

NATIONAL WEATHER SERVICE

NWS Trace Gas Observations -Assimilation and Verification

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Cory Martin¹, Alicia Bentley¹, Jianping Huang¹, Jeff McQueen¹, Daryl Kleist¹, Ivanka Stajner¹, Partha Bhattacharjee², Hyundeok Choi², Ho-Chun Huang³, Andrew Tangborn², Yaping Wang², Hongli Wang⁴, Ruifang Li⁴

¹NOAA NWS NCEP EMC | ²SAIC @ NOAA NWS NCEP EMC | ³Lynker @ NOAA NWS NCEP EMC | ⁴CIRES @ NOAA GSL



Current and Planned Operational Systems

Operational:

- GEFSv12 single aerosol member out to 5 days
- AQMv7 regional AQ model (operational implementation is imminent)
- HRRR-Smoke

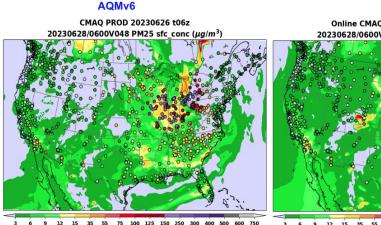
Planned:

- GEFSv13 aerosols with radiative feedback in all members
- GFSv17 aerosol tracers (no rad. feedback) in DA forecast cycle only
- RRFSv1 smoke and dust tracers in one member
- RRFSv2 regional AQ forecast member as part of the RRFS

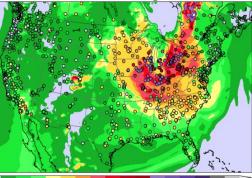
AQMv7

- Transitioning from an offline system (with GFS meteorology) to an online system with coupled FV3 and CMAQ
 - 13km resolution, 65 layers, CONUS, AK, HI all in one large domain

AQMv7 improves PM_{2.5} prediction during Quebec Fires in June 2023



AQMv7 Online CMAQ V70C84 20230626 t06z 20230628/0600V048 PM25 sfc conc (µg/m³)



3 6 9 12 15 35 55 75 100 125 150 250 300 400 500 600 750



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Usage of Atmospheric Composition Observations

Assimilation

- GFSv17/GEFSv13
 - VIIRS Aerosol Optical Depth assimilation
- Regional AQ Model
 - TROPOMI NO₂, VIIRS AOD, surface PM
 - TEMPO NO_2 , O_3 , AOD?
- State / Emissions Adjustment
 - Longer term plan to improve NRT emissions through coupled DA

Validation/Verification



Joint Effort for Data assimilation Integration (JEDI) Infrastructure for Unified Data Assimilation

JEDI is a project within the Joint Center for Satellite Data Assimilation (JCSDA)

JEDI provides a software infrastructure for data assimilation that

- □ is model agnostic
- is generic and portable, from toy models running on laptops to operational Earth system coupled models running in the cloud.
- enables DA on the model native grid
- does not impose one specific DA methodology or algorithm
- provides a framework for rapid uptake of new observations into operations with generic observation handling and modeling
- encourages implementation of model-independent observation operators
- provides a unified Interface for Observation Data Access (IODA)

JEDI is intended for scientific exploration and operational forecasting.

The keys to success are separation of concerns and interfaces.





GFSv17 Aerosol DA Plans

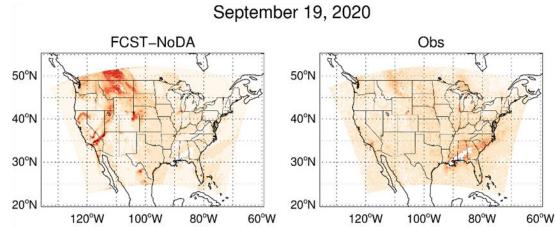
Currently one of the few (only?) operational centers to not have aerosol DA initializing their aerosol prediction system

- 6-hourly cycles 4x a day with early and late cycles
 - Early cycle to initialize the GEFS long forecasts (one aerosol analysis provided, up to the ensemble forecast group to decide if/how to perturb)
 - Late cycle to initialize the high resolution GDAS forecast (without radiative feedback)
- Analysis resolution C384L127 (~0.25 deg); background resolution C1152L127 (~9km)
- 3DVar FGAT with 3-hourly backgrounds
- VIIRS EPS 550nm AOD from S-NPP, N20, N21

TROPOMI NO₂ Assimilation

In collaboration between NWS/EMC and JCSDA, a generic column retrieval forward operator has been developed in JEDI with the first application being TROPOMI NO₂ retrievals.

