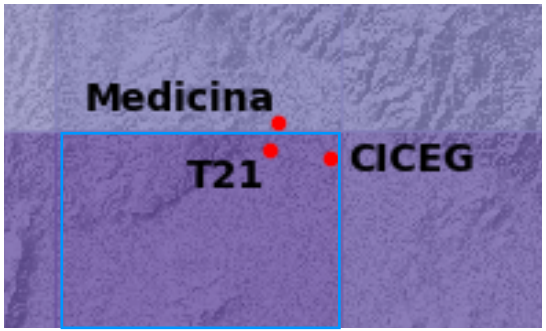
Use machine learning to correct for small scale variability and/or model biases



- Algorithm: gradient boosted decision trees (XGBoost)
- Train separate algorithm for each site

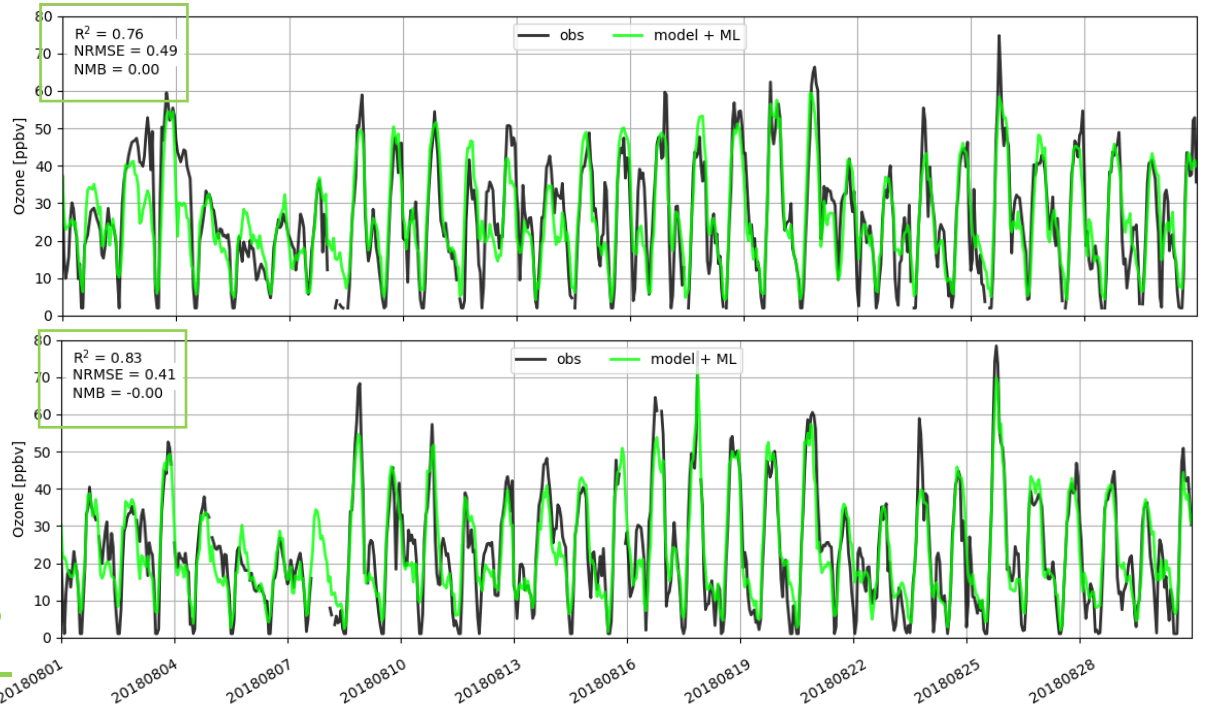
Keller et al., 2021 ACP

Improve local forecasts using statistical bias correction



Two observation sites in the same grid box

- GEOS-CF+ML captures diurnal variability at sub-grid scale



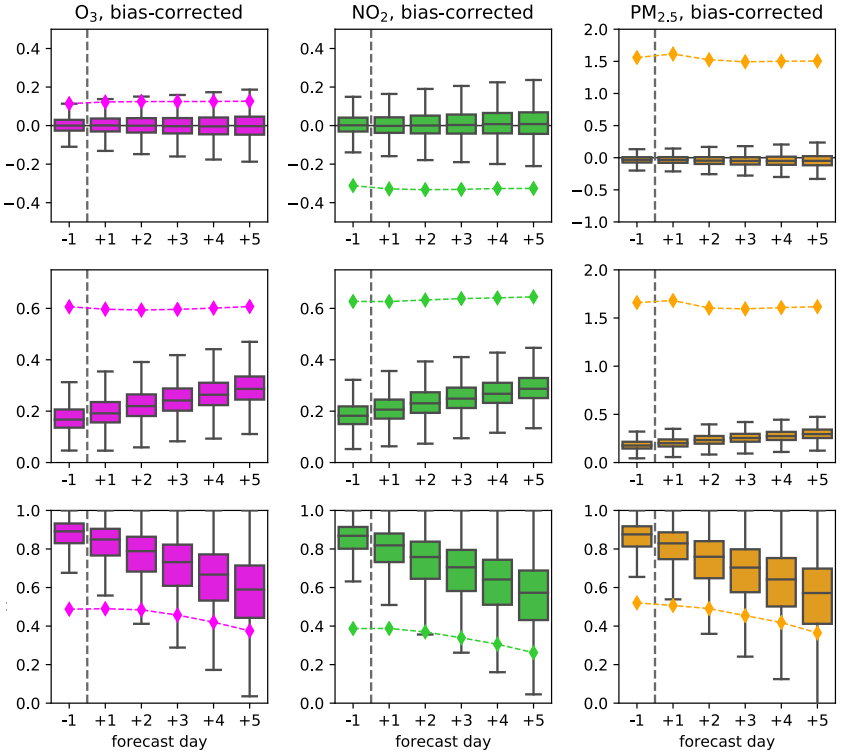
Observations Model + ML

GEOS CF Forecast skill

Normalized Mean Bias (NMB)

Normalized Root Mean Square Error (NRMSE)

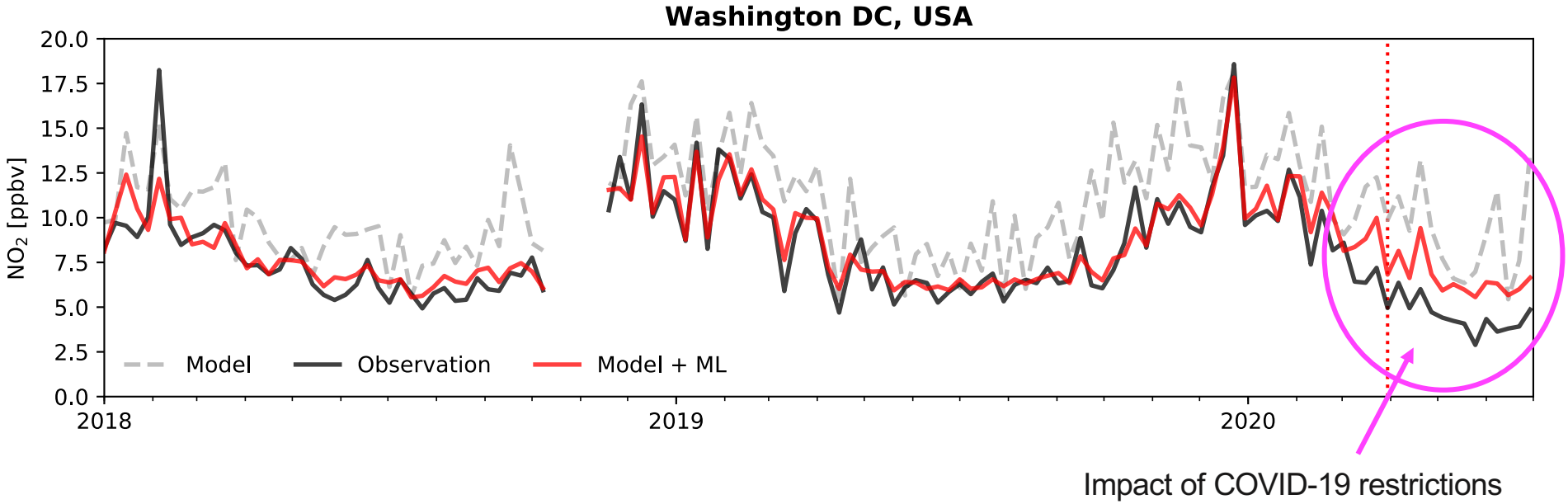
Pearson Correlation Coefficient (R)



- ✓ Using a Machine Learning (ML) algorithm to calculate bias-correction term for each monitoring site can drastically improve the forecast skill at the individual locations

