George Mason University
Cooperative Institute for Satellite Earth System Studies (CISESS)
National Oceanic and Atmospheric Administration, U.S. Department of Commerce
Environment and Climate Change Canada
Environnement et Changement climatique Canada

Ongoing Research and Developments for NOAA's Next Generation Air Quality Model

Patrick C. Campbell[1,2,3], Wei Li[1,2,3], Beiming Tang[1,2,3], Youhua Tang[1,2,3], Barry Baker[3], Irena Ivanova[1,2], Wei-Ting Hung[1,2,3], Zachary Moon[3,4], Chi-Tsan Wang[1], Daniel Tong[1], B.H. Baek[1], Siqi Ma[1], Paul Makar[5], Fanglin Yang[6], Jianping Huang[6,7], Ivanka Stajner[6], and Raffaele Montuoro[6]

[1]George Mason University, [2]Cooperative Institute for Satellite Earth System Studies, [3]NOAA Air Resources Laboratory, [4]Earth Resources Technology, Inc., [5]Environment Climate Change Canada, [6]NOAA Environmental Monitoring Center , [7]I.M. Systems Group Inc., Rockville, MD, USA

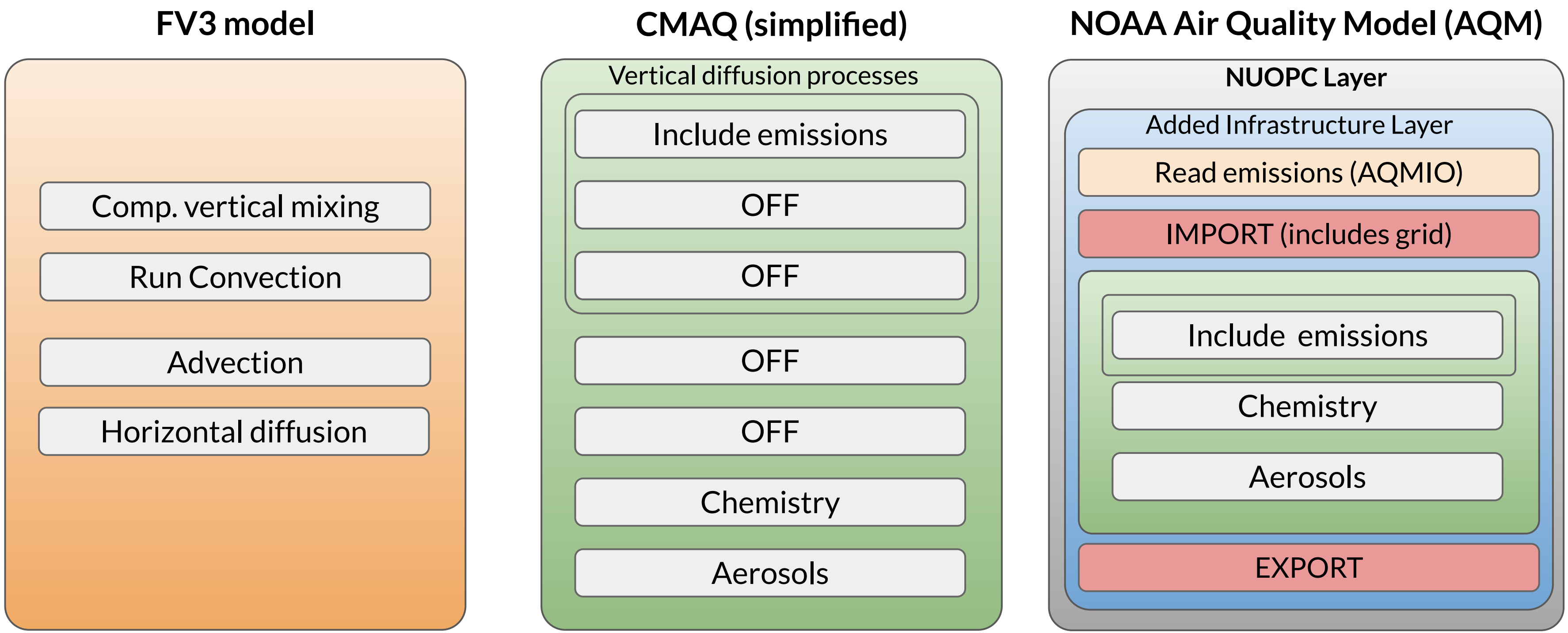
UFS Webinar: April 11th, 2024

Outline

1. NOAA's UFS-AQM component and major science updates.
2. Moving beyond the "big-leaf" model in the UFS-AQM.
3. Updating the anthropogenic emissions in the UFS-AQM.

