AGES Forecasting and modeling team presentations

Pierce (moderator):

- NOAA CSL (Schwantes)
- NOAA GSL (Schnell)
- NSF (Carlton)
- NCAR (Kumar)
- Wisconsin (Pierce)
- Post-Campaign (Jathar)
- NASA (Knowland)

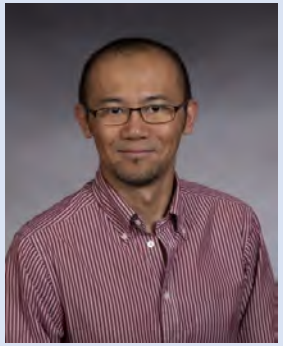
September 29 Morning: Logistics, Flight Planning, Coordination, Data Management

NOAA CSL Forecasting / Flight Preparation Plans for AEROMMA & CUPiDS

Plans:

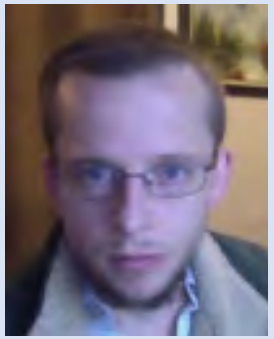
- Prepare climatologies and other useful information before the campaign
- Provide slides and a forecasting discussion each day for the AEROMMA and CUPiDS campaigns
- Goal for each day is to produce concise slides that specifically help to answer the following:
  - Should we fly today or tomorrow?
  - What should the target be?
  - Which flight pattern do we choose?
- If needed, this team will also provide support during the flight as well

The Team


Siyuan Wang

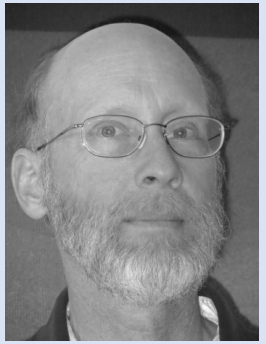

Harold Gamarro


Jian He


Edward Strobach


Graham Feingold


Jan Kazil


Wayne Angevine


Congmeng Lyu

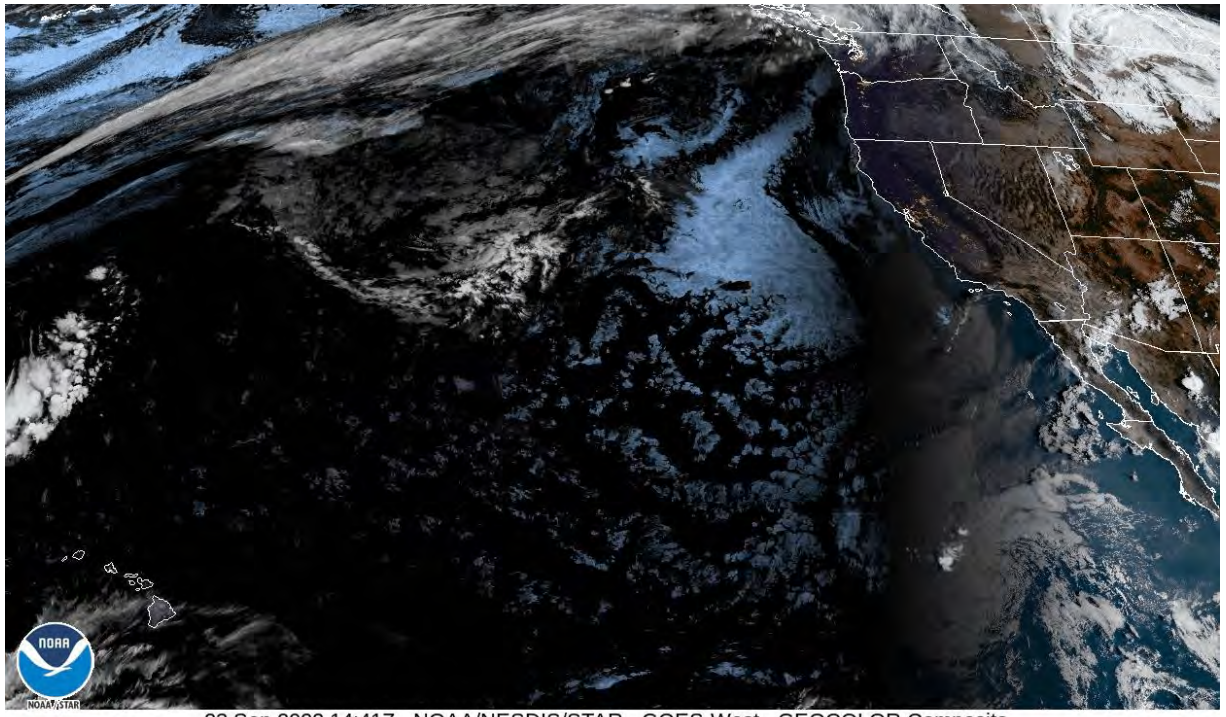

Meng Li

Forecasting / Flight Preparation Plans for AEROMMA - Marine

Provide the following information prior to the flight:

- Regional and local meteorological forecast
- GOES satellite products to monitor clouds
- Cloud forecasts (RAP or HRRR)
- Surface wind forecasts (windy.com)
- DMS climatology and daily satellite chlorophyll and SST products
- Offshore NO_x forecasts (RAP-Chem or HRRR-Chem)
- Tropical Tidbits for forecasting and satellite products

GOES



23 Sep 2022 14:41Z - NOAA/NESDIS/STAR - GOES-West - GEOCOLOR Composite

Provide the following information during the flight:

- Use the GOES satellite products to identify specific cloud morphologies in order to potentially change targets during the flight

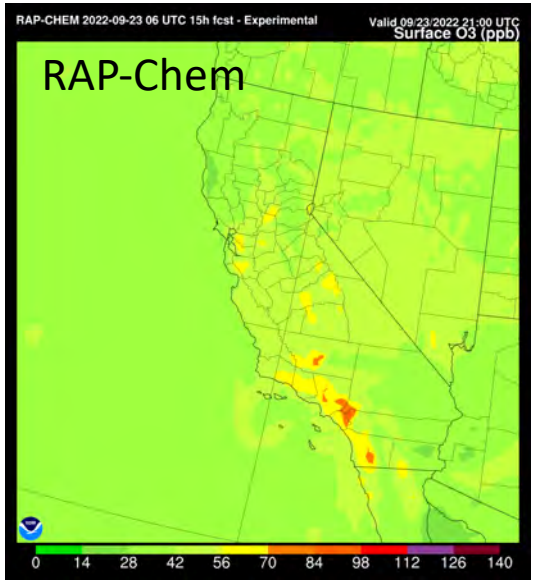
Let us know what other products are useful

Forecasting / Flight Preparation Plans for AEROMMA – Urban & CUPiDS

Provide the following information prior to the flight:

- Regional and local meteorological forecast including the NWS Discussions
- Plan to involve local meteorologists
- GOES satellite products to monitor clouds
- NEXRAD radar for clouds, precipitation, and winds
- Surface wind forecasts (windy.com)
- Commercial Aircraft Sondes (AMDAR) data to assess the mixing layer height and the PBL height forecasts (RAP-Chem or HRRR-Chem)
- Wildfires and prescribed burns impacting the region including smoke forecasts from HRRR-Smoke
- AirNow AQI Forecast and Ozone and $PM_{2.5}$ Forecasts (RAP-Chem or HRRR-Chem)
- Tropical Tidbits for forecasting and satellite products

Let us know what other products are useful



Experimental air quality forecasting with the Rapid-Refresh model coupled to chemistry (RAP-Chem)

Jordan L. Schnell (jordan.schnell@noaa.gov)

w/ contributions from Ravan Ahmadov, Gregory J. Frost, Stuart A. McKeen, Brian C. McDonald, Brian Jamison, Mackenzie Arnold, Jian He, Meng Li, Megan M. Bela, Rebecca H. Schwantes, Barry Baker, Joseph B. Olson, Wayne M. Angevine, Eric P. James, Ka Yee Wong, R. Bradley Pierce, Matthew Coggon, Colin Harkins, Georg A. Grell