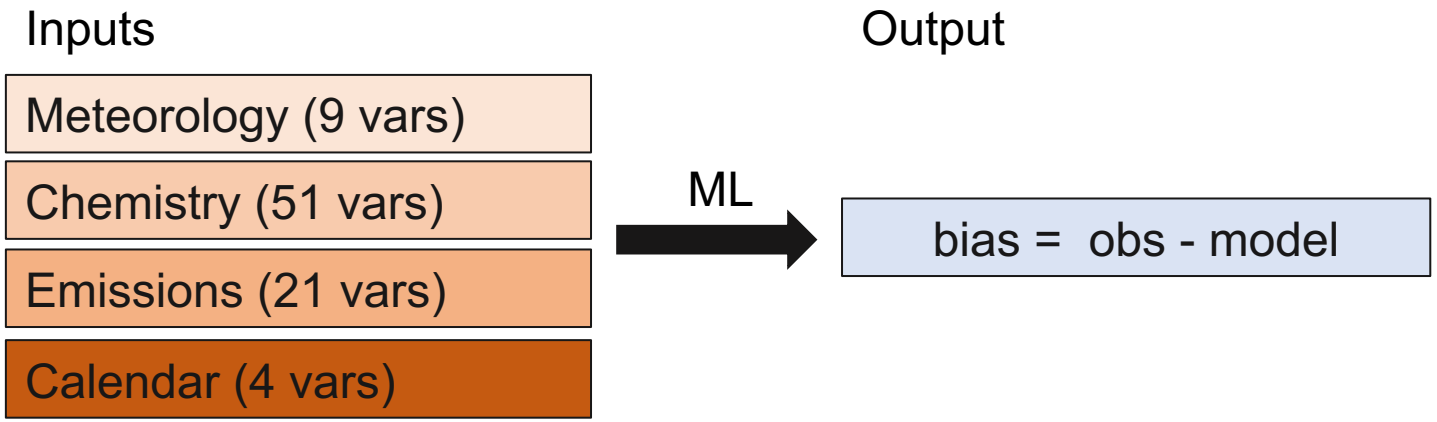
Keller et al., in review JAMES

New application of the GEOS-CF ML algorithm



Keller et al., 2021 ACP

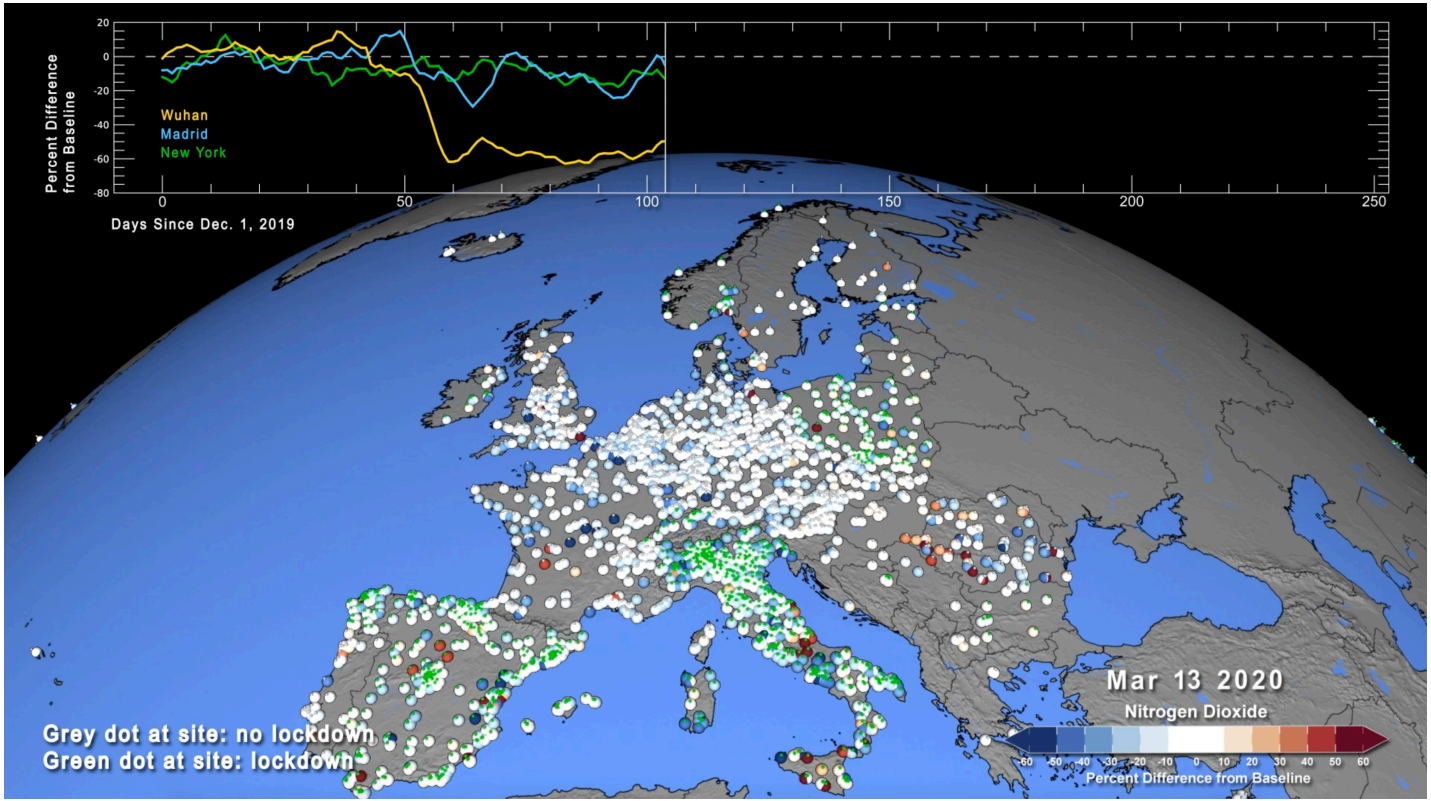
Apply bias-correction to model output using machine learning (using historical observation-model comparisons)



- Algorithm: gradient boosted decision trees (XGBoost)
- Training: 2018-2019 (8-fold cross validation)

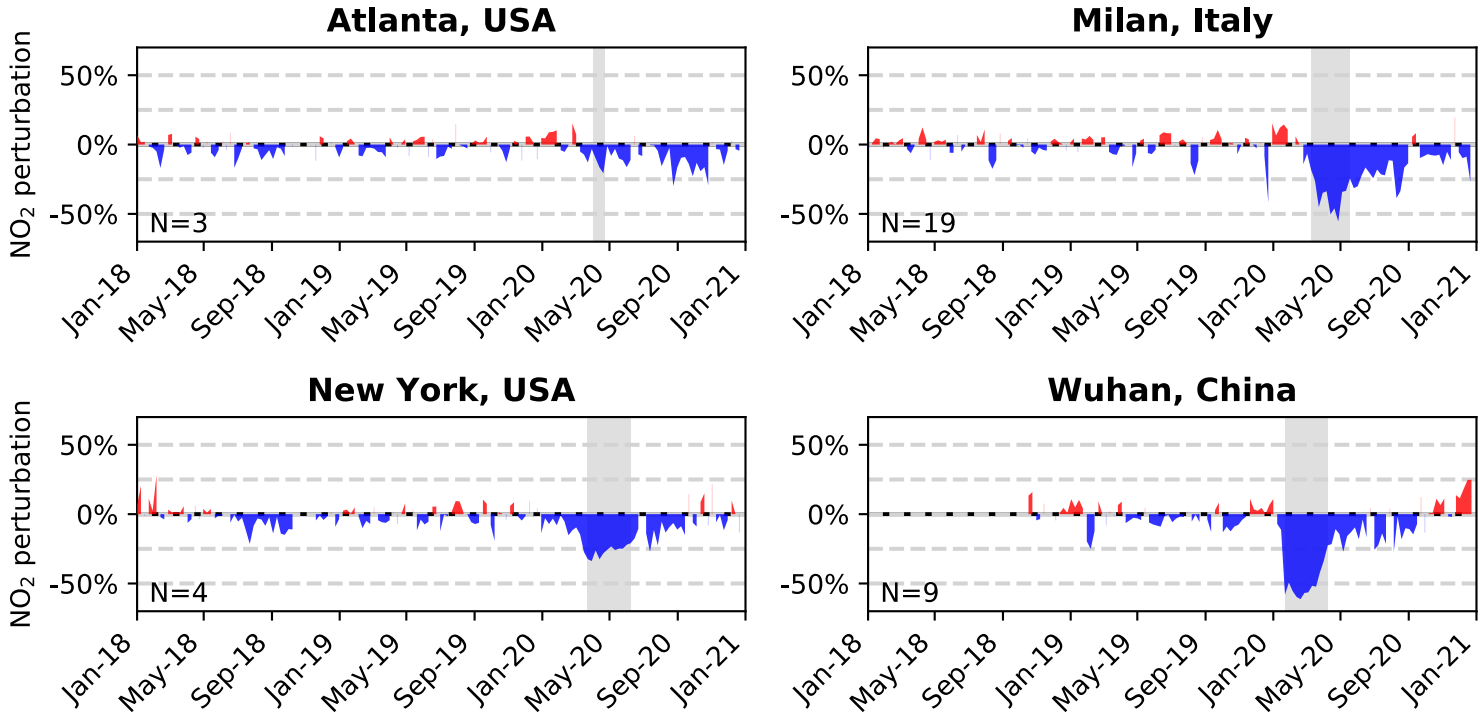
Keller et al., 2021 ACP

Apply analysis to 5756 sites worldwide



https://www.nasa.gov/feature/goddard/2020/nasa-model-reveals-how-much-covid-related-pollution-levels-deviated-from-the-norm