NOAA's Next-Generation Online-Coupled Air Quality Model

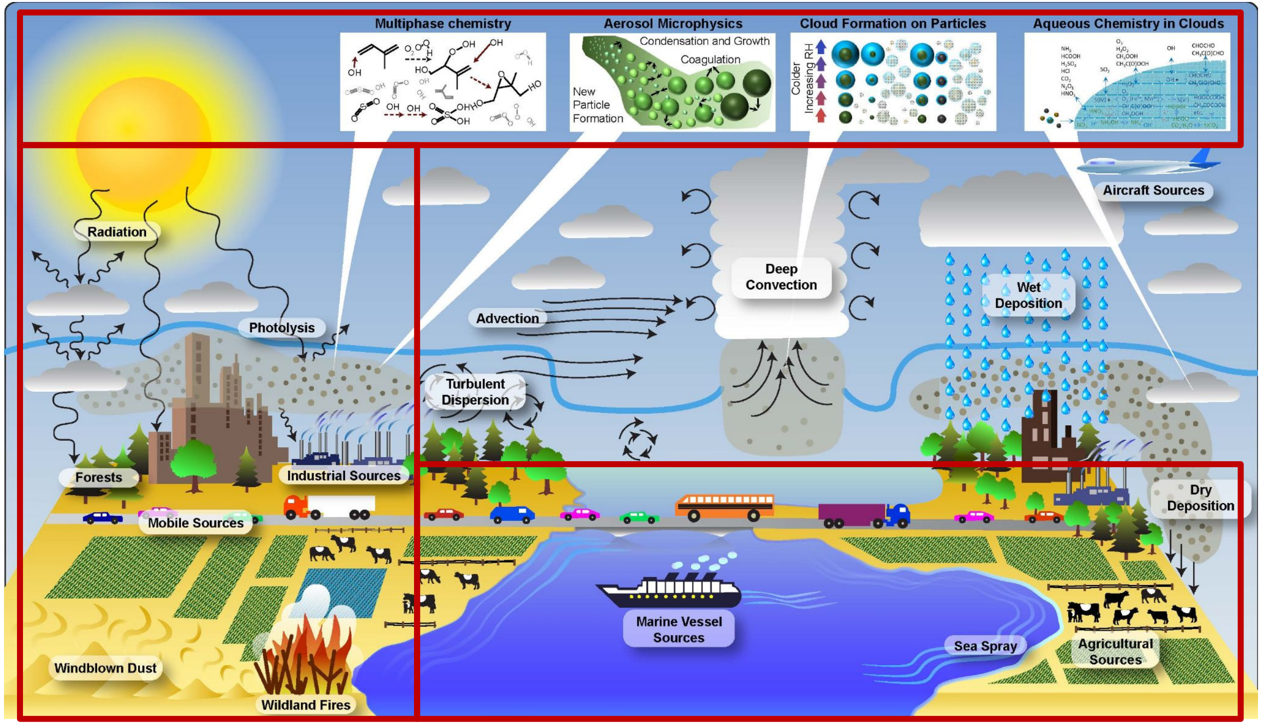
The Unified Forecast System (UFS) is a community-based, coupled, comprehensive Earth modeling system.



https://github.com/ufs-community

NOAA's Current UFS Air Quality Model (UFS-AQM)

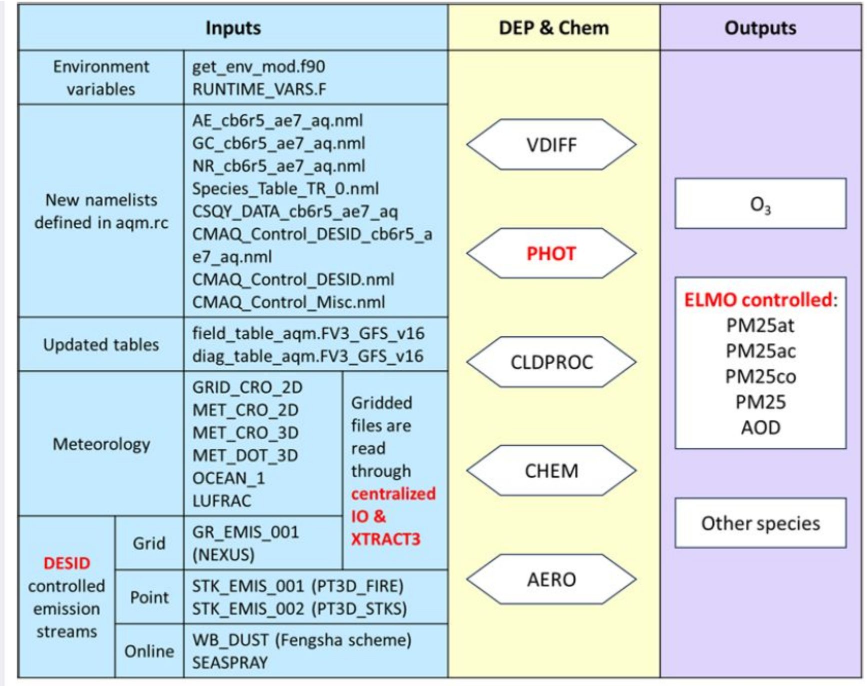
AQM Version 7 (AQMv7) Chemical Component: Based on the U.S. EPA's Community Multiscale Air Quality Model (CMAQ) Version 5.2.1. Version released in June 2017.