AGES Workshop | September 29, 2022

University of Colorado Boulder

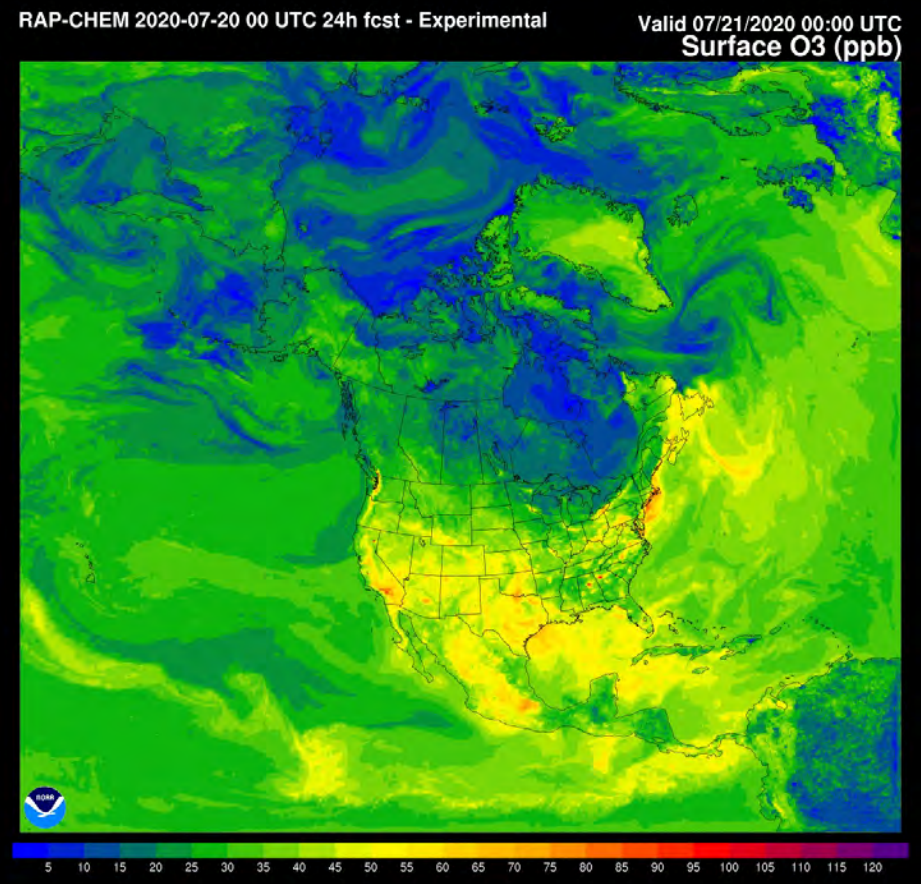
CIRES

NOAA

Photo Credit: Patrick Cullis, CIRES

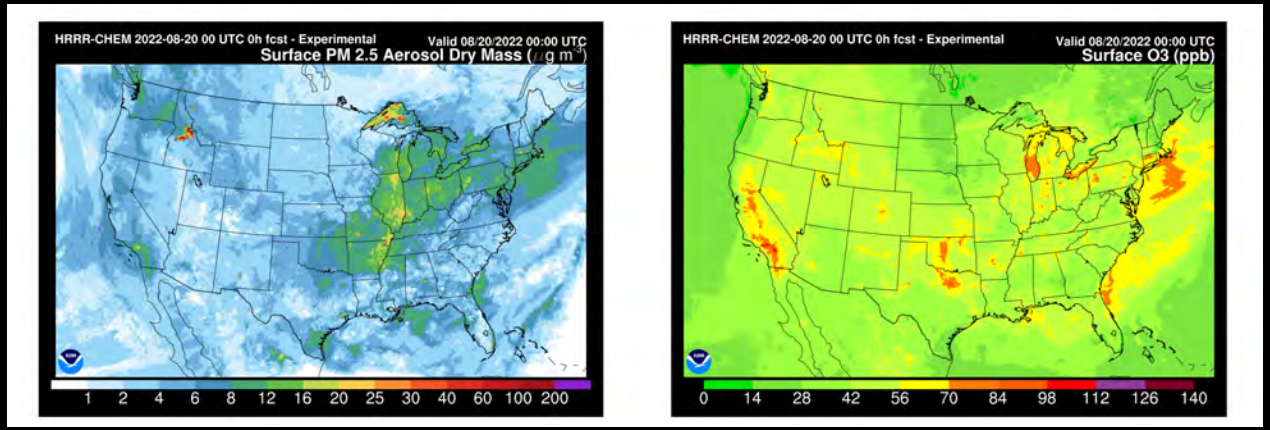
RAP-Chem Overview

- **13.5 km** resolution using **operational RAP IC/BCs**
- **36-h** forecasts **initialized at 06Z and 18Z**
- **Plots** available online: **https://rapidrefresh.noaa.gov/RAPchem/**
- **Chemical mechanism**: simplified carbon-bond coupled to VBS-SOA (**85 species, 96 RXNs** vs 217 species, 366 RXNs in NOAA/NWS NAQFC)
- **Online emissions**: dust (FENGSHA), sea salt, biogenics (BEIS), and wildfires + plumerise as a *f* (FRP)
- **Photolysis**: TUV + aerosol direct effects
- **Radiation**: RRTMG + aerosol direct effects
- **MP**: Thompson-Eidhammer Aero-aware (*loosely coupled*)
- **Chemical vertical mixing**: Inline with MYNN EDMF
- **Chemical LBCs from RAQMS**
- **Automated NRT AQS/AERONET surface verification and comparison with TROPOMI NO_2, HCHO, CO**
- **Workflow** easily modified for specific output/diagnostics



(maybe) coming soon: HRRR-Chem @3km

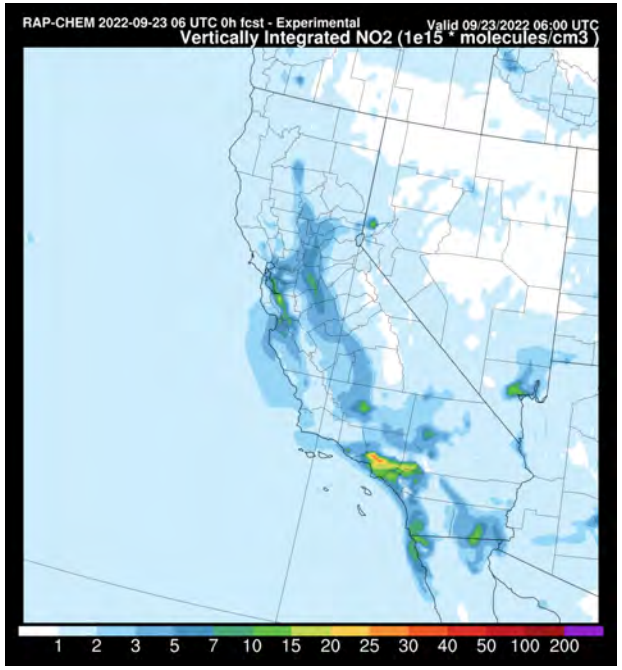
- All features from RAP-Chem are carried over except no cumulus parameterization (3 km vs. 13 km) & associated convective transport/scavenging
- Forecast is currently being tested, but there is SIGNIFICANT computational overhead (~15K core-hours/forecast day = 6x RAP-Chem

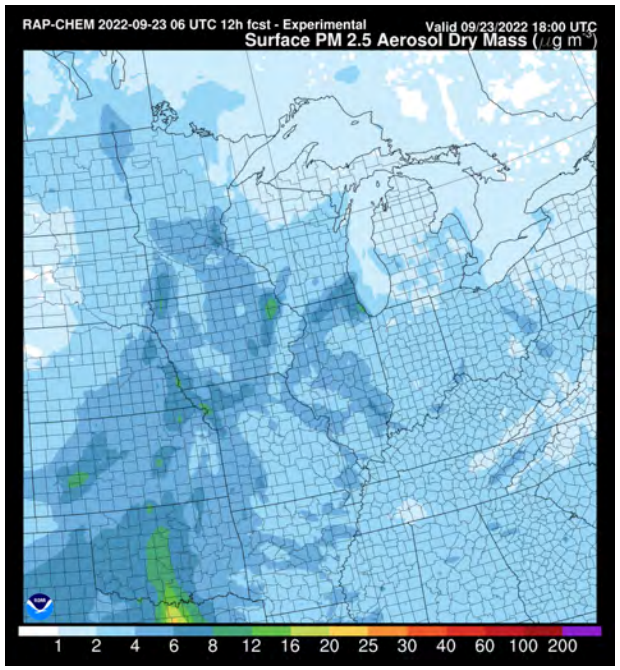


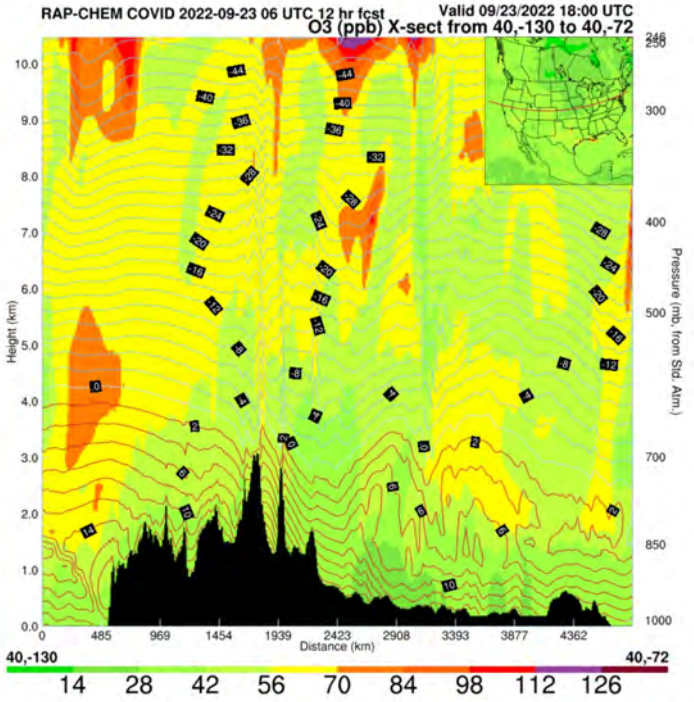
https://rapidrefresh.noaa.gov/RAPchem/

2m temp	✓	✓
10m wind	✓	✓
1h precip	✓	✓
PBL height	✓	✓
UV index	✓	✓
Surface Visibility	✓	✓
Fire Radiative Power	✓	✓
Surface O3	✓	✓
Surface CO	✓	✓
Surface NO2	✓	✓
Surface HCHO	✓	✓
Surface isoprene	✓	✓
Surface NH3	✓	✓
Surface N2O5	✓	✓
Vertically integrated CO	✓	✓
Vertically integrated NO2	✓	✓
Vertically integrated HCHO	✓	✓
HCHO/NO2 column ratio	✓	✓
Surface PM2.5	✓	✓
Surface PM10	✓	✓
Surface Dust	✓	✓
Surface Pollen	✓	✓
Surface Organic Aerosol	✓	✓
Surface nitrate aerosol	✓	✓
Vertically integrated PM2.5	✓	✓
AOD at 550nm	✓	✓
Air Quality Index	✓	✓

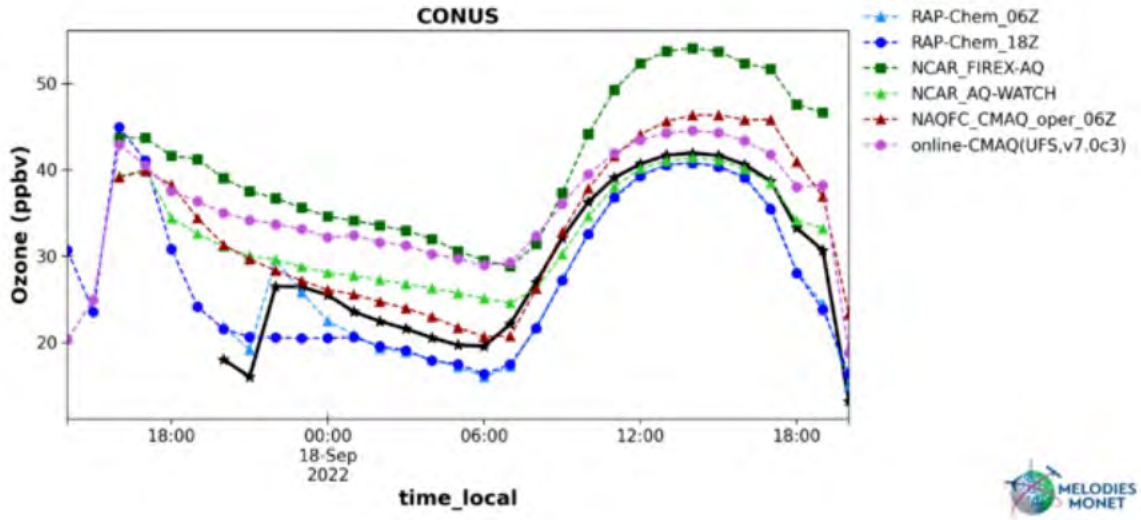
x-section 40N O3	✓	✓
x-section 40N PM2.5	✓	✓
x-section 45N O3	✓	✓
x-section 45N PM2.5	✓	✓
x-section ATL O3	✓	✓
x-section ATL PM2.5	✓	✓