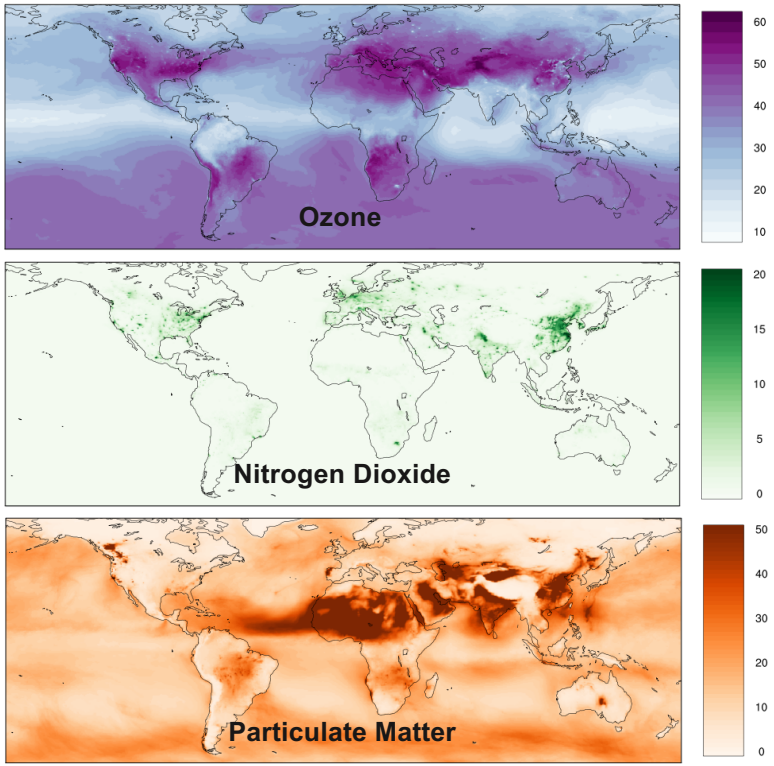
Observation-model differences indicate city-wide NO_2 declines of up to 50% early on and a halting recovery since then



Updated through Dec 27, 2020

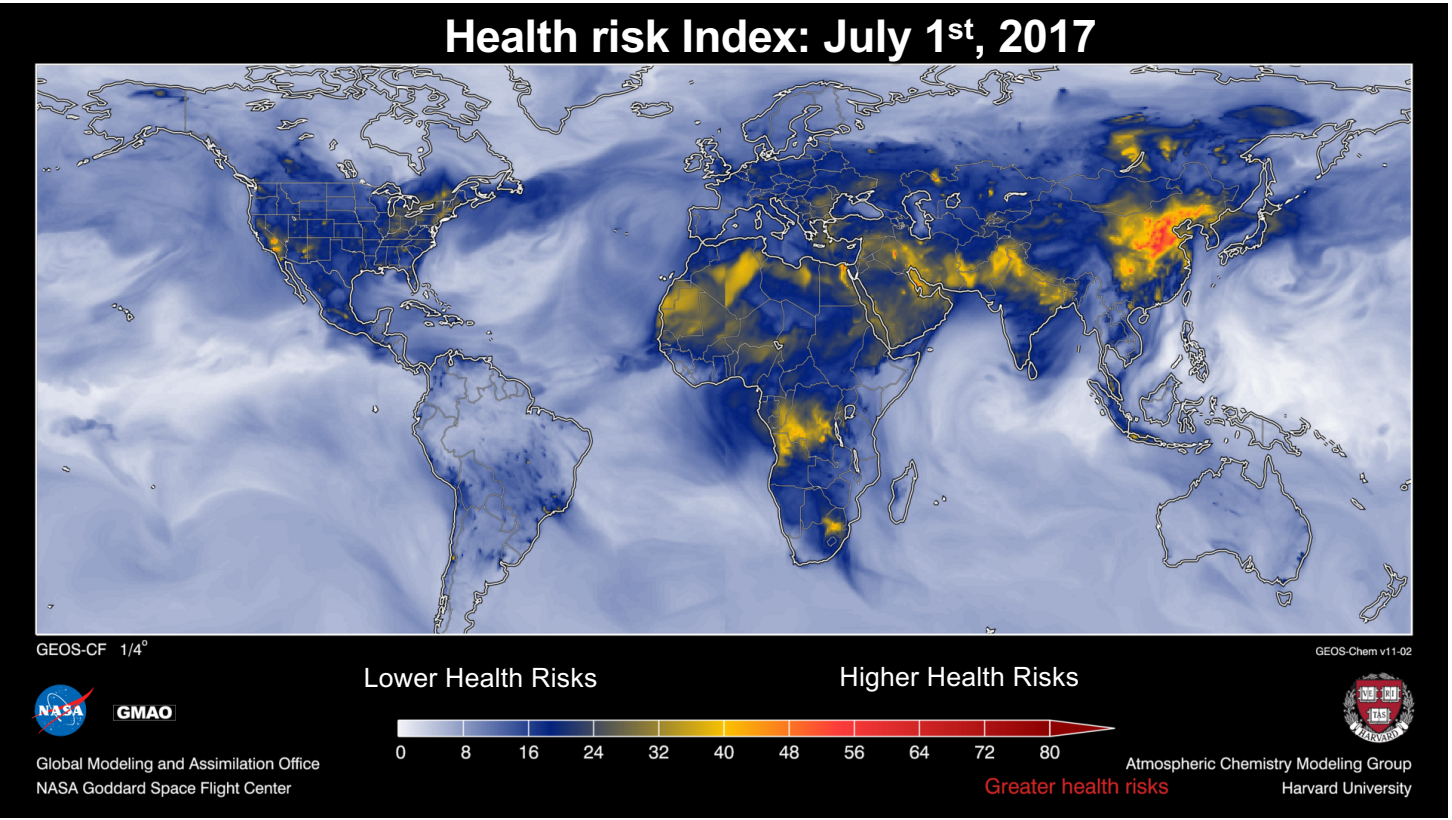
Keller et al., 2021 ACP

Forecast Application: Multi-pollutant Health Risk Index



- O_3 influences Background levels
- NO_2 is Short-lived
- Extreme gradients
- $PM_{2.5}$ driver of spatial gradients

Forecast Application: Multi-pollutant Health Risk Index



Multi-pollutant index, developed by Kevin Cromar (NYU)

- Maximum daily 8-hour average (MDA8) O_3
- 24-hour-average NO_2
- 24-hour-average $PM_{2.5}$

GMAO Mission Support for Field Campaigns

Global Modeling and Assimilation Office GMAO

Weather | Mission Support | CF | Reanalysis | Seasonal

Navigation

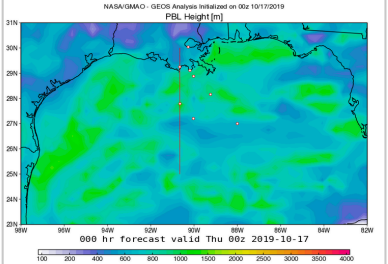
» FLUID Overview
» Contact

Active Missions

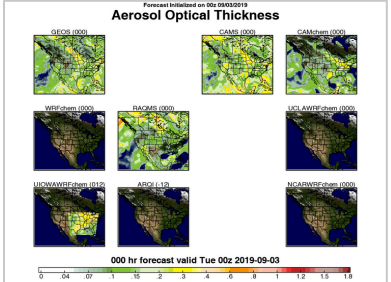
» SCOAPE
» FIREX-AQ
» CAMP2EX
» AEOLUS-CALVAL
» SOCRATES
» ORACLES
» EPOCH
» ACE-ENA
» ABOVE
» ATOM
» MOSAIC

GMAO Active Mission Support

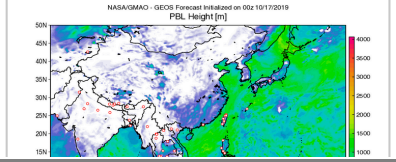
SCOAPE



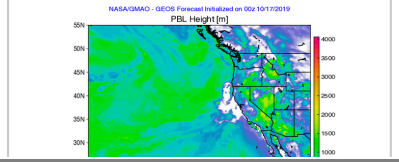
FIREX-AQ



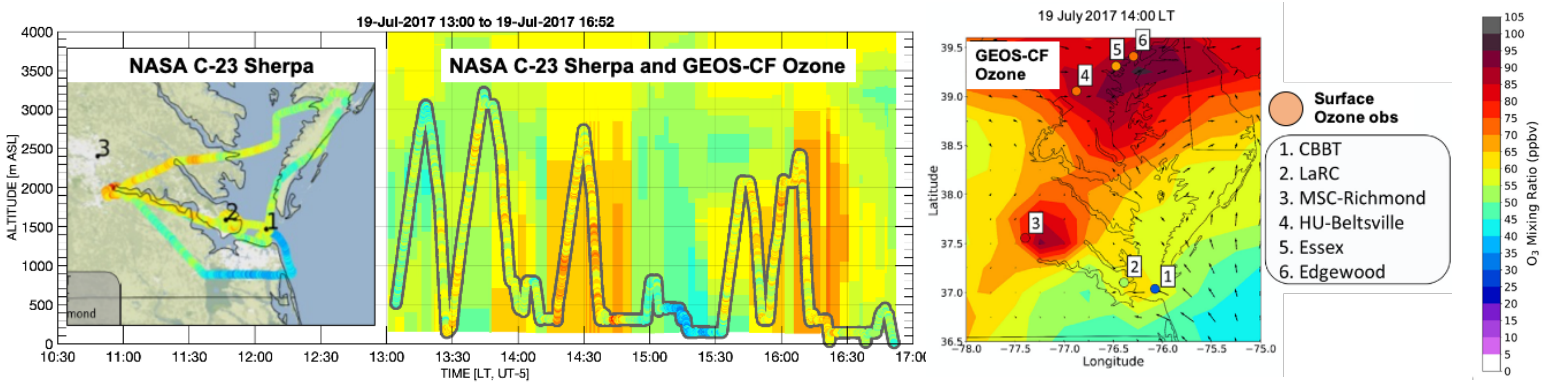
CAMP2EX



AEOLUS-CALVAL



GEOS-CF evaluation with NASA's OWLETS campaign observations



NASA's Ozone Water-Land Environmental Transition Study (OWLETS) campaign, Summer 2017, targeted the potentially large pollutant gradients at the water-land interface of the Chesapeake Bay. This interface can be difficult for air quality models to simulate, with potentially both water and land in the same model grid-box. GEOS-CF has the highest horizontal resolution of a global composition forecast system at 25 km x 25 km, facilitating comparison to observations in this region.