→ NOAA-ARL has updated the AQM chemical component from CMAQv5.2.1 to CMAQv5.4 (includes interim CMAQv5.3 updates)

→ Major code structure and scientific changes

Overview of Major Structural Changes to UFS-AQM



Li et al., 2024, GMD, in prep.

- Emission reading, mapping, and scaling are controlled in the Detailed Emissions Scaling, Isolation, and Diagnostic (DESID) module.
- Opening, description, extraction, and interpolation of the meteorological and emission variables are encapsulated in the centralized I/O (CIO) module.
- Introduction of the Explicit and Lumped air quality Model Output (ELMO) module is included that can synthesize the definition, calculation, and maintenance of individual or aggregate gas and particulate matter online, i.e., simplifies CMAQ output.

Overview of Major Scientific Changes to UFS-AQM

Major science updates from CMAQv5.2.1 → v5.3+ → CMAQv5.4

- Updated chemical mechanism (CB6r3 → CB6r5), photochemistry (e.g., halogen chemistry and DMS), and photolysis rates.
- Updated aerosol module (AERO6 □ AERO7) and both inorganic and organic aerosol formation (anthropogenic species, monoterpenes, water uptake, etc.).
- Other updated processes (e.g., ozone and aerosol dry deposition, ammonia bidirectional fluxes, extended biogenic emissions options, etc.).
- Lead to significant changes in predictions of near-surface air quality, such as O_3 and $PM_{2.5}$.
- Summary of impact comparisons for updating from CMAQv5.2.1 to CMAQv5.3+ and CMAQv5.4.

UFS-AQM Model Components and Configurations

Model attributes	Configuration	Reference
Domain	North America Cantered on 50° N 118° W	N/A
Horizontal resolution	13km	N/A
Vertical resolution	64 levels from near the surface up to the top of the stratosphere	N/A
Meteorological ICs and BCs	FV3GFSv16.3	https://nws.weather.gov/ (last access: 25 November 2023)
Chemical ICs and BCs	Static monthly AM4 for gases and aerosol species and GEFS-Aerosol for dynamic smoke and dust	Horowitz et al. (2020); Tang et al. (2021)
Microphysics	GFDL six-category cloud microphysics scheme	Lin et al. (1983); Lord et al. (1984); Krueger et al. (1995); Chen and Lin (2011, 2013)
PBL physics scheme	sa-TKE-EDMF	Han and Bretherton (2019)
Shallow and deep cumulus parameterization	SAS scheme	Han and Pan (2011); Han et al. (2017)
Shortwave and longwave radiation	RRTMg	Mlawer et al. (1997); Clough et al. (2005); Iacono et al. (2008)
Land surface model	Noah land surface model	Chen and Dudhia (2001); Ek et al. (2003); Tewari et al. (2004)
Surface layer	Monin-Obukhov	Monin and Obukhov (1954); Grell et al. (1994); Jimenez et al. (2012)
Anthropogenic emissions (CONUS)	Area Sources: NEIC2016v1 Point Sources: NEIC2016v1 with Briggs plume rise	NEI (2019); Briggs (1965)
Anthropogenic emissions (Outside CONUS)	CEDSv2; HTAPv2.2; OMI-HTAP SO_2 2019	O'Rourke et al. (2021); Janssens-Maenhout et al. (2015); Liu et al., 2018
Biogenic emissions	MEGAN2.1 driven by GFSv16 meteorology	Guenther et al. (2012)
Wildfire emissions	RAVE with Sofiev plume rise	Li et al., (2022); Sofiev et al. (2012)
Other Inline/Offline emissions	FENGSHA windblown dust scheme	Fu et al. (2014); Huang et al. (2015); Dong et al. (2016)
	Sea spray emissions	Kelly et al. (2010); Gantt et al. (2015)