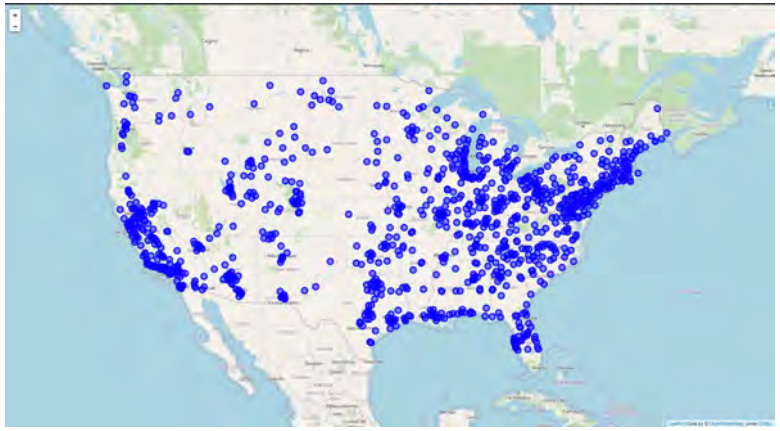




https://rapidrefresh.noaa.gov/RAPchemEPA/



https://rapidrefresh.noaa.gov/RAPchemEPAsites/

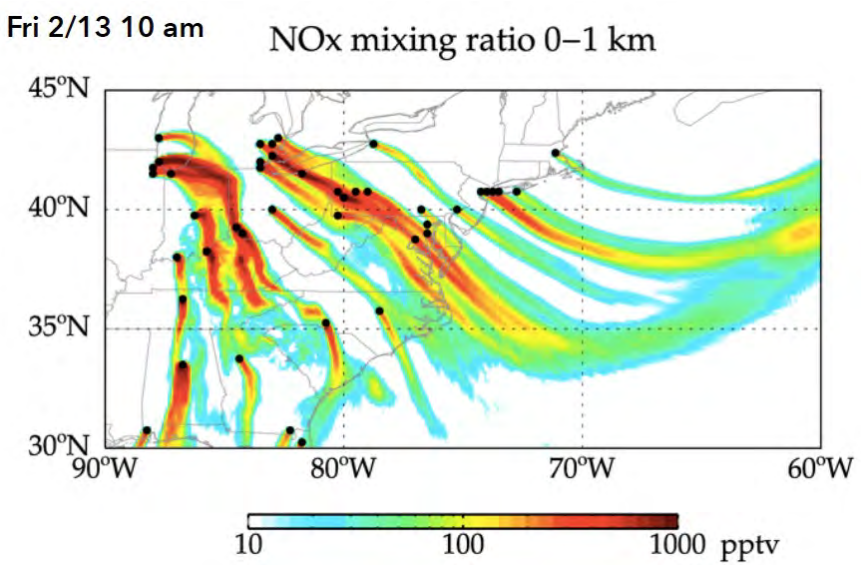


Modeling in multiple stages: campaign planning, in-field forecasts (L. Jaegle UW) & post campaign synthesis (L. Jaegle, A. Carlton)

Forecasting tools to be used for GOTHAAM (Jaegle):

- Meteorological forecasts & FLEXPART forecast trajectories to identify plumes
  - 5-day forecasts: Urban NOx tracer + BVOC tracer with fixed lifetimes
- NASA/GMAO GEOS-FP and GEOS-CF chemical forecasts (5-day forecasts. 25 km resolution)
- Near-Real-Time GEOS-Chem chemical transport simulations for comparison to aircraft observations in the field

FLEXPART Urban NOx forecast



GOTHAAM mission forecasting and modeling

GEOS-Chem modeling for data analysis after the mission:

Nested grid simulation 0.25º x 0.3125º (~25 km) over N. America

GEOS-FP assimilated meteorology

Aerosol-oxidant simulation (HO_x-NO_x-O_3- VOC-Br/Cl/I + SO_4^{2-}-NH_4^+-NO_3^-, BC, organic aerosol, dust, sea salt

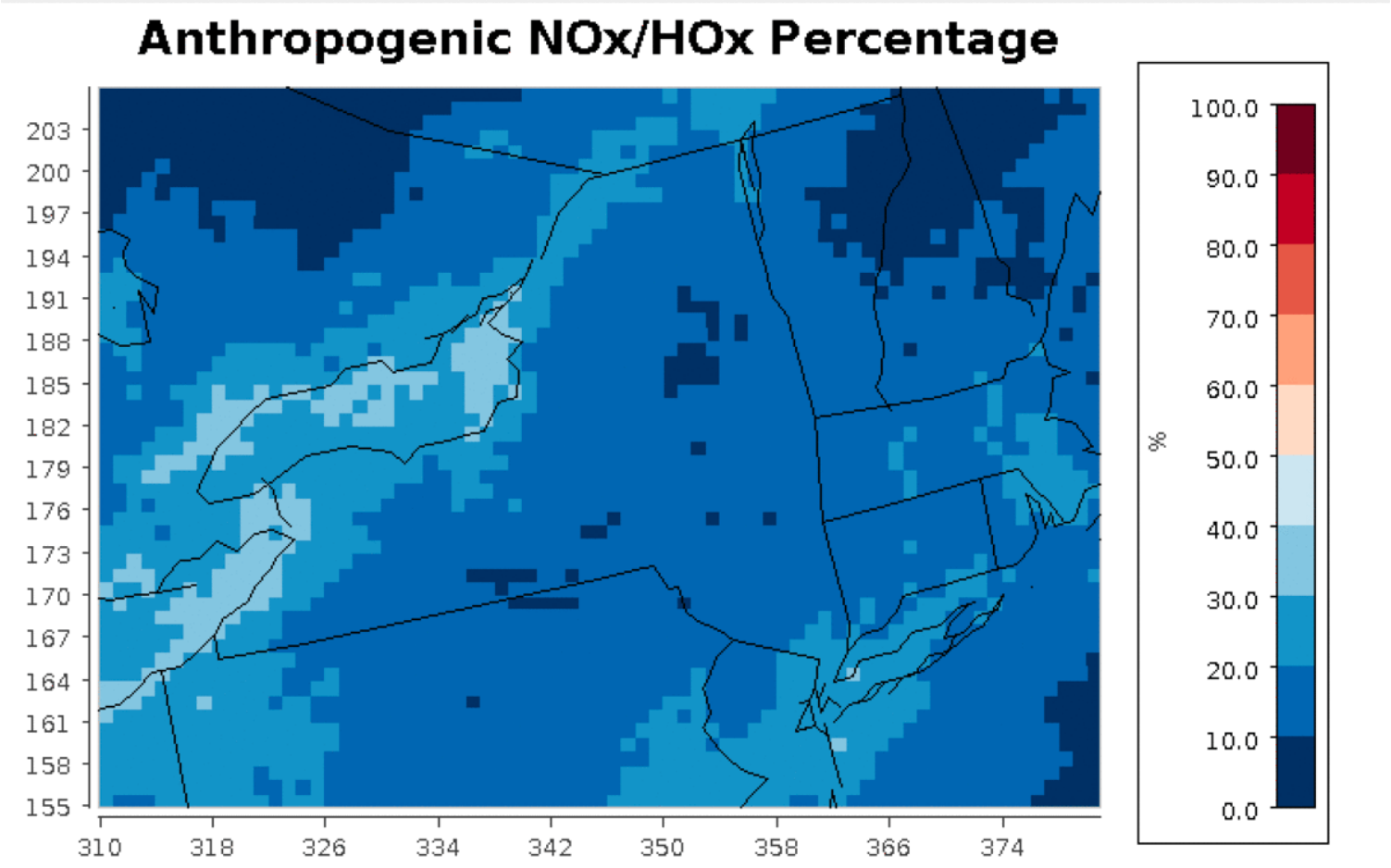
WRF-CMAQ modeling for data analysis after the mission:

Initial and boundary layer conditions from GEOS-Chem

WRF assimilated meteorology

Extensive gas-phase VOC oxidation and complex SOA module

Nighttime flights needed: example objective for why

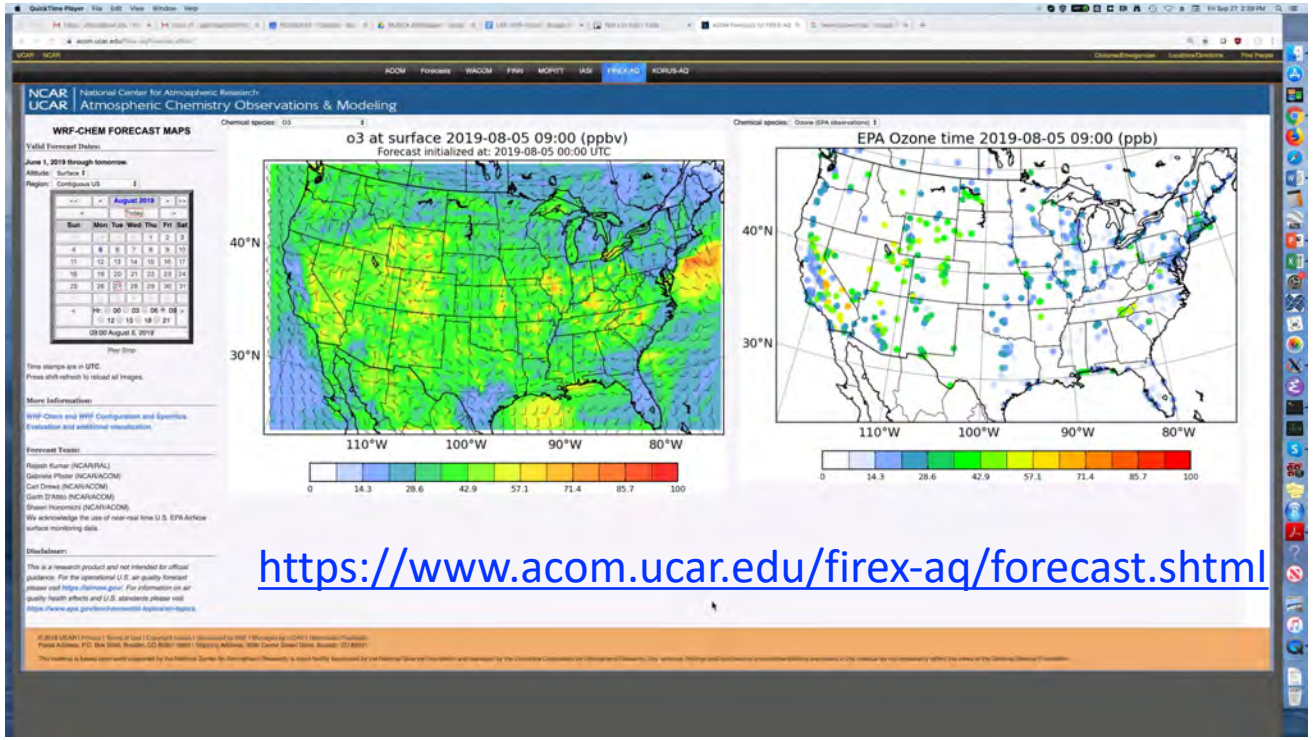


Objective 3. Quantify the relative importance of the various oxidation processes for both gas phase and aerosol species, and how the relative importance of these processes vary across the diel cycle and as a function of the chemical system (biogenic/urban/marine).