Dacic et al. (2020) used the GEOS-CF simulated ozone to put the OWLETS observations in 'the big picture', using the combined meteorology and chemistry to represent the synoptic conditions that lead to the observed ozone exceedances at surface observation sites.

From where the model and the observations diverged, we learned where there are missing local marine emission sources and errors in the boundary layer chemical and dynamical processes in the model over the Chesapeake Bay.

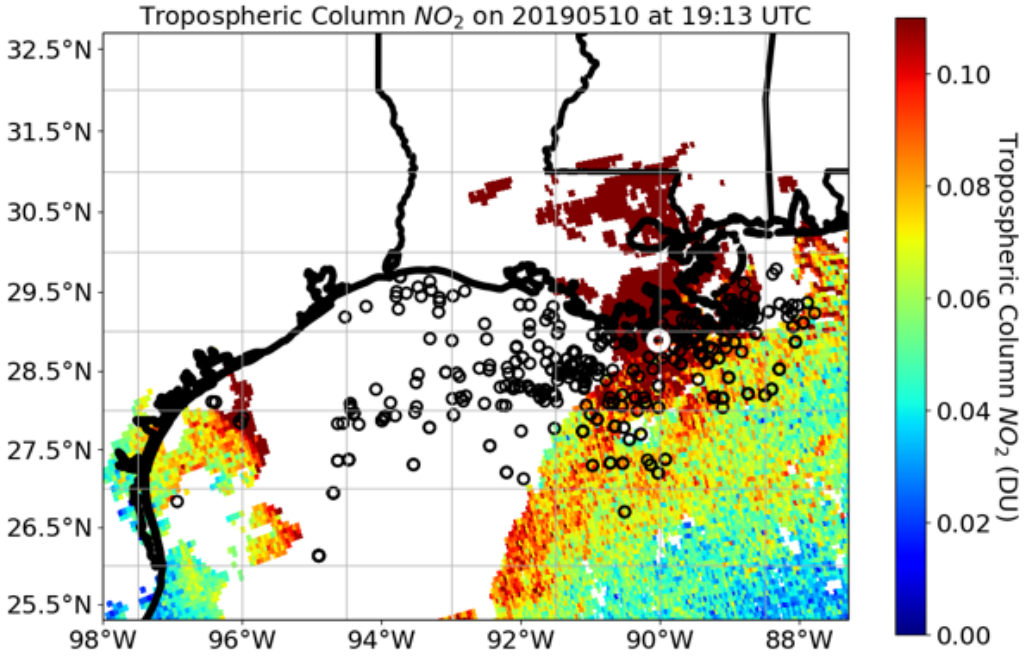
Dacic, N. et al., 2020, Atmos. Environ. "Evaluation of NASA's high-resolution global composition simulations: Understanding a pollution event in the Chesapeake Bay during the summer 2017 OWLETS campaign"

Satellite Coastal and Oceanic Atmospheric Pollution Experiment (SCOAPE)

BOEM
Bureau of Ocean Energy Management

"Can we use NASA resources to monitor off shore sources in the Gulf of Mexico which are impacting air quality onshore?"

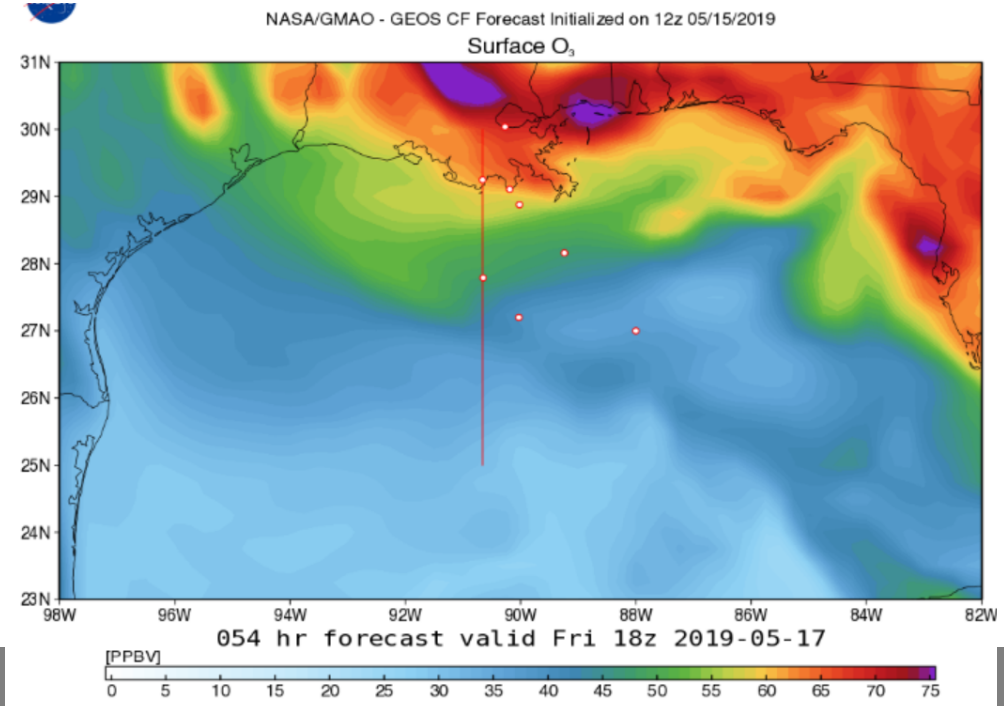
- **The Gulf of Mexico is a complex region for both meteorology and composition**
- **Frequent cloud cover**
- **Onshore and off shore flow**
  - **Recirculation of onshore pollution**



Satellite Coastal and Oceanic Atmospheric Pollution Experiment (SCOAPE)

BOEM
Bureau of Ocean Energy Management

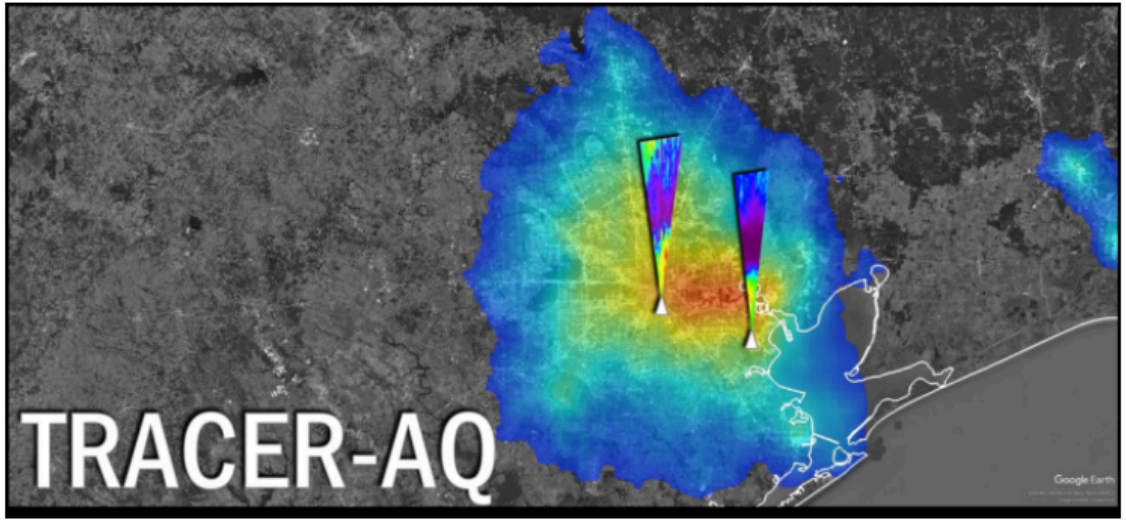
"Can we use NASA resources to monitor off shore sources in the Gulf of Mexico which are impacting air quality onshore?"