This operator has been shown to work with both total column and averaging kernel observations of constituents.

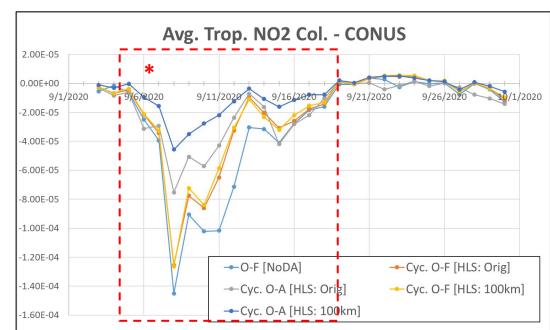


This is the first step towards high resolution trace gas assimilation at NWS.



TROPOMI NO₂ Assimilation

- Example of initial results from assimilating TROPOMI NO₂ retrievals in a development version of our AQM:
- Overall, DA improves NO₂ forecast during the fire season in September 2020.
- Initial tuning of background error and horizontal length scales is showing sensitivity to analysis performance
- * Huge negative values are related to the NO₂ plumes that model simulated, but observation didn't see.





Planned TEMPO Assimilation

- S5P only provides 1-2 observations (some overlap) per day for the coterminus US, with an overpass in the early afternoon local time
- For real-time air quality prediction, our forecast models will benefit greatly from geostationary observations of trace gases / aerosols for multiple reasons
 - Higher temporal resolution (hourly; daytime only)
 - Greater chance of cloud-free retrievals
 - Data availability in the morning so that the AQ forecast can initialize early enough to provide a useful, same-day air quality prediction for the afternoon



Assimilation of Trace Gas Obs

Short-Term Plans

• Use TROPOMI + TEMPO to constrain ICs using NO $_2$, O $_3$, and other assimilation quality retrievals

Future Plans

- Meteorology is an initial value problem, AQ is more sensitive to emissions (anthropogenic, biogenic, fires, etc.) and for regional, LBCs
- Using strongly coupled DA, can use retrievals + in situ obs to constrain state and adjust emissions concurrently (fire emissions already based on observations)
- Challenges:
 - Computational cost (4DVar; ensemble approaches)
 - Could AI help with either or both?

Operational Validation Datasets

- EVSv1 (EMC Verification System) recently went into operations (https://www.emc.ncep.noaa.gov/users/verification/)
 - Current operational EVS is only validating with in situ surface PM2.5 and O₃ observations for the regional AQM
- EVSv2 plans to include a comprehensive composition validation suite:
 - Smoke and or dust AOD from satellites, Total AOD from satellites and AERONET
 - \circ Surface NO₂ and SO₂
- Future EVS implementations could include additional remotely-sensed verification datasets
 - TEMPO: O₃ (tropospheric and PBL), NO₂, HCHO, aerosol products, O₃ profiles (ex: OMPS)



Development Datasets

Operational use of observations comes with stipulations and challenges

• Latency, limited resources for ingest/storage, etc.

But, observations from TEMPO will be useful to NWS as soon as they are publicly available

- Verification / validation of systems under development and pre-operational implementation
- Development of future assimilation systems
- "offline" validation of currently operational systems
 - Used to define areas of focus for model upgrades



Summary

- No operational assimilation of aerosol / trace gas observations (yet)
 - JPSS VIIRS AOD coming soon, TROPOMI/TEMPO trace gas shortly after
- Observations are/can be used to validate operational model performance
- Long term plans include simultaneous state and emissions adjustment through strongly coupled DA

Questions: cory.r.martin@noaa.gov