NCAR ACOM/RAL Regional Air Quality Prediction System

Rajesh Kumar and Gabriele Pfister

- Support of field campaigns and air quality research from local processed to pollution transport to wildfires to stratospheric intrusions.
- Information for policy makers (e.g. used by CDPHE) – complements NOAA's operational forecasts.
- Early identification of model errors and biases.



Configuration: WRF-Chem V3.9.1, MOZCART Chemistry, inert tracers, 12 x12 km^2 over CONUS, 4 km^2 Coloaado; daily 48-hr forecasts

Visualization

Parameters:

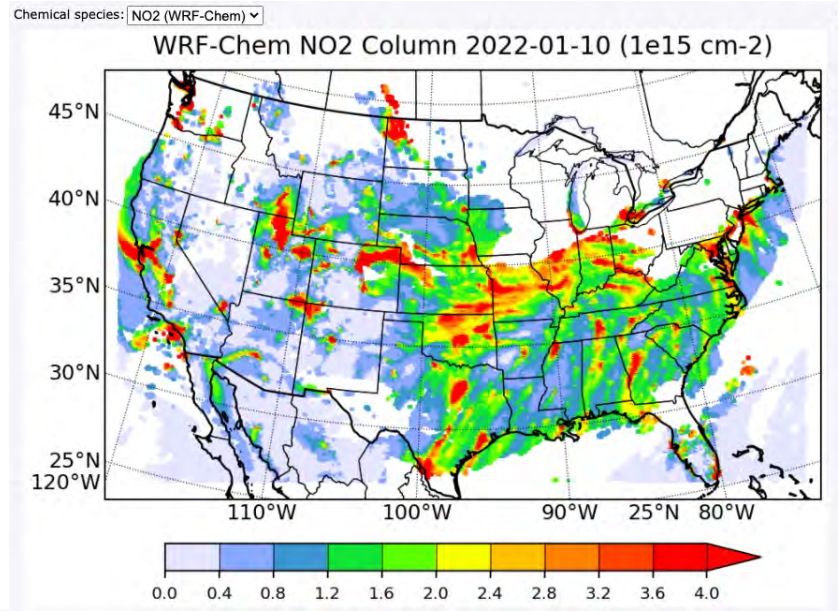
Surface Obs Ozone & $PM_{2.5}$
Ozone, NO_x
PM_{10} & $PM_{2.5}$ (surface)
AOD 550 nm
CO, CO anthro, CO boundary cond. , CO fires
CO fires boundary cond., CO chemical
PBLH, SWDOWN } per CDPHE request
CO asia
Ventilation Index**

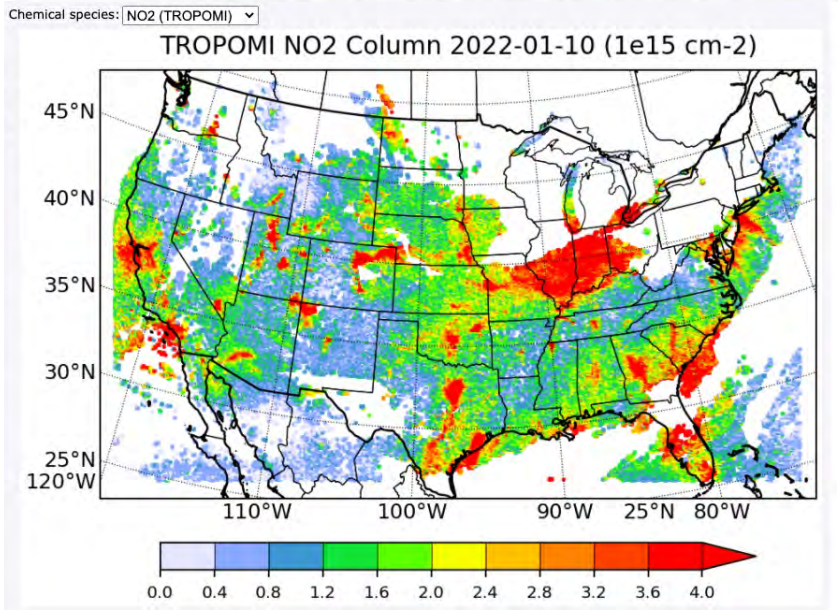
Altitudes: Surface, 3 , 5, 8 km

Regions: CONUS
Colorado
Front Range

Special products:

TOLNET forecasts
TROPOmi and WRF-Chem NO_2
MODIS and WRF-Chem AOD





** In process: WRF only forecasts at 1.3 x 1.3 km^2 over Colorado Front Range

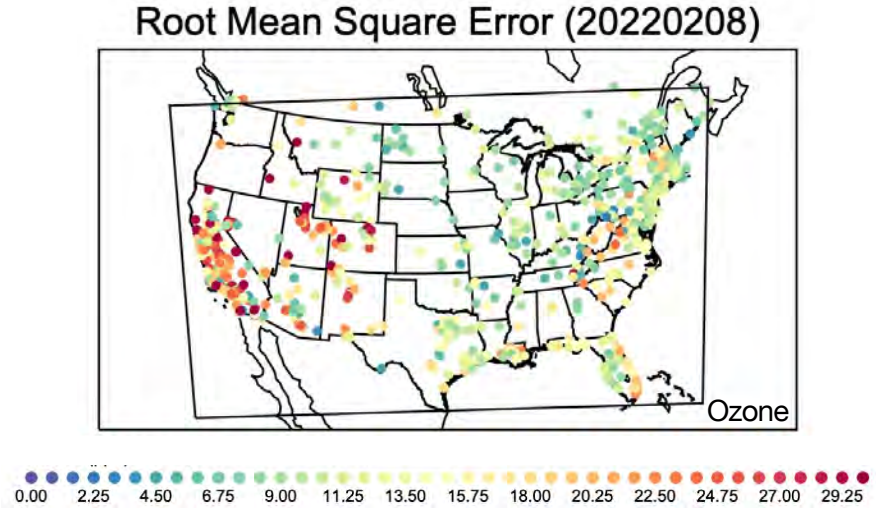
Online Evaluation

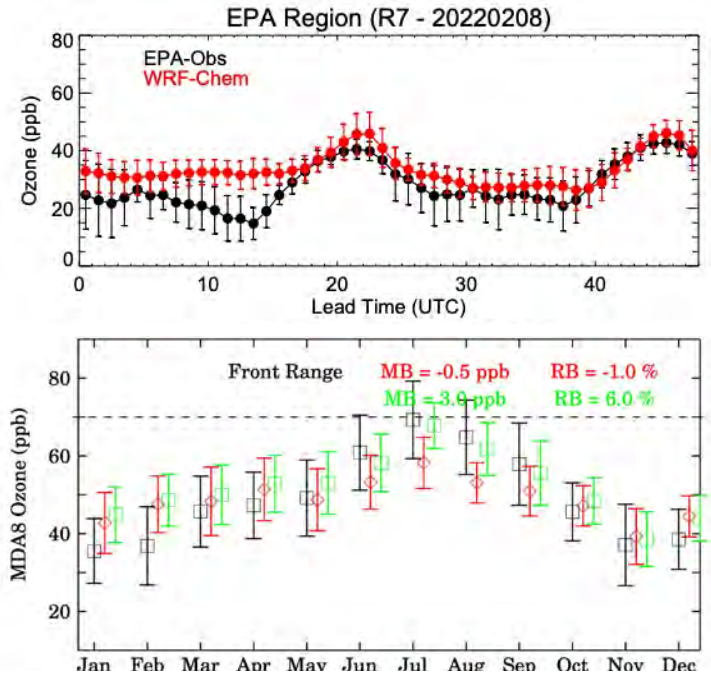
- AIRNOW Ozone and $PM_{2.5}$ NRT observations
  48-hour forecast statistics (timeseries + maps) for
  10 EPA regions + Colorado + Front Range

Offline Evaluation

- AIRNOW Ozone and $PM_{2.5}$ NRT observations – Monthly Statistics
- U.S. EPA surface wind observations
- MOPITT CO
- MODIS AOD
- NASA TOLNET Ozone Lidar (case studies)

We will be happy to add other products in support of upcoming field campaigns!