- **May 2019 measurement campaign**
- **GSFC support**
  - **Mission planning**
  - **Post mission analysis**

k.e.knowland@nasa.gov
christoph.a.keller@nasa.gov

Future missions



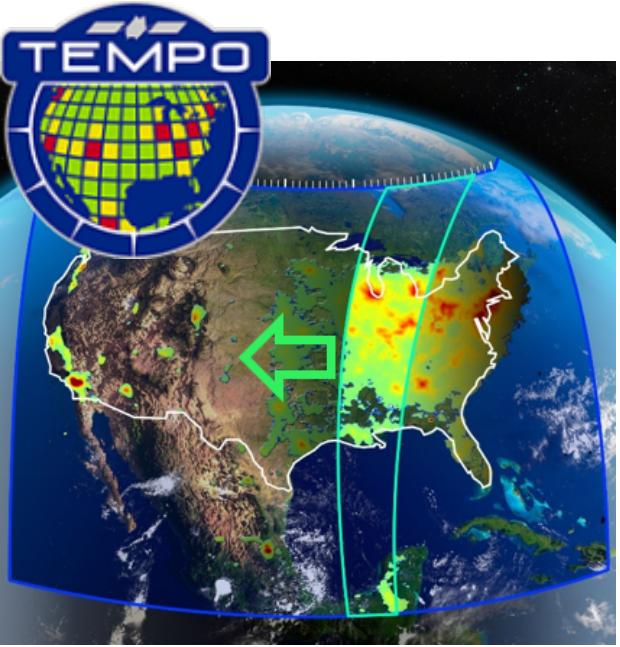
Banner image includes annual average TROPOMI Tropospheric NO_2 columns over the Houston region (April 2019-March 2018) with the approximate proposed locations for TOLNET lidars illustrating their capability for ozone profiling.

GEOS products to support the upcoming TRACER-AQ campaign September 2021

https://www-air.larc.nasa.gov/missions/tracer-aq/

Daily *atmospheric composition* forecast

GEOS - CF



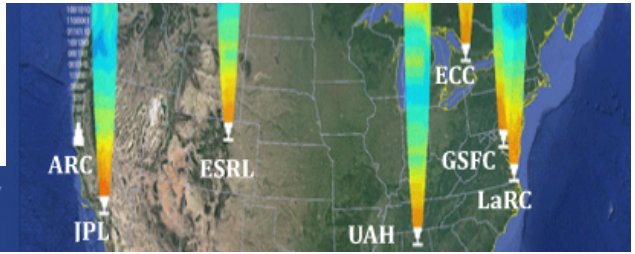
A realistic stratosphere in GEOS-CF is essential to support a broad range of NASA applications, including:



- Satellite retrievals of trace gases
- Airborne campaigns
- Stratosphere-troposphere exchange

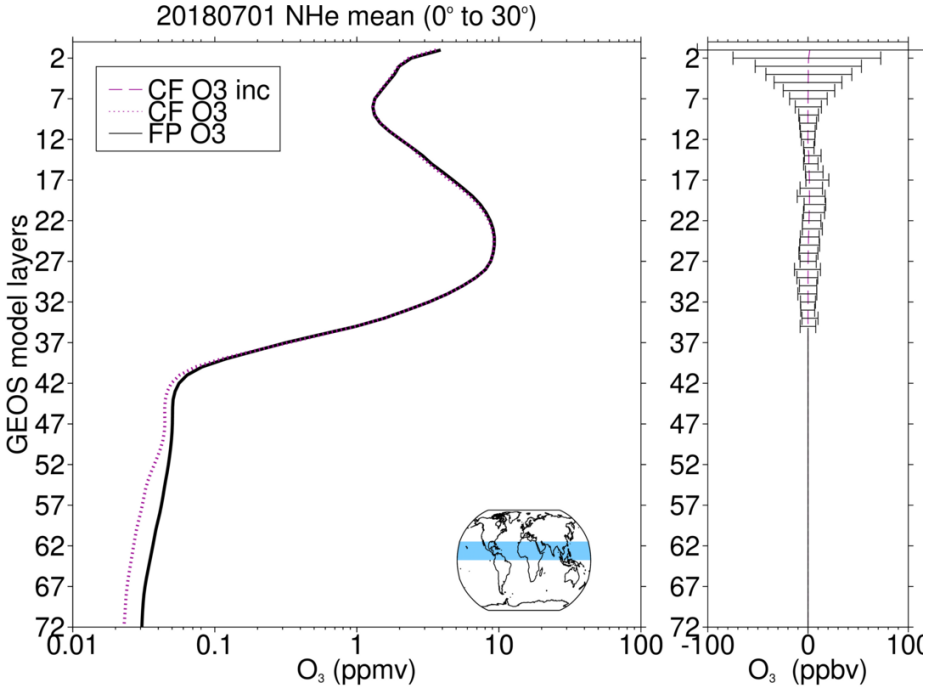
TOLNET

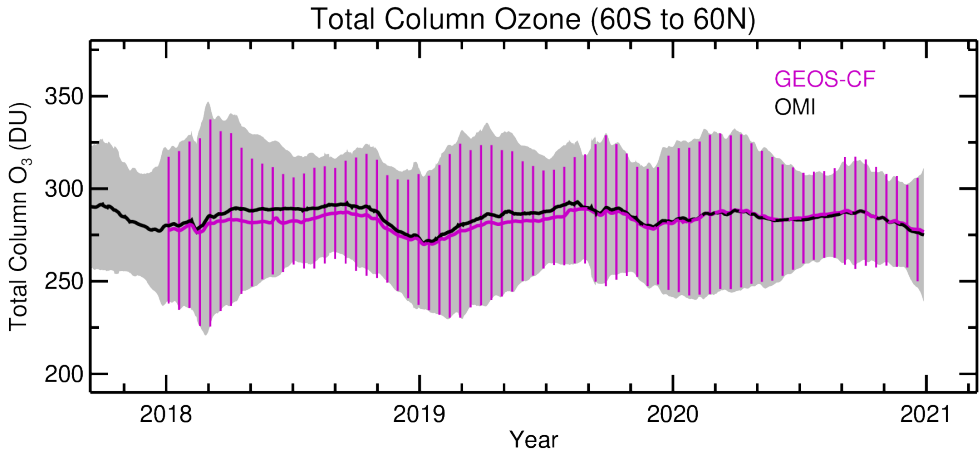
Tropospheric Ozone LIDAR Network



Near-real time updates from satellite data

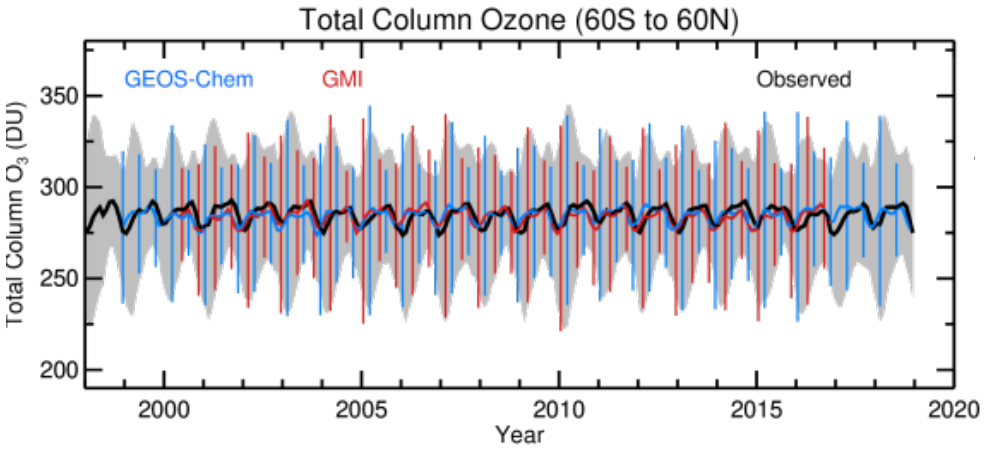
- GEOS-CF Stratospheric O_3 is weakly nudged to the GEOS FP assimilated O_3