Major Configuration, Components, and Inputs

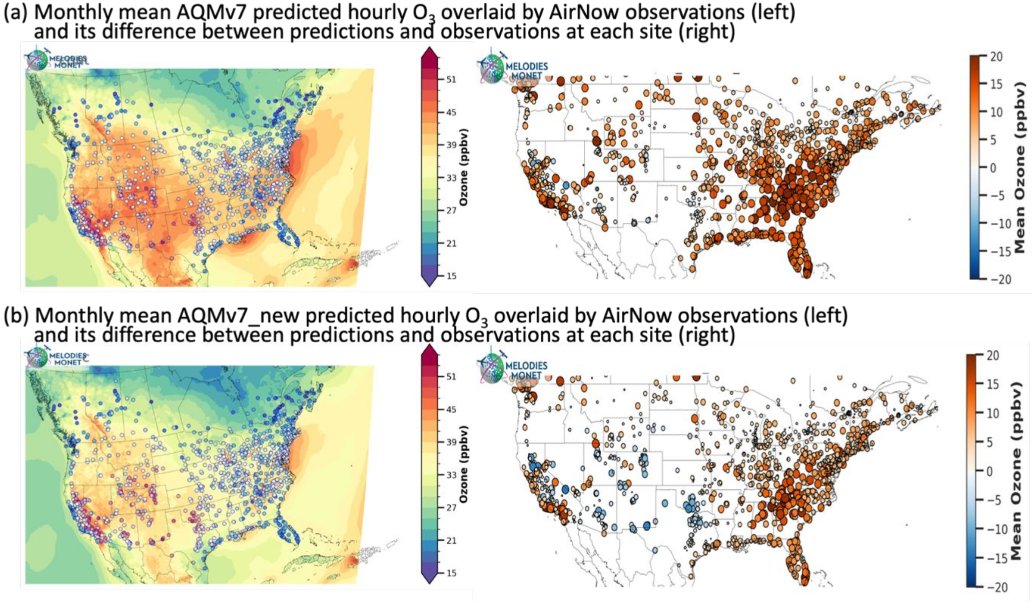
- Domain: North America @ 13x13 km horizontal resolution, 64 vertical levels.
- CCPP FV3-GFSv16.3 physics.
- Anthropogenic Emission: CEDSv2, HTAPv2.2, OMI-HTAP SO2 2019, and NEIC2016v1.
- Biogenic Emission: Inline MEGANv2.1
- **Wildfire Emission: RAVE with Sofiev Plume Rise.**
- Other Emission: Inline FENGSHA dust and inline sea-spray.

1-month warm start test simulation (August 2023), all conditions same except for CMAQv5.2.1 (AQMv7) vs. CMAQv5.4 update (AQMv7_new).

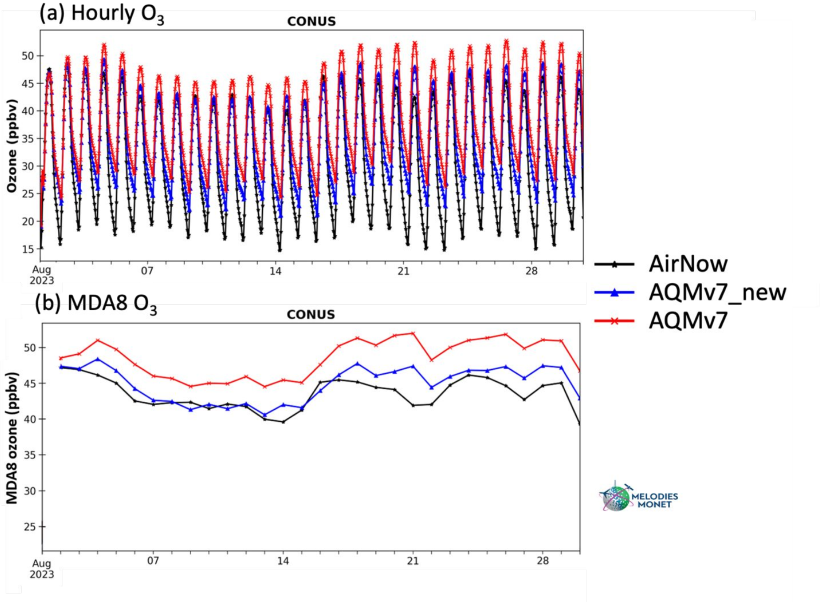
Impact of Updates on Near-Surface Ozone Predictions

August 2023

Mean O_3 for AQMv7 (a) and AQMv7_new (b)