UW-Madison AGES Forecasting

Maggie Bruckner
UW-Madison AOS

Jerrold Acdan
UW-Madison AOS

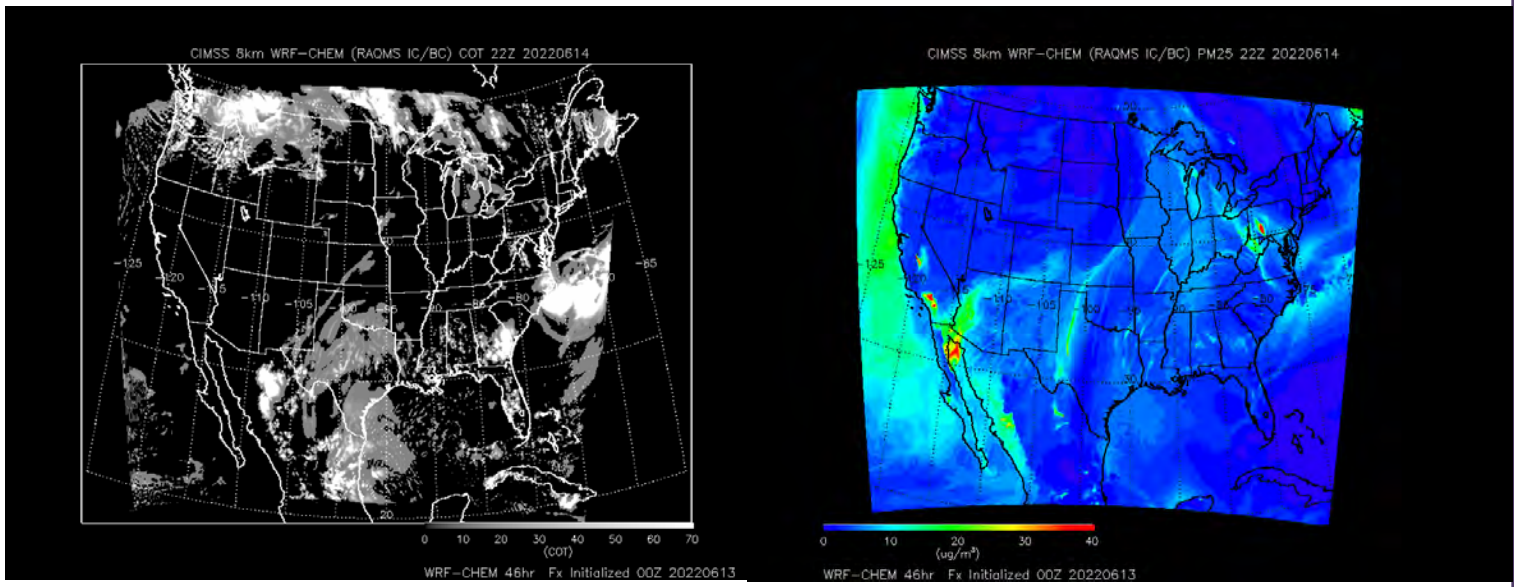
Aditya Kumar
UW-Madison SSEC

Allen Lenzen
UW-Madison SSEC

Brad Pierce
UW-Madison SSEC/AOS

- 8km CONUS nested RAQMS/WRF-Chem (aerosol/clouds/meteorology)
- 4km LADCO nested RAQMS*/WRF-Chem (chemistry/aerosols/clouds/meteorology)

*Currently conducting retrospective testing with WACCOM

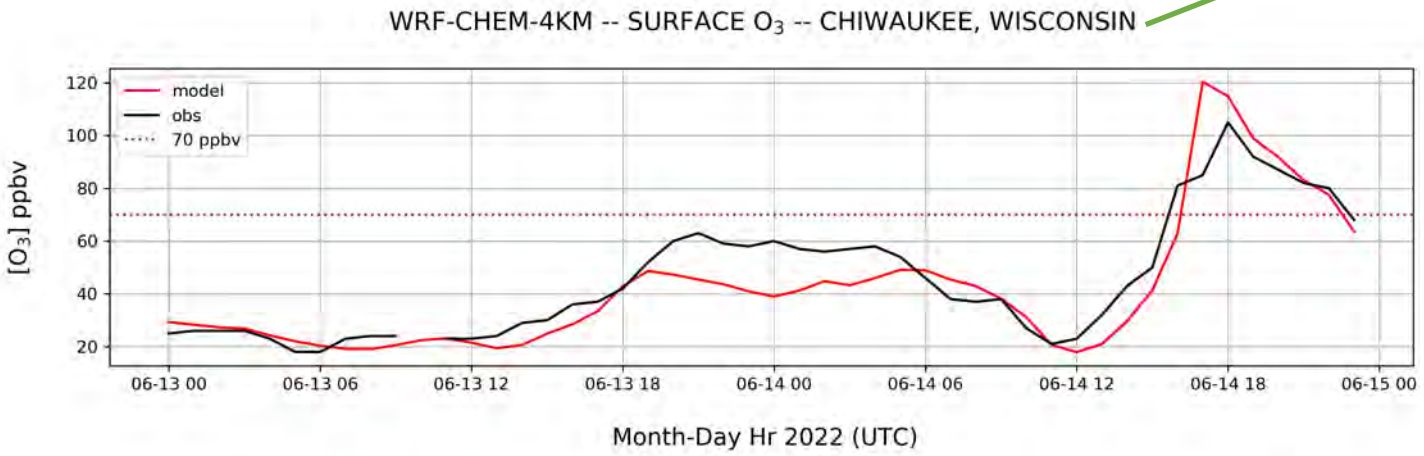


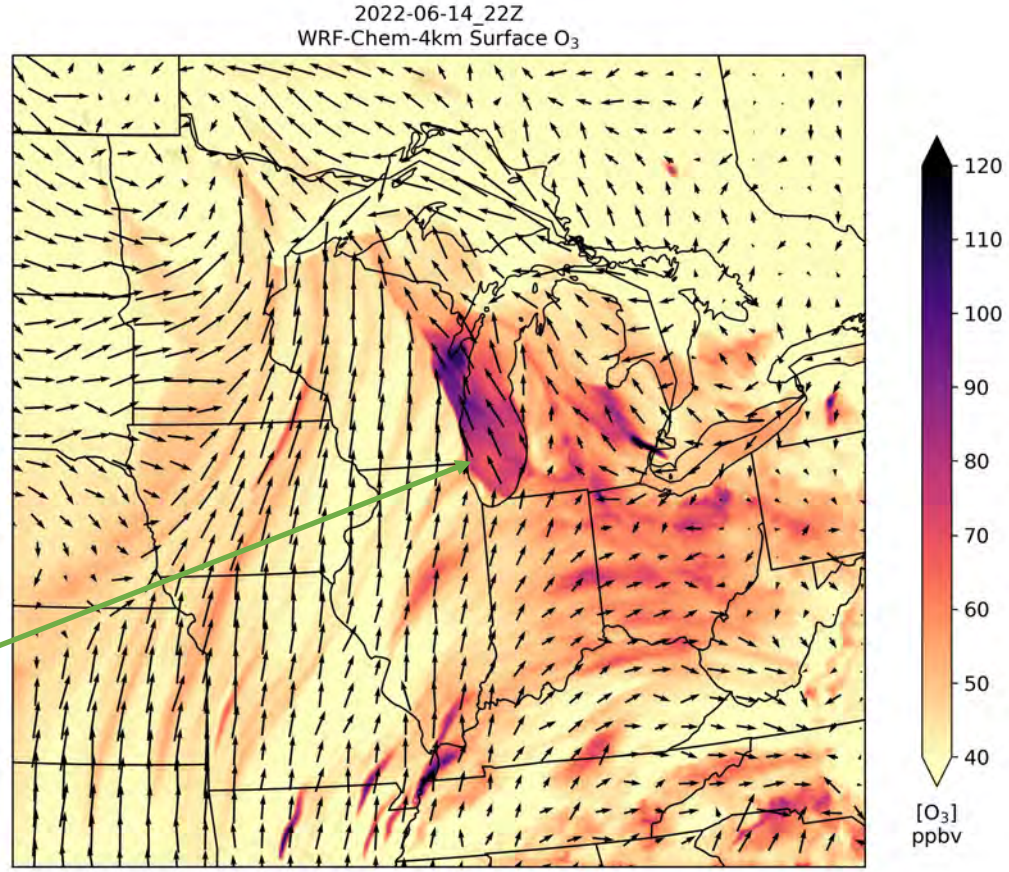
Contact: rbpierce@wisc.edu

4km WRF-Chem V.4.4 (Developed in collaboration with Gabi Pfister, ACOM)

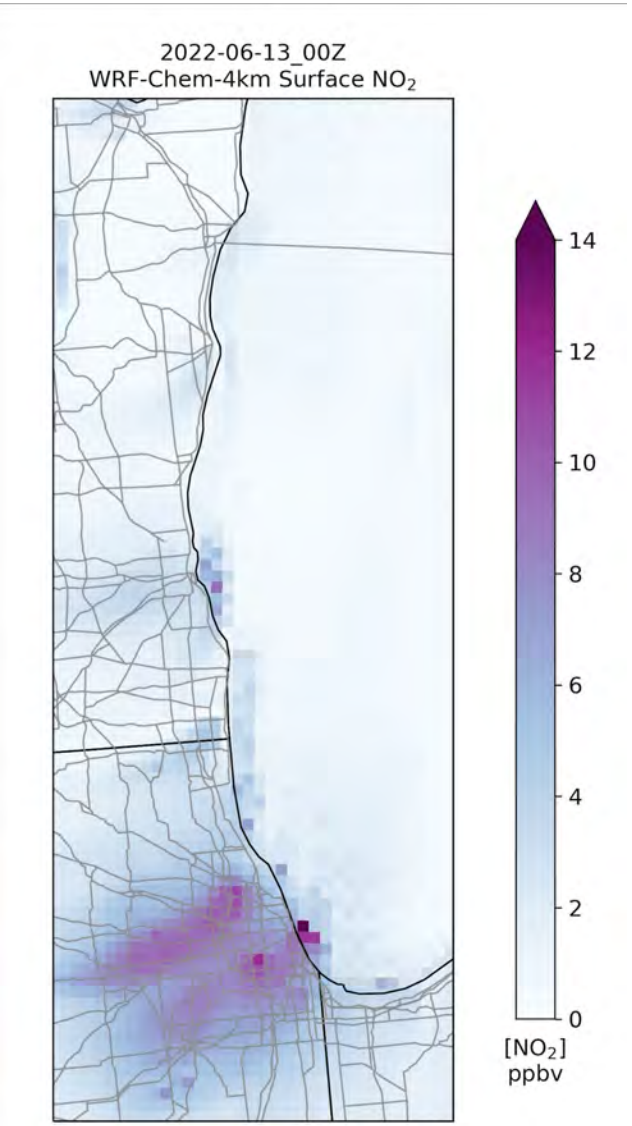
Meteorology	HRRR 3-km
Anthropogenic emissions	NEI17 12-km (non-trended)*
Biogenic emissions	MEGAN v2
Fire/biomass burning emissions	FINN v1.5
Sea surface temperature	GLSEA
Chemistry mechanism	T1_MOZCART
Photolysis option	TUV