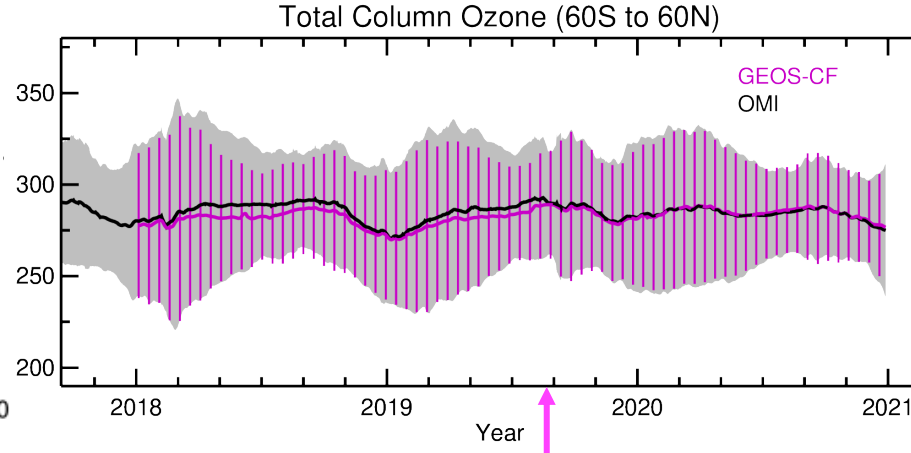




GEOS-CF captures the spread of OMI column O_3

Stratospheric Composition Evaluation

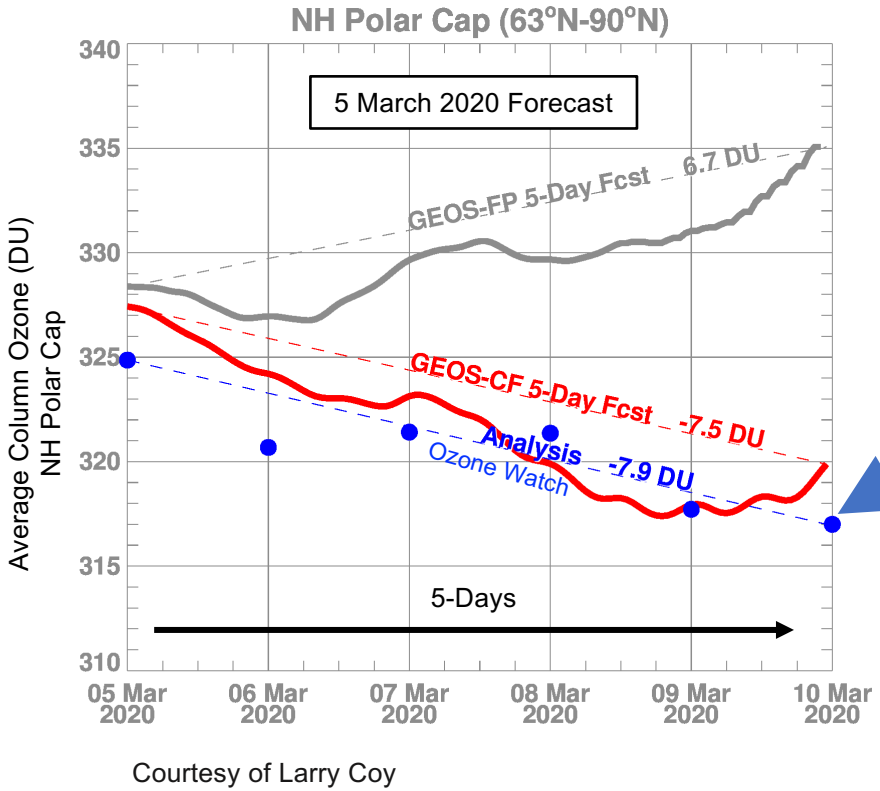




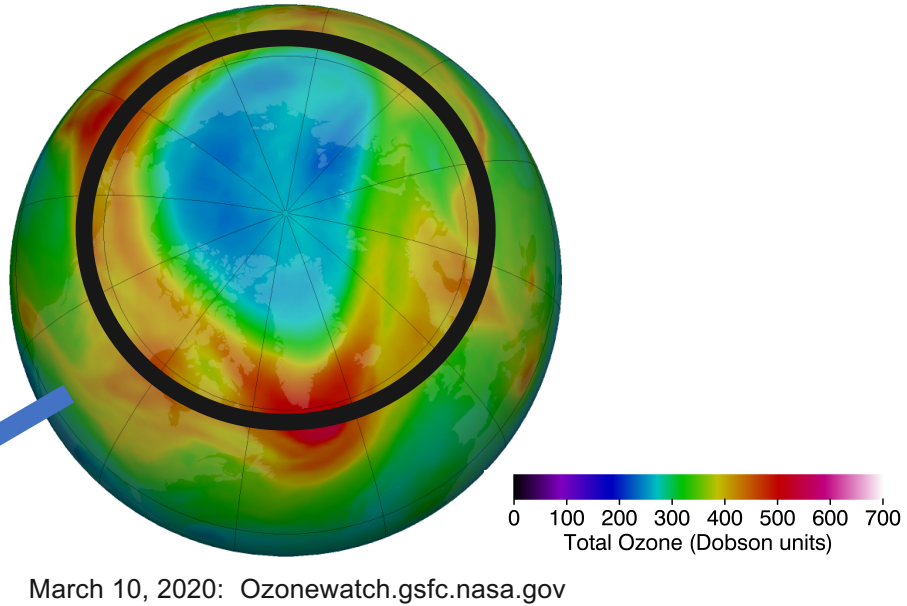
Updates were made to GEOS-Chem in GEOS-CF based on experience from the GSFC Chemistry Climate Modeling (CCM) group with GMI

Figures courtesy of Pam Wales

GEOS-CF has realistic stratospheric ozone forecasts



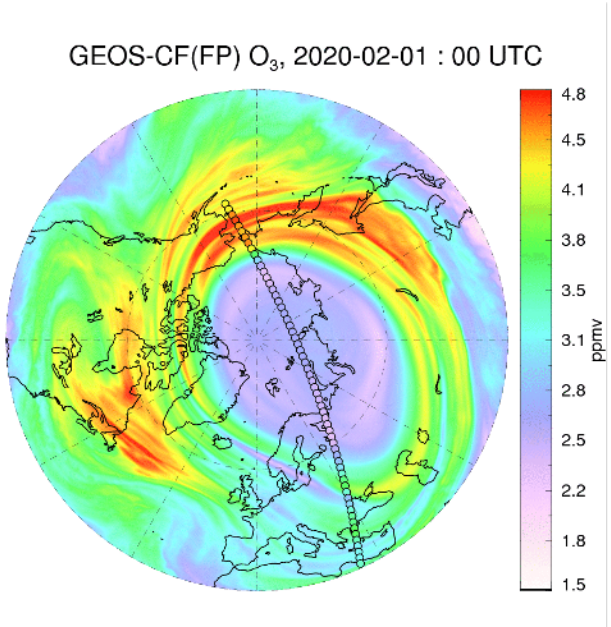
Courtesy of Larry Coy

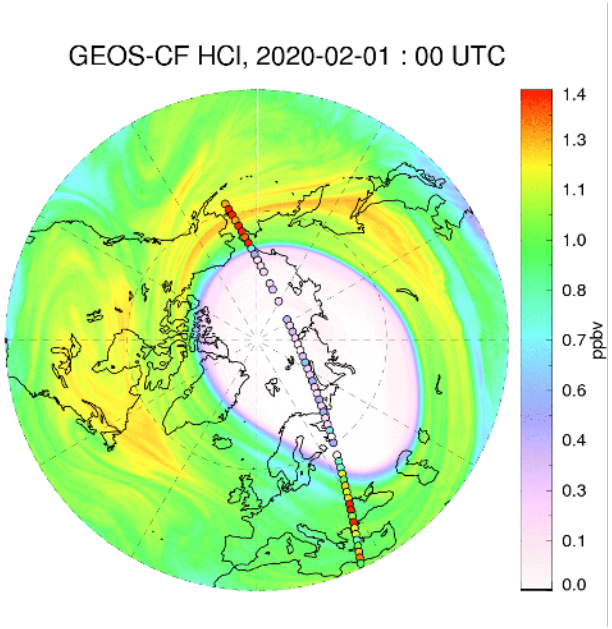


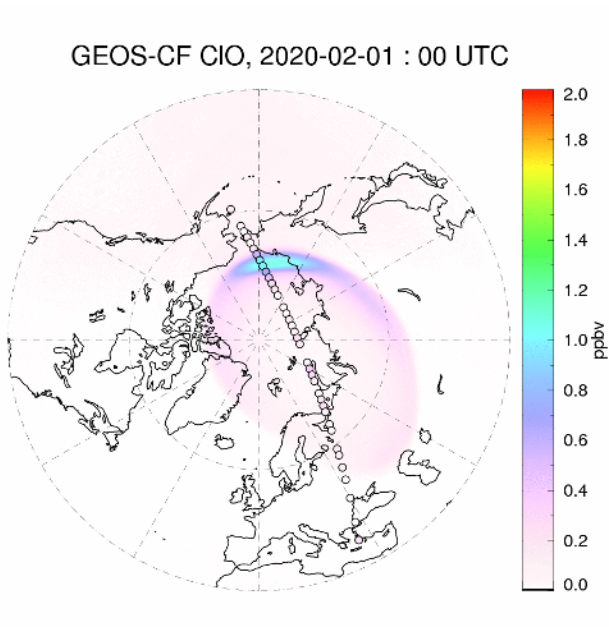
March 10, 2020: Ozonewatch.gsfc.nasa.gov

The GEOS-CF with stratospheric chemistry is responsible for the improved ozone forecasts adding realistic near-real-time stratospheric ozone forecasting capability to the NASA GMAO.