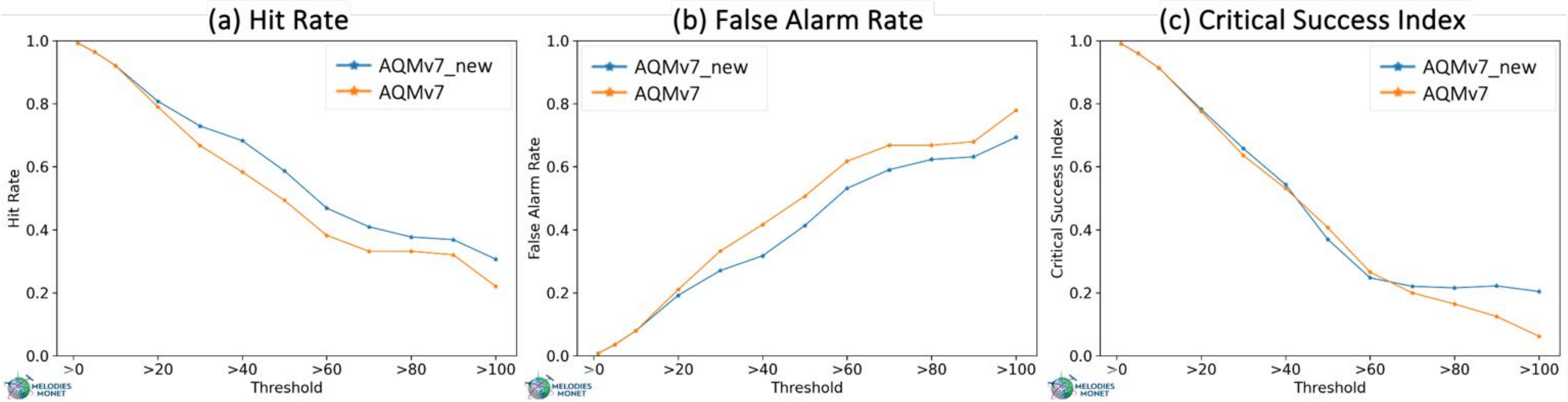
Time series of hourly (a) and MDA8 (b) O_3



Li et al., 2024, GMD, in prep.

Impact of Updates on Near-Surface Ozone Predictions

August 2023



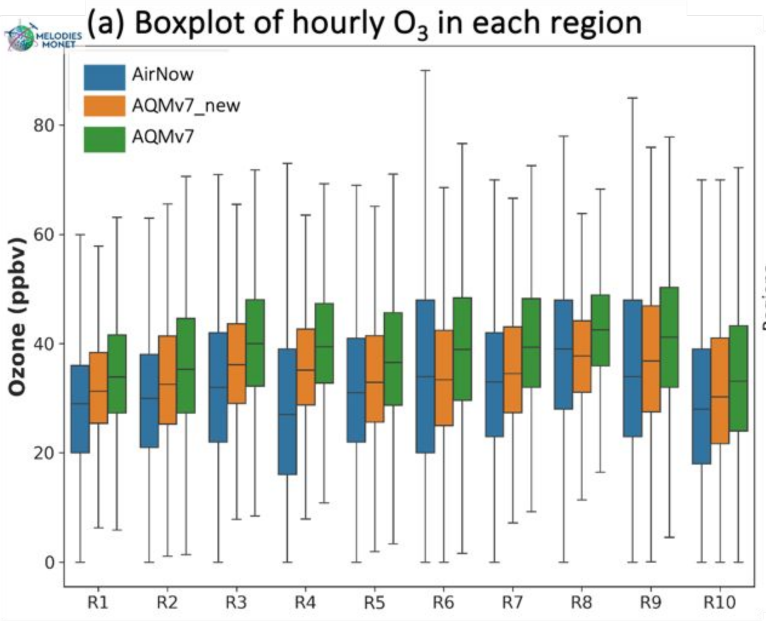
Region	Model	MB (ppb)	NMB (%)	MdnB (ppb)	NMdnB (%)	R^2	RMSE (ppb)	IOA
CONUS	AQMv7	7.06	22.64	6.35	21.16	0.50	13.36	0.79
	AQMv7_new	**3.55**	**11.38**	**2.79**	**9.28**	**0.51**	**11.71**	**0.82**

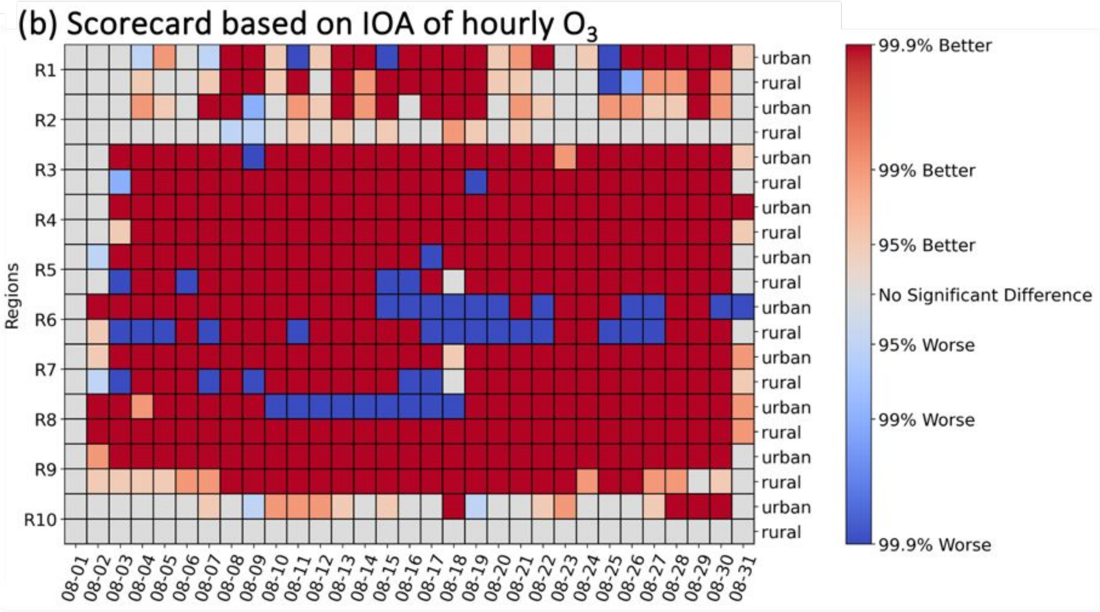
Li et al., 2024, GMD, in prep.