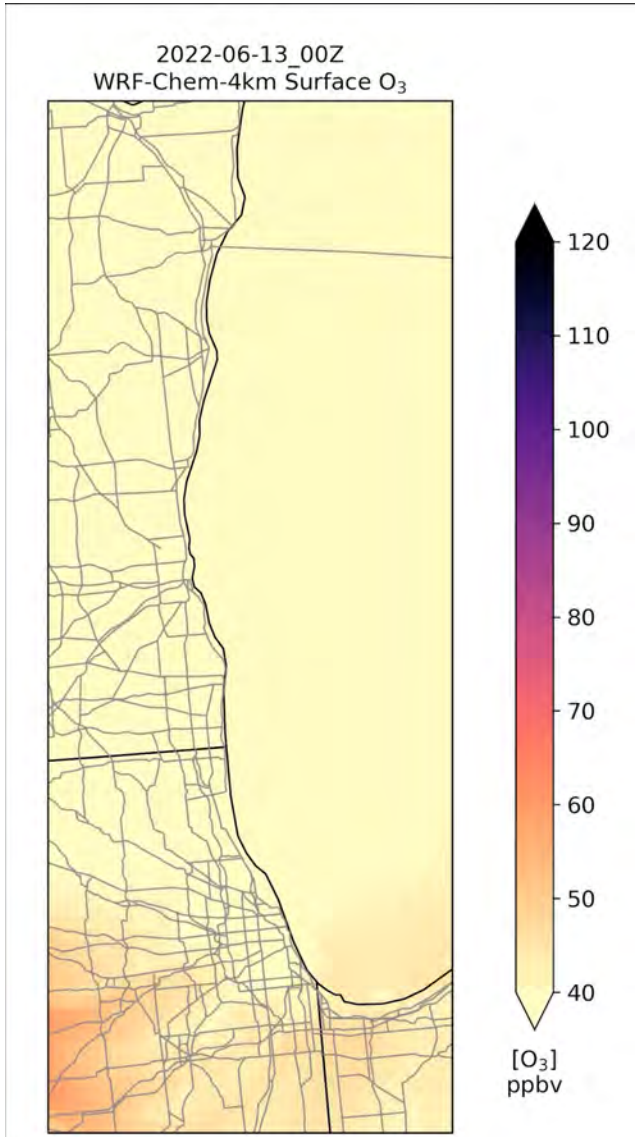
*Will update to trended NEI17 4km (Kirk Baker)

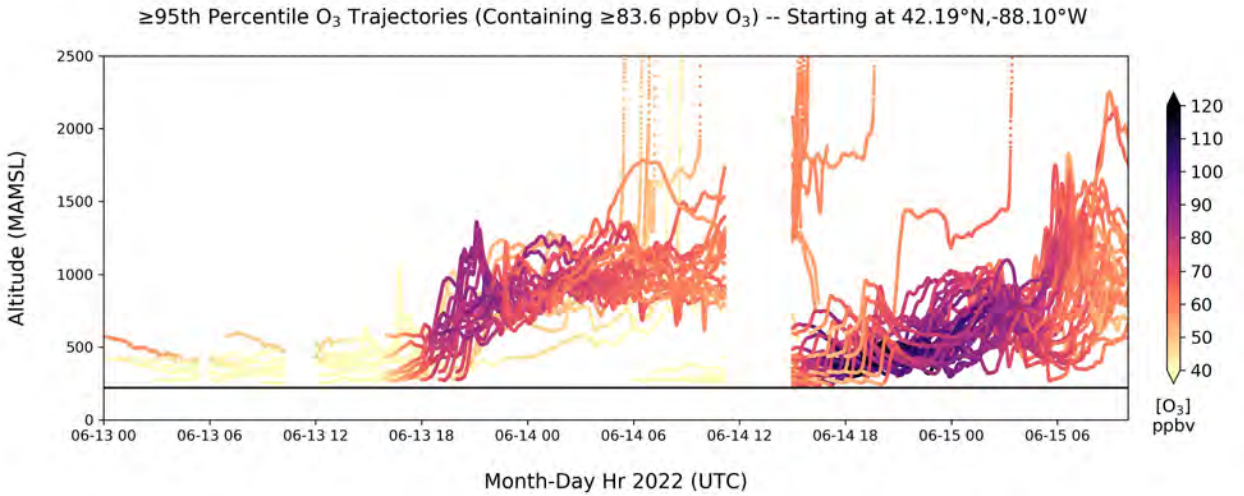


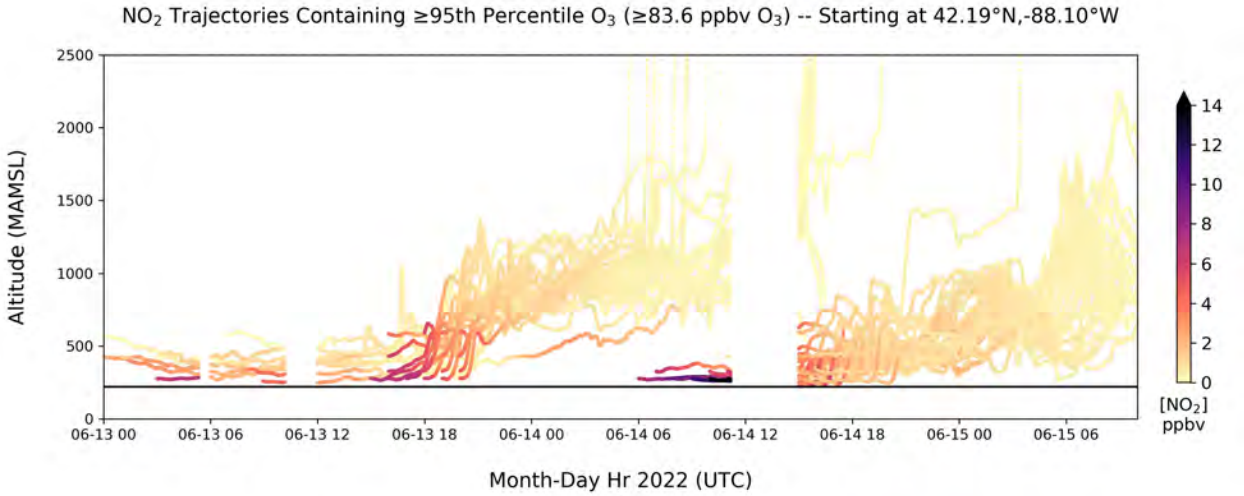


4km WRF-Chem V.4.4 Trajectory Analysis









- Will allow Lagrangian diagnostics of ozone production and ozone precursors
- Will provide link between emissions and aircraft/satellite measurements

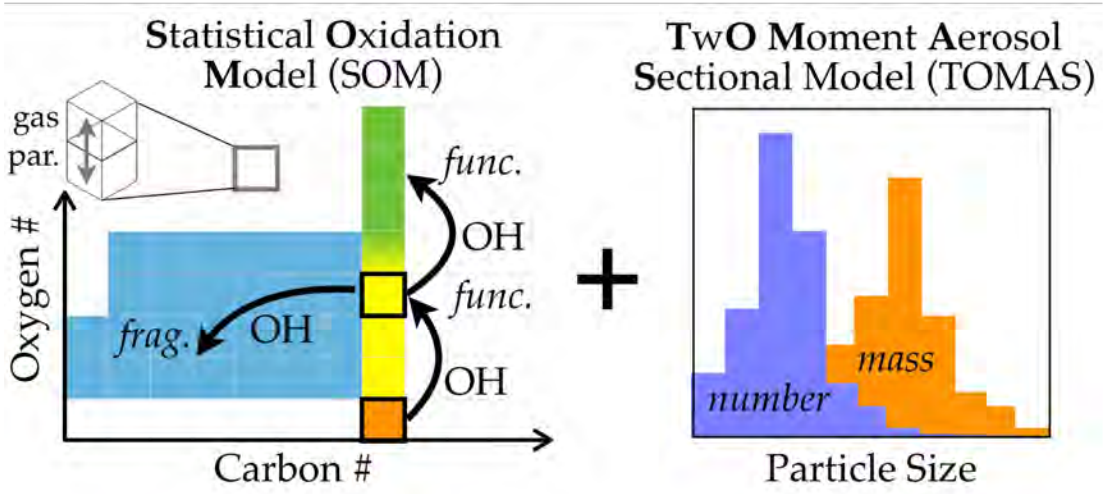
Studying the Emerging Contribution of VCPs and Food Cooking to Urban and Regional Air Quality