Evaluation GEOS-CF against MLS at 45 hPa





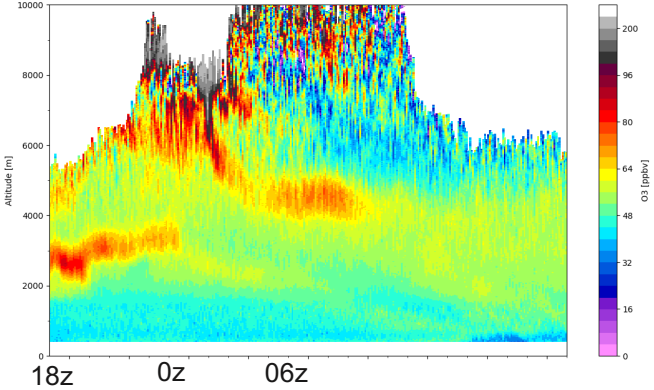


Figures courtesy of Kris Wargan



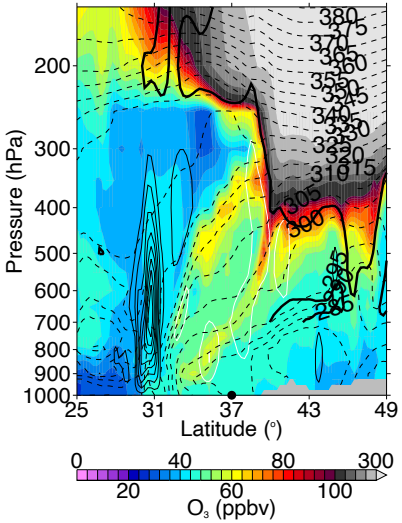
Stratosphere Troposphere Exchange

NASA LaRC Feb 13-14, 2019

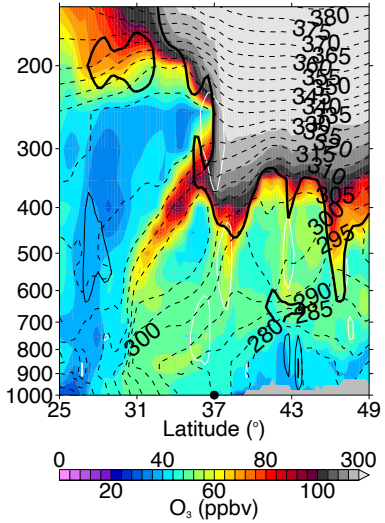


LMOL lidar plot courtesy of G. Gronoff

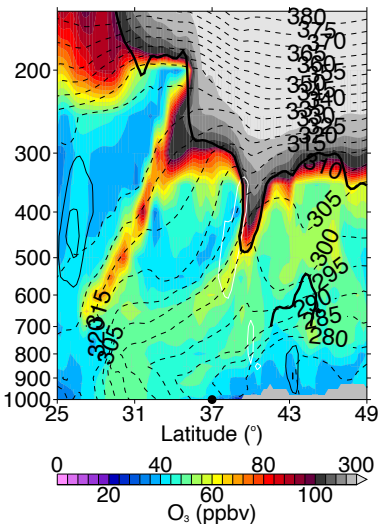
GEOS-CF
Feb 13, 2019 18z



Feb 14, 2019 00z



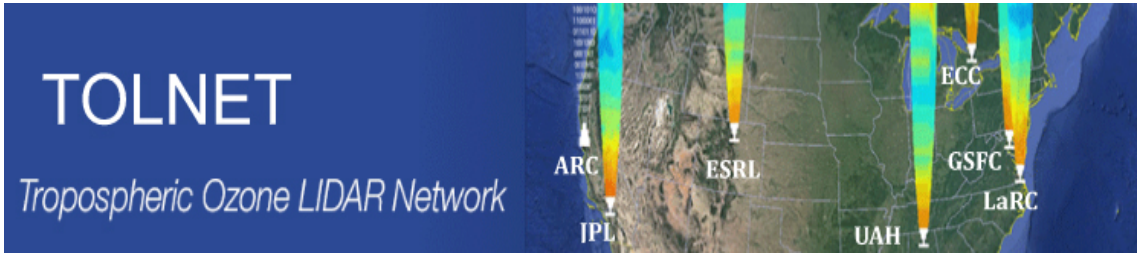
Feb 14, 2019 06z

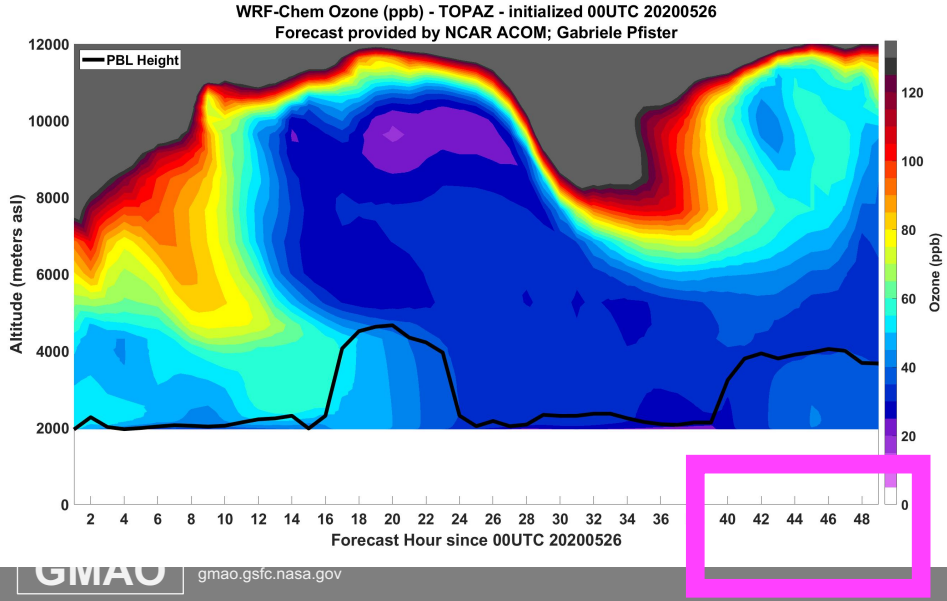


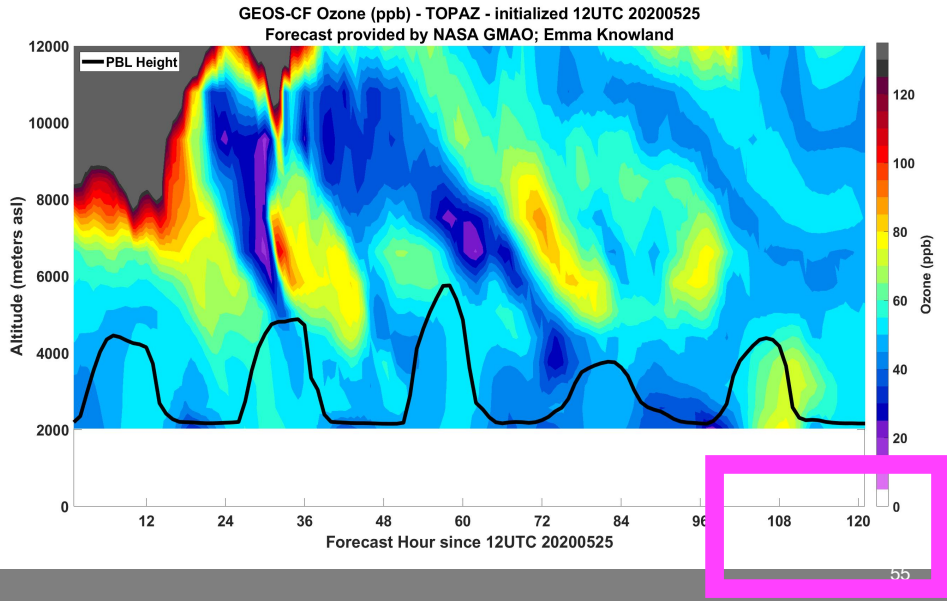
Model-Data Comparison of Stratospheric Intrusions over Hampton, Virginia
Gronoff et al., Submitted to Atmospheric Environment

Daily alerts to NASA TOLNet Lidar teams sent by Matt Johnson, NASA AMES

WRF-Chem 48-hour (left) and GEOS-CF 120-hour (right) Ozone forecasts for TOPAZ on May 26, 2020.

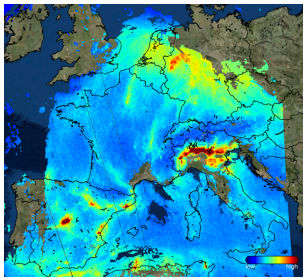


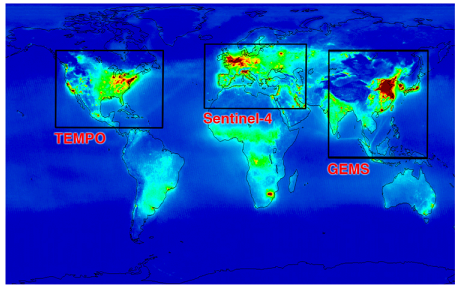


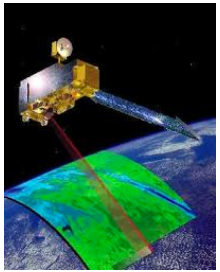


Planned upgrades for GEOS-CF

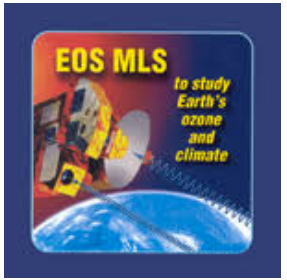
- Model update to GEOS-Chem v13.0
  - Improvements to ozone deposition
  - Updates to NO_3 washout ⇢ likely reduce PM2.5 bias
- Meteorology update to GEOS-FP
- Coupling GEOS-Chem aerosols with GOCART aerosols
- Constituent Data Assimilation System (CoDAS)
  - Multi-constituent assimilation with O_3, CO, NO_2
  - Satellite-based emission scale factors (already tested for COVID-19 experiment)