Impact of Updates on Near-Surface Ozone Predictions

August 2023

Mean O_3 for box-whisker (a) and IOA scorecard (b)





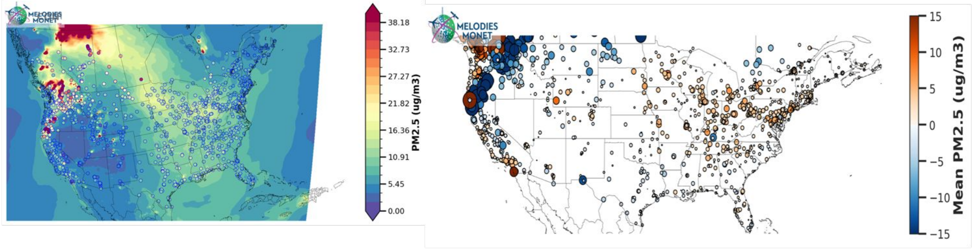
Li et al., 2024, GMD, in prep.

Impact of Updates on Near-Surface $PM_{2.5}$ Predictions

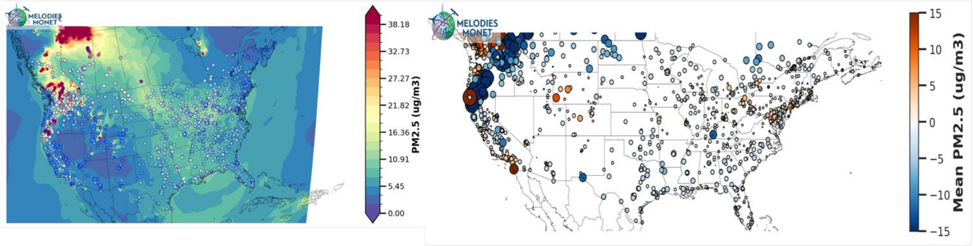
August 2023

Mean $PM_{2.5}$ for AQMv7 (a) and AQMv7_new (b)

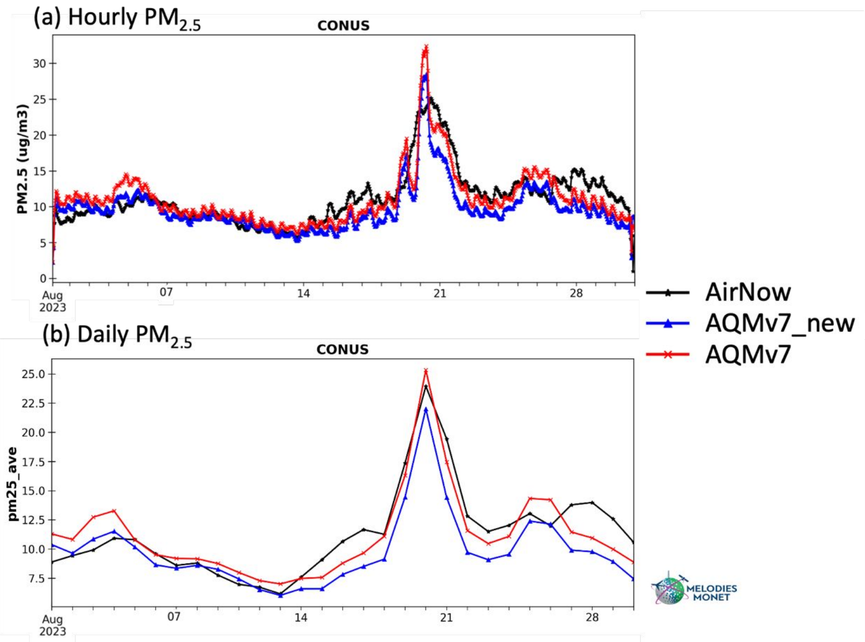
(a) Monthly mean AQMv7 predicted hourly $PM_{2.5}$ overlaid by AirNow observations (left) and its difference between predictions and observations at each site (right)



(b) Monthly mean AQMv7_new predicted hourly $PM_{2.5}$ overlaid by AirNow observations (left) and its difference between predictions and observations at each site (right)