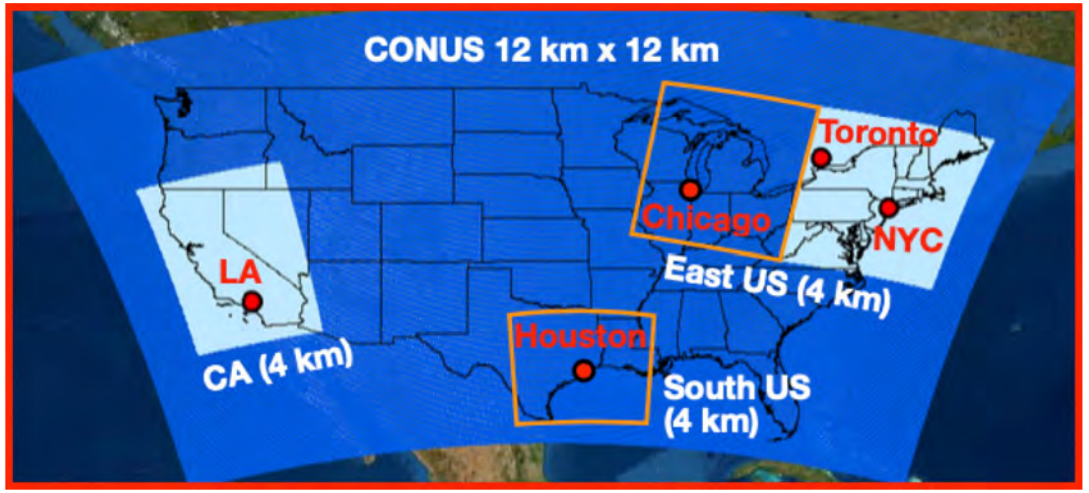
Shantanu Jathar

Jeffrey Pierce

En Li

TBD

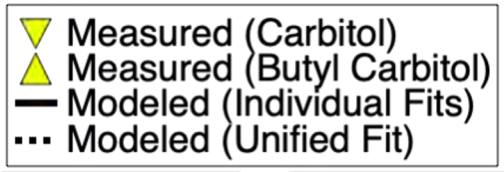


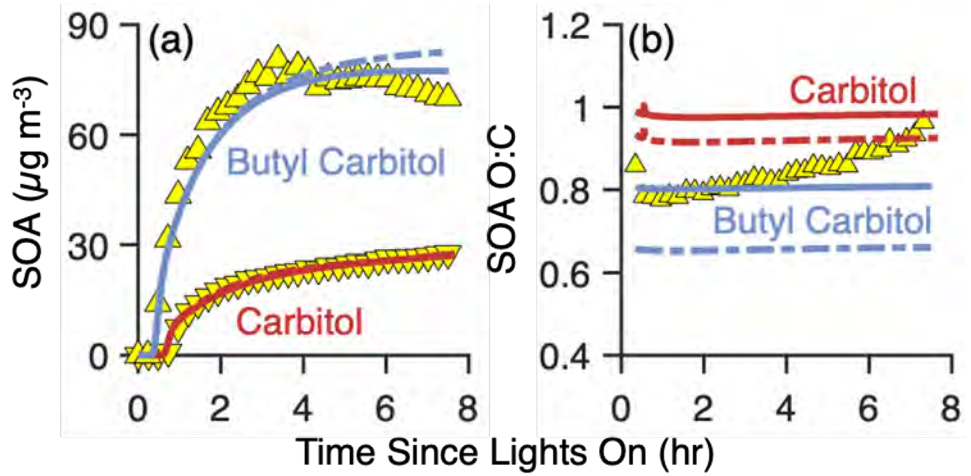


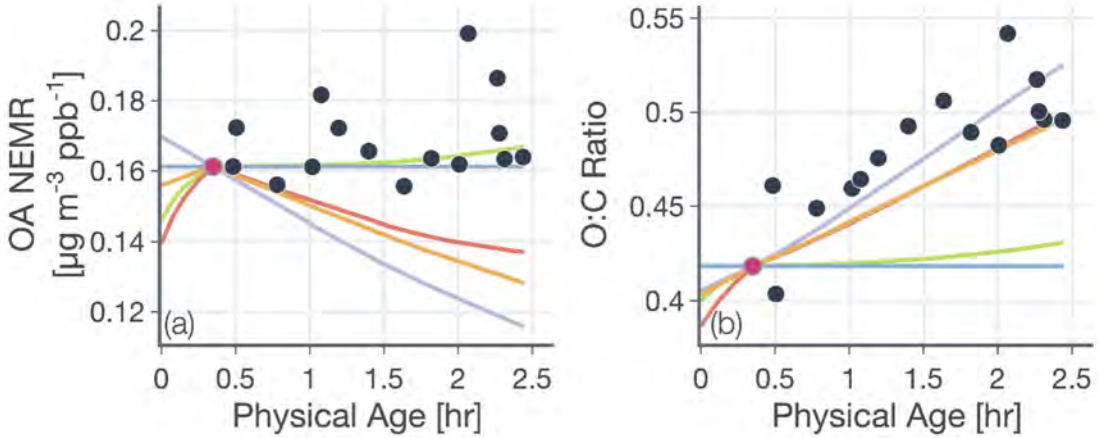
Partnerships/Collaborations: *NOAA (Warneke, Schwantes, McDonald; AEROMMA), UC Riverside (David Cocker; VCP SOA), CMU (Presto; VCP SOA), Helsinki (Ehn, Jokinen; monoterpene SOA), Toronto (Chan; cooking), Hong Kong (Chan; cooking)*

Objective 1: Use kinetic box models to develop SOA parameterizations from laboratory experiments

Sasidharan et al., In Prep





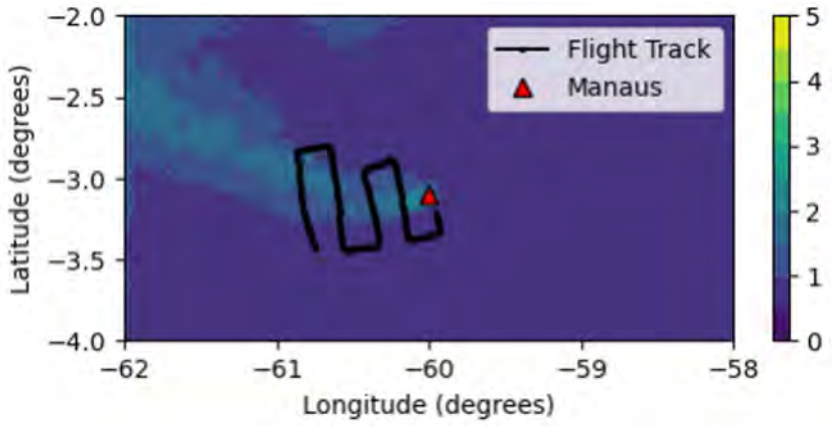


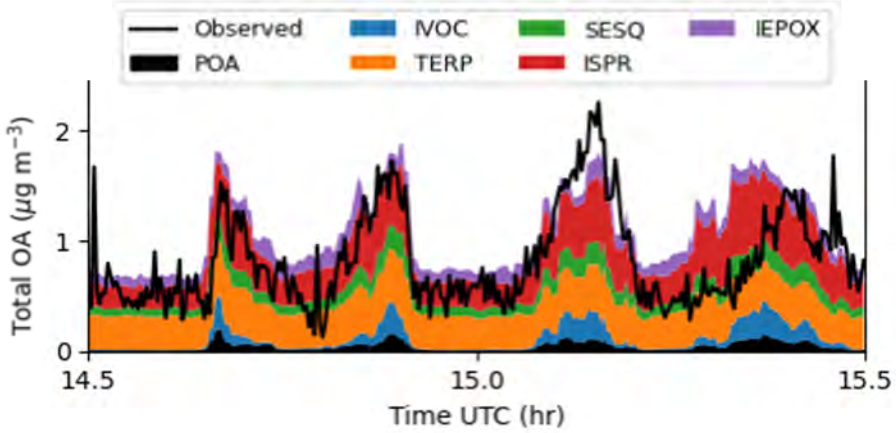
Akherati et al., ESA, 2022

Objective 2: Use Lagrangian models to study the aerosol evolution in urban plumes

Objective 3: Use a 3D model (WRF-Chem) to study atmospheric impacts

He, Bilsback et al., In Prep





Secondary organic aerosol Chamber Experiments for Non-Traditional Species (**SCENTS**)

- Studied SOA formation from <u>14 oxygenated VOCs and 2 VOC mixtures across 34 experiments</u> (Spring and Summer 2022)
- OVOC classes: carbitols, furans, terpenoids, acetates, siloxanes, adhesives
- Data will be used to inform VCP VOC chemistry on AEROMMA modeling project

Supporting NASA missions with the GEOS Composition Forecast System, "GEOS-CF"

K. Emma Knowland

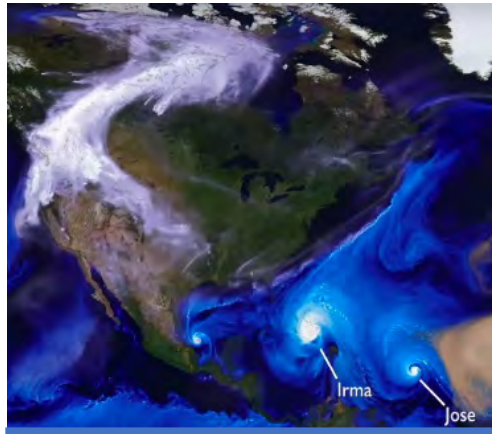
Morgan State University/GESTAR-II

NASA Global Modeling and Assimilation Office (GMAO)

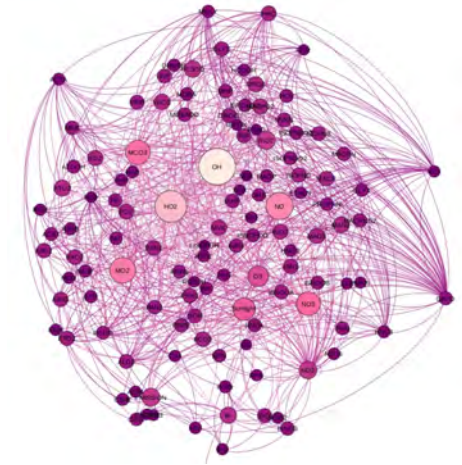
In collaboration with:

Christoph Keller, Pamela Wales, Lesley Ott, Joe Ardizzonne, Christine Bloecker, Austin Conaty, Meredith Nichols, Callum Wayman, Steven Pawson

GEOS Composition Forecast



GEOS NWP



GEOS-Chem

GEOS - CF

Version 12.0.1
Tropospheric and Stratospheric chemistry

Keller, C. A., Knowland, K. E., et al. (2021). **Description of the NASA GEOS composition forecast modeling system GEOS-CF v1.0**. *Journal of Advances in Modeling Earth Systems (JAMES)*, 13, e2020MS002413. https://doi.org/10.1029/2020MS002413

Knowland, K. E., Keller, C. A., et al. (2022). **NASA GEOS Composition Forecast Modeling System GEOS-CF v1.0: Stratospheric Composition.** *JAMES* https://doi.org/10.1029/2021MS002852

https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

k.e.knowland@nasa.gov

GEOS NWP with Coupled GEOS-Chem chemistry

GEOS-CF v1.0

One **5-day forecast** per day

- Initialized at 12z
- 1-day meteorological replay ("analysis")
- 5-day forecast
- c360 (0.25°, **~25x25 km^2**)
- 72 layers (surface to 0.01hPa)
- GEOS-Chem v12.0.1

Data distributed via OpenDAP and HTTPS:

- 2D output at 15 minute and hourly frequency
- 3D output at hourly and three hourly frequency, 1-hour 2D & 3D output, **including specific TEMPO file for trace-gas retrievals**

Emissions:

- HTAP v2.2 (global bottom-up) for anthropogenic
- Near real-time fires (QFED)
- Online dust, sea salt, plant emissions

Observation-constraints:

- Currently no direct data assimilation of constituents in GEOS-CF
- GOCART aerosols constrained by satellite measurements of AOD
- Biomass burning emissions from QFED