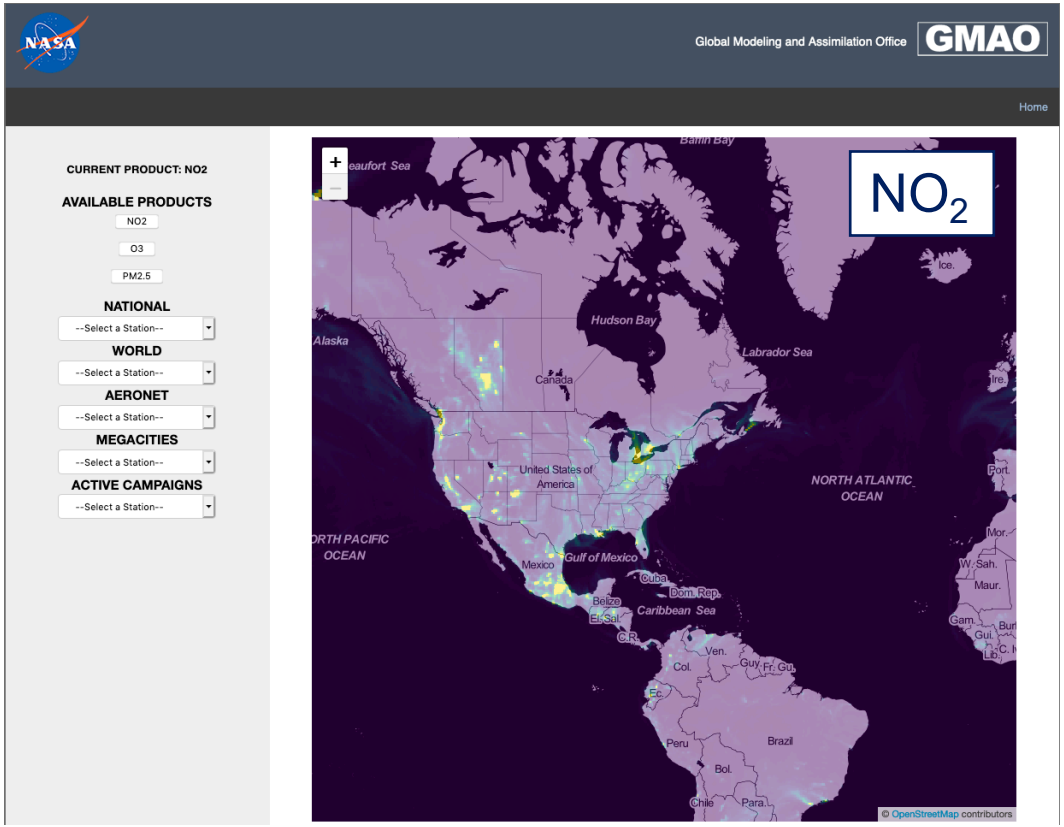




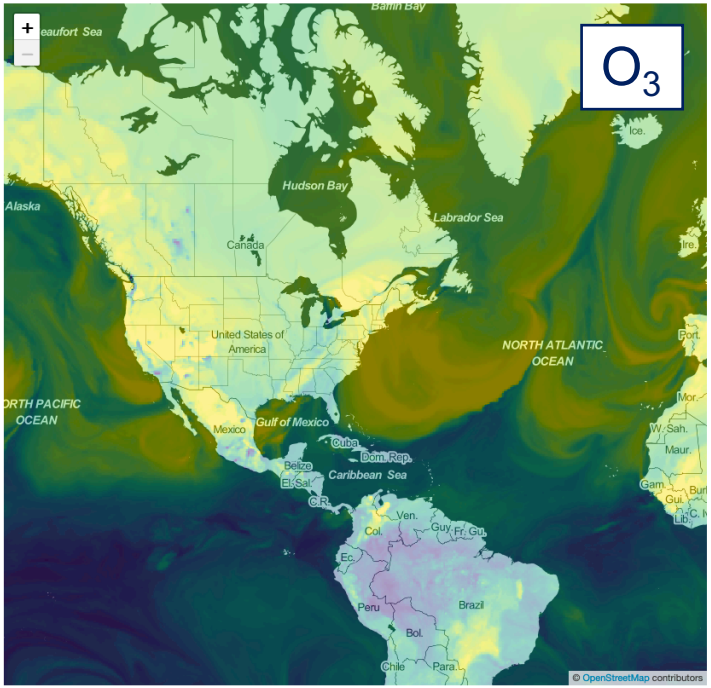
Summary of GEOS-CF Status

- GEOS-CF daily global composition forecasts at 25km resolution are generated in near-real time:
  - High-resolution replay segments are available since January 2018
    - ✓ Model realisticly captures global distribution of the major pollutants, though aerosols and SO2 are biased high, when compared against surface observations, ozonesondes and satellite.
    - ✓ Due to grid-box size, model skill is typically worse for the urban sites (OpenAQ) than the background sites (GAW)
  - Forecasts accessible via data servers for two weeks, or since January
    - ✓ Forecast skill is improved using ML algorithm in post-processing step.
    - ✓ Now have realistic stratospheric ozone 5-day forecasts
- Emerging applications users, including:
  - NASA field missions (SCOAPE, FIREX-AQ, ACT-America, TRACER-AQ)
  - Daily alerts sent to NASA TOLNet lidar teams (Matt Johnson, NASA Ames)
  - TEMPO a priori for trace gas product

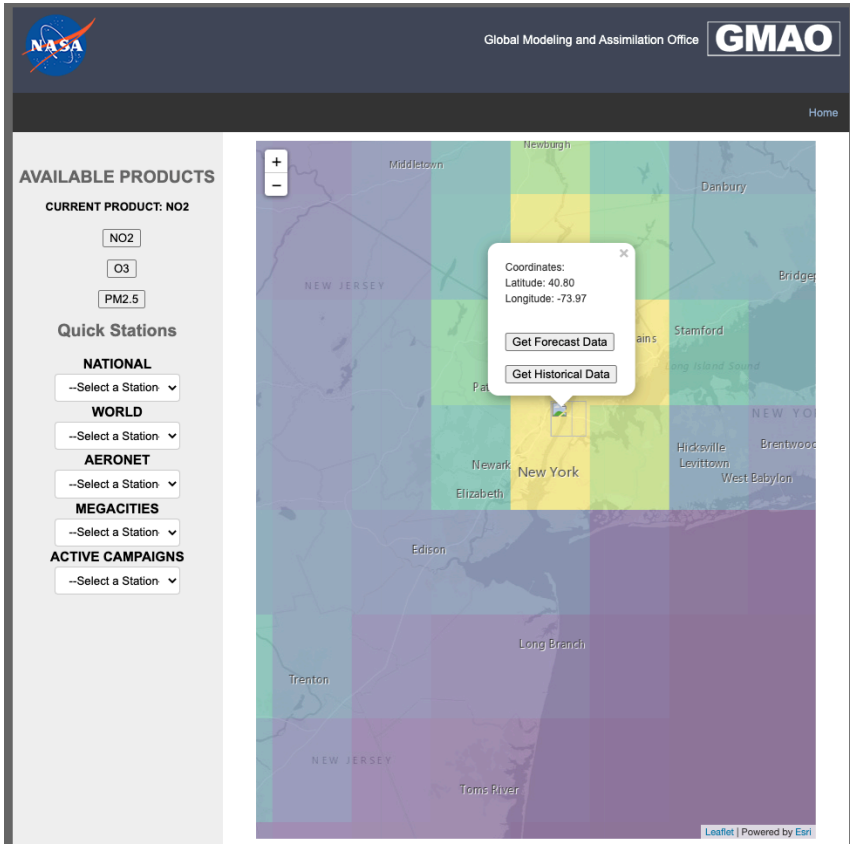
Emerging FLUID Features *in Development*



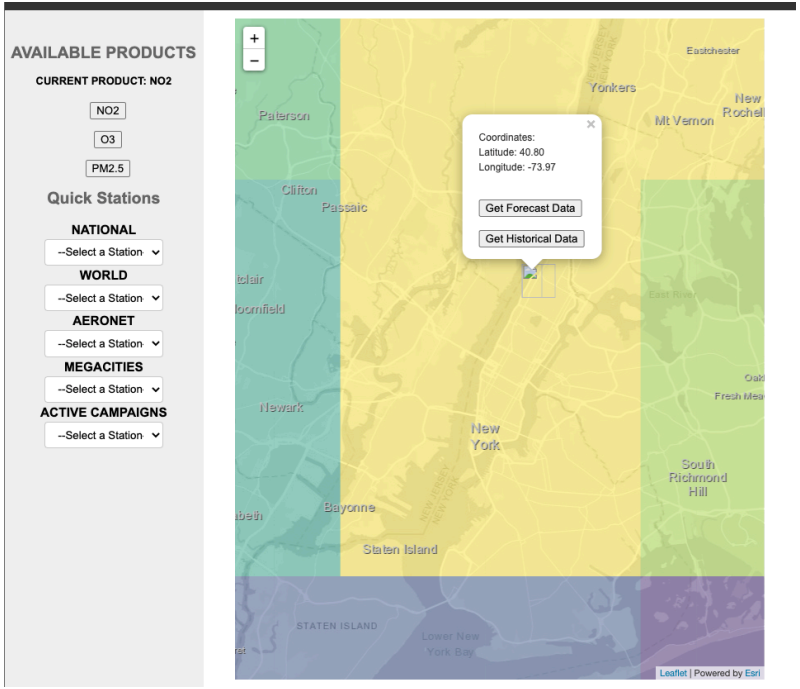
Support from NASA HQ Applied Sciences and Army Public Health Center



Emerging FLUID Features *in Development*



Capability to zoom in and select data for any grid box



Thank you!