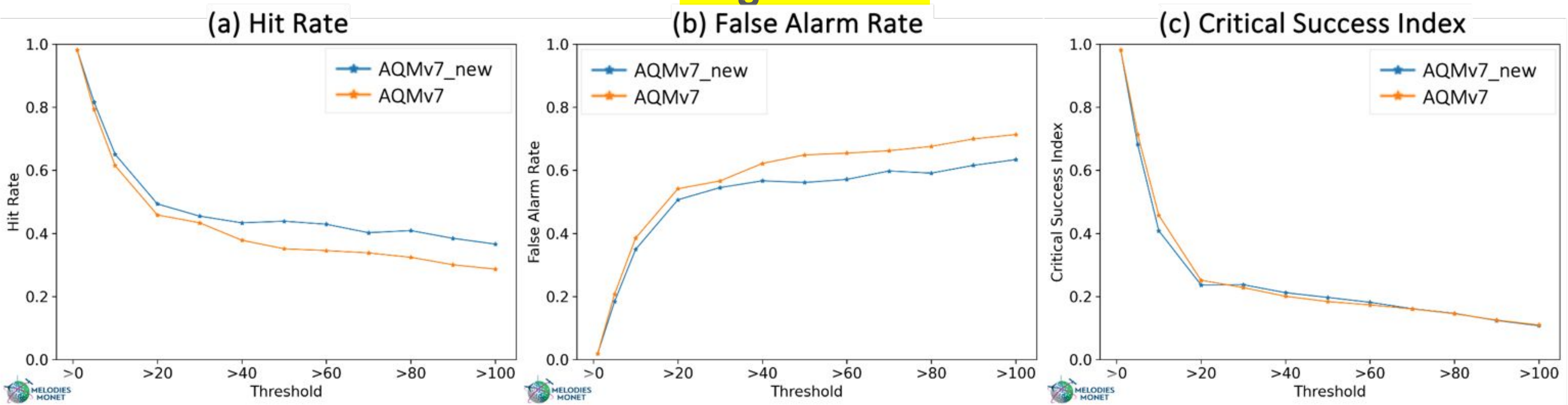
Time series of hourly (a) and daily (b) $PM_{2.5}$



Li et al., 2024, GMD, in prep.

Impact of Updates on Near-Surface $PM_{2.5}$ Predictions

August 2023



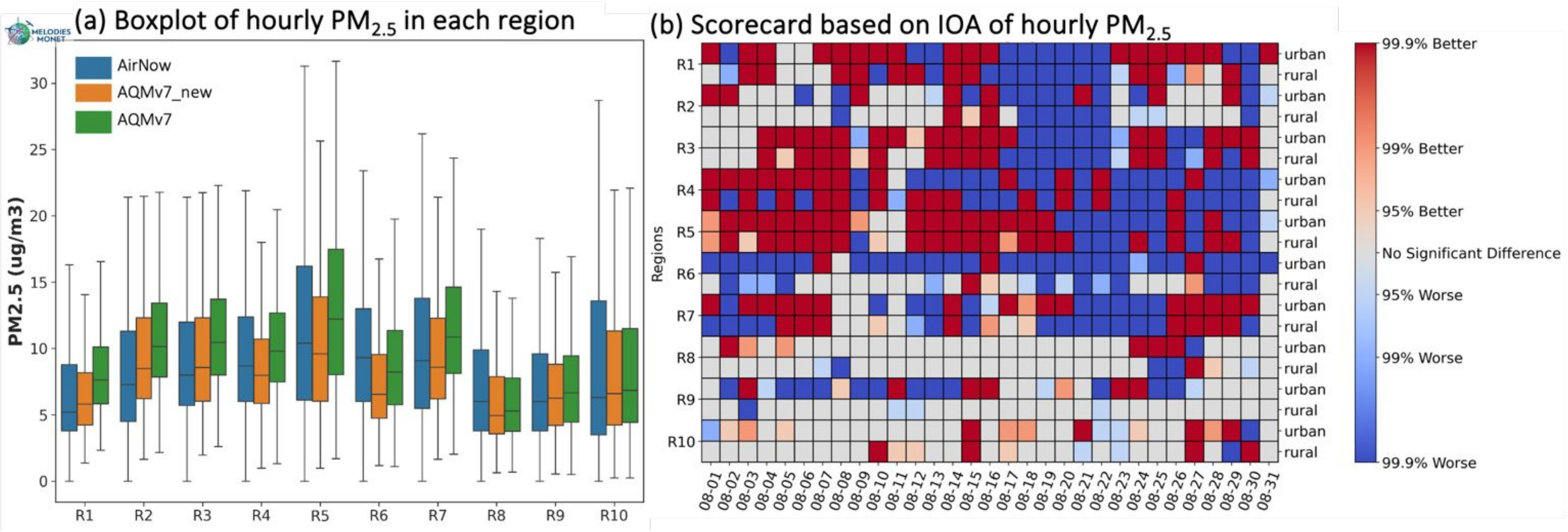
Region	Model	MB (μg/m^3)	NMB (%)	MdnB (μg/m^3)	NMdnB (%)	R^2	RMSE (μg/m^3)	IOA
CONUS	AQMv7	-0.05	-0.44	0.77	9.94	0.07	32.43	0.38
	AQMv7_new	-1.40	-12.47	**-0.34**	**-4.35**	0.06	**31.92**	0.38

Li et al., 2024, GMD, in prep.