Knowland et al., 2022. "File Specification for GEOS-CF Products." *GMAO Office Note No. 17 (Version 1.2), available from http://gmao.gsfc.nasa.gov/pubs/office_notes*

https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/

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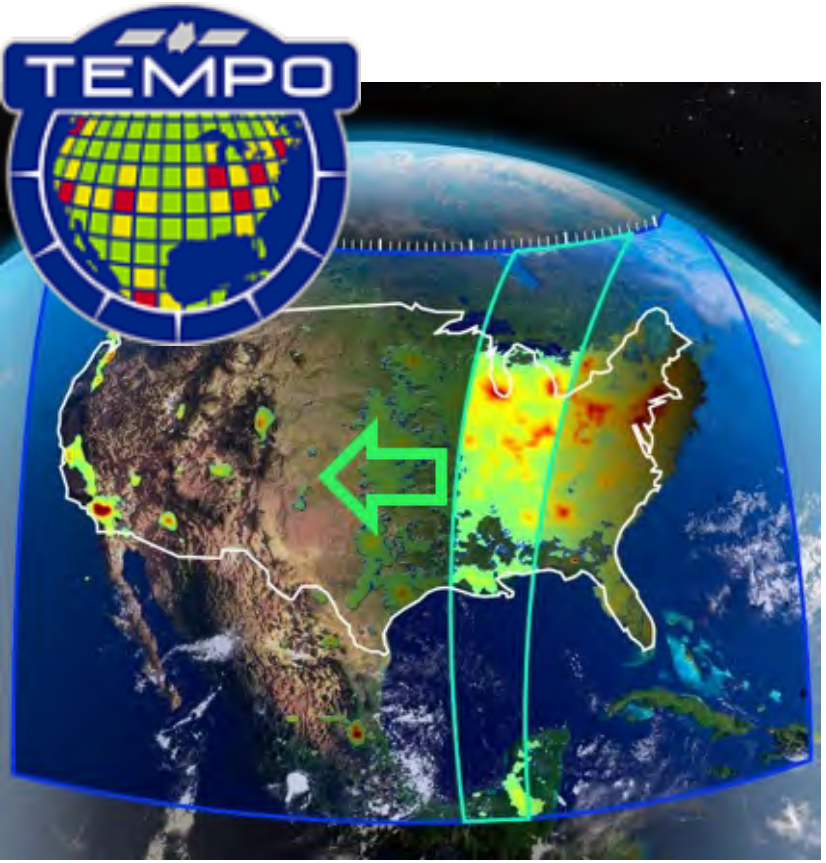
Support a broad range of NASA applications

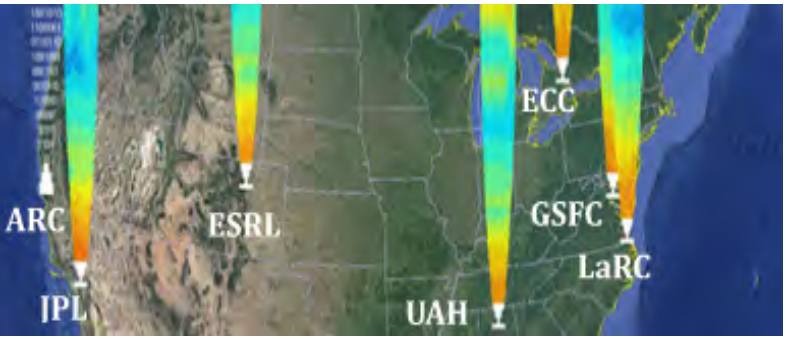
GEOS - CF



- Realistic atmospheric composition in the troposphere **and** stratosphere in GEOS-CF is essential to support a broad range of NASA applications measuring trace gases and aerosols, including:
  - Airborne campaigns
  - Satellite retrievals of trace gases
  - Stratosphere-troposphere exchange

TOLNET

Tropospheric Ozone LIDAR Network



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GMAO Mission Support for Field Campaigns

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

Global Modeling and Assimilation Office GMAO

Weather | Mission Support | CF | Reanalysis | Carbon

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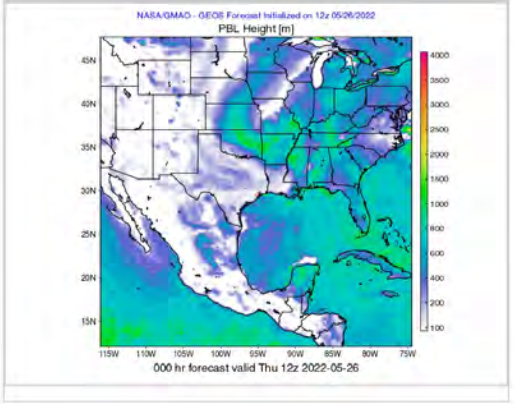
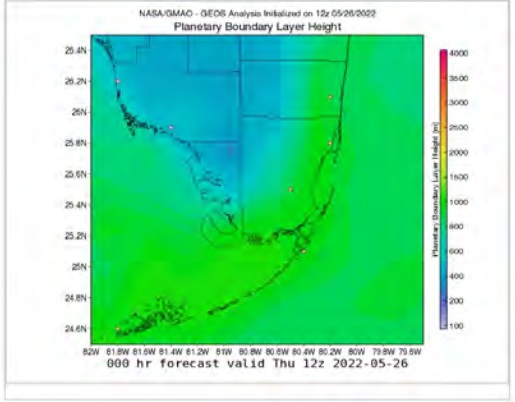
- » SCOAPE
- » SOCRATES
- » TRACER-AQ

GMAO Active Mission Support

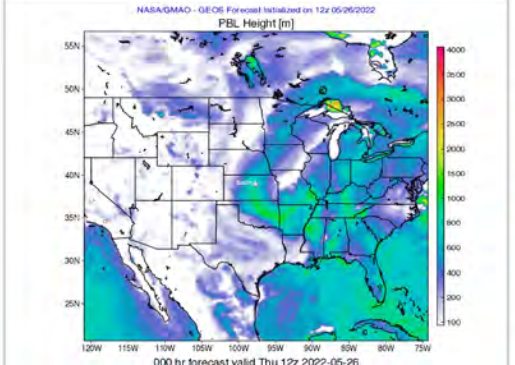
ACCLIP



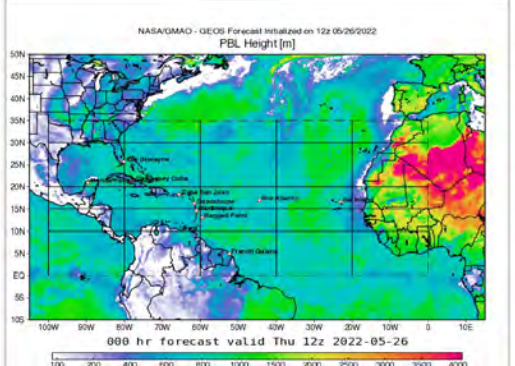
BLUEFLUX



DCOTSS



PRDUST



https://gmao.gsfc.nasa.gov/field_campaigns/real_time_support_requests.php

To request GMAO Real-Time Support for NASA Field Campaigns

realtimesupportrequests@gmao.gsfc.nasa.gov

1. NASA field campaign name
2. Brief overview of the campaign
3. Requester's contact information
4. Time period when support is required
5. URL of the campaign website
6. Brief description of the real-time support requested in terms of GEOS products and any campaign-specific needs

Request as soon as possible, but no later than 3 months prior to the start of campaign

TEMPO specific collection: “sat_inst_1hr_r721x361_v72”

- **Regional Chemistry and Meteorology Diagnostics to support TEMPO satellite**

- **Frequency:** *hourly instantaneous from 00:00 UTC*
- **Spatial Grid:** *3D, model-level, subset region of full horizontal resolution*
- **Dimensions:** *longitude=721, latitude=361, every 0.25º*
  - **longitude:** 0º to -180º
  - **latitude:** 0º to 90º
- **vertical level:** *72 layers*
- **Granule Size:** *~258 MB per file*
- **Start date:** 00 UTC 1 January 2022
- **Mode:** Replay only; Forecasts available based on mission requirements

- Knowland et al., 2022. "File Specification for GEOS-CF Products." *GMAO Office Note No. 17 (Version 1.2), available from http://gmao.gsfc.nasa.gov/pubs/office_notes*

Name	Dim	Description	Units
BrO	tzyx	Bromine monoxide (BrO, MW = 96.00 g mol-1) volume mixing ratio dry air	mol mol-1
FRSEAICE	tyx	ice covered fraction of tile	1
FRSNO	tyx	fractional area of land snowcover	1
GLYX	tzyx	Glyoxal (CHOCHO, MW = 58.00 g mol-1) volume mixing ratio dry air	mol mol-1
HCHO	tzyx	Formaldehyde (CH2O, MW = 30.00 g mol-1) volume mixing ratio dry air	mol mol-1
HNO2	tzyx	Nitrous acid (HNO2, MW = 47.00 g mol-1) volume mixing ratio dry air	mol mol-1
IO	tzyx	Iodine monoxide (IO, MW = 143.00 g mol-1) volume mixing ratio dry air	mol mol-1
NO2	tzyx	Nitrogen dioxide (NO2, MW = 46.00 g mol-1) volume mixing ratio dry air	mol mol-1
O3	tzyx	Ozone (O3, MW = 48.00 g mol-1) volume mixing ratio dry air	mol mol-1
OClO	tzyx	Chlorine dioxide (OClO, MW = 67.00 g mol-1) volume mixing ratio dry air	mol mol-1
PHIS	tyx	surface geopotential height	m+2 s-2
PS	tyx	surface pressure	Pa
Q	tzyx	specific humidity	kg kg-1
SNODP	tyx	snow depth	m
SNOMAS	tyx	Total snow storage land	kg m-2
SO2	tzyx	Sulfur dioxide (SO2, MW = 64.00 g mol-1) volume mixing ratio dry air	mol mol-1
T	tzyx	air temperature	K
TROPPB	tyx	tropopause pressure based on blended estimate	Pa
U2M	tyx	2-meter eastward wind	m s-1
V2M	tyx	2-meter northward wind	m s-1
ZPBL	tyx	planetary boundary layer height	m

https://gmao.gsfc.nasa.gov/weather_prediction/GEOS-CF/
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Summary of GEOS-CF Status

- GEOS-CF daily global composition forecasts at 25km resolution are generated in near-real time:
  - High-resolution historical estimates for fields are available since January 2018
  - Forecasts remain available on data servers for two weeks
  - The forecasts of the five most-requested surface pollutants (O_3, NO_2, CO, PM2.5, and SO_2) remain accessible via data servers for January 2019-present
- Forecast visualizations and links to data available at: fluid.nccs.nasa.gov/cf and /cf_map
- Applications users include:

Keller, C. A., Knowland, K. E., et al. (2021). **Description of the NASA GEOS composition forecast modeling system GEOS-CF v1.0**. *Journal of Advances in Modeling Earth Systems*, 13, e2020MS002413. https://doi.org/10.1029/2020MS002413

Knowland, K. E., Keller, C. A., et al. (2022). **NASA GEOS Composition Forecast Modeling System GEOS-CF v1.0: Stratospheric Composition.** *JAMES* https://doi.org/10.1029/2021MS002852

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