Impact of Updates on Near-Surface $PM_{2.5}$ Predictions

August 2023

Mean $PM_{2.5}$ for box-whisker (a) and IOA scorecard (b)

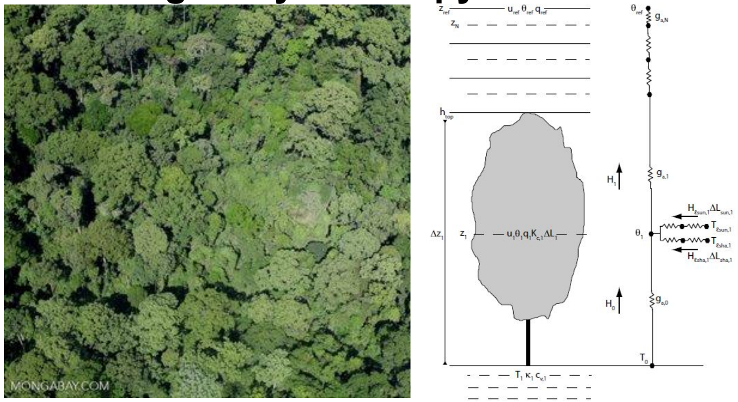


Li et al., 2024, GMD, in prep.

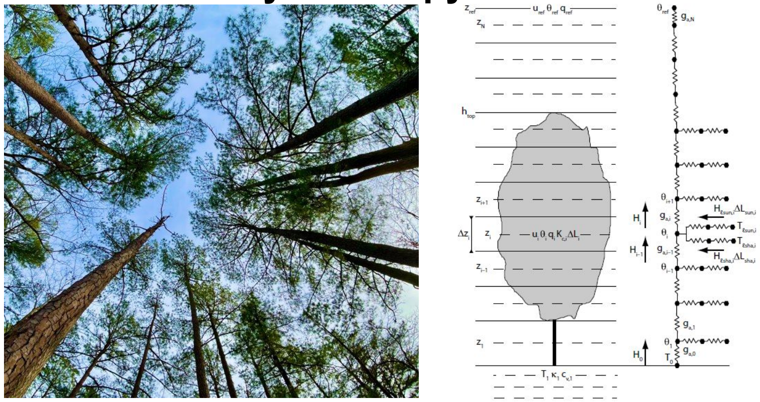
Beyond the “big-leaf” model in UFS-AQM

- The big-leaf approach is widely used in land, weather, climate, and air quality models, and typically represent the plant canopies as a homogeneous single layer without real vertical structure.
- Multi-layer canopy models are more costly, but can better represent the vertical variation of within canopy physical, dynamical, and chemical traits.

Single-Layer Canopy



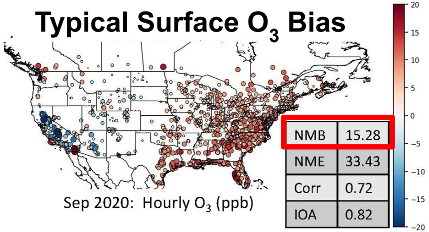
Multi-Layer Canopy



- Application of multilayer approaches to already costly air quality forecasting models with complex chemistry at regional scales presents further challenges (especially in UFS-AQM).

Beyond the "Big-Leaf" Model in UFS-AQM

- Systematic ozone overpredictions in CTMs are linked to distinct vertical gradients of ozone measured within dense forest canopies of the U.S. □ Incorporate canopy parameters associated with **photolysis** and the attenuation of light (Makar et al., 2017):



$$P(\theta, z) = e^{-\frac{G(\theta)\,\Omega(\theta)\mathrm{LAI}(z)}{\cos(\theta)}}$$

Probability of beam penetration (i.e., fractional light penetration; Nilson, 1971; Monsi and Saeki, 1953) depends on LAI, leaf projection (G), clumping index (Ω), and solar zenith angle (θ).

- In-canopy **vertical diffusivity** is also modified based on the Raupach (1989) near-field theory for turbulence within the forest canopy (Makar et al., 2017):

$$K_{\mathrm{can}}(z) = \frac{K_{\mathrm{mod}}(z_1)}{K_{\mathrm{est}}\left(\frac{z_1}{h_c}\right)} K_{\mathrm{est}}\left(\frac{z}{h_c}\right),$$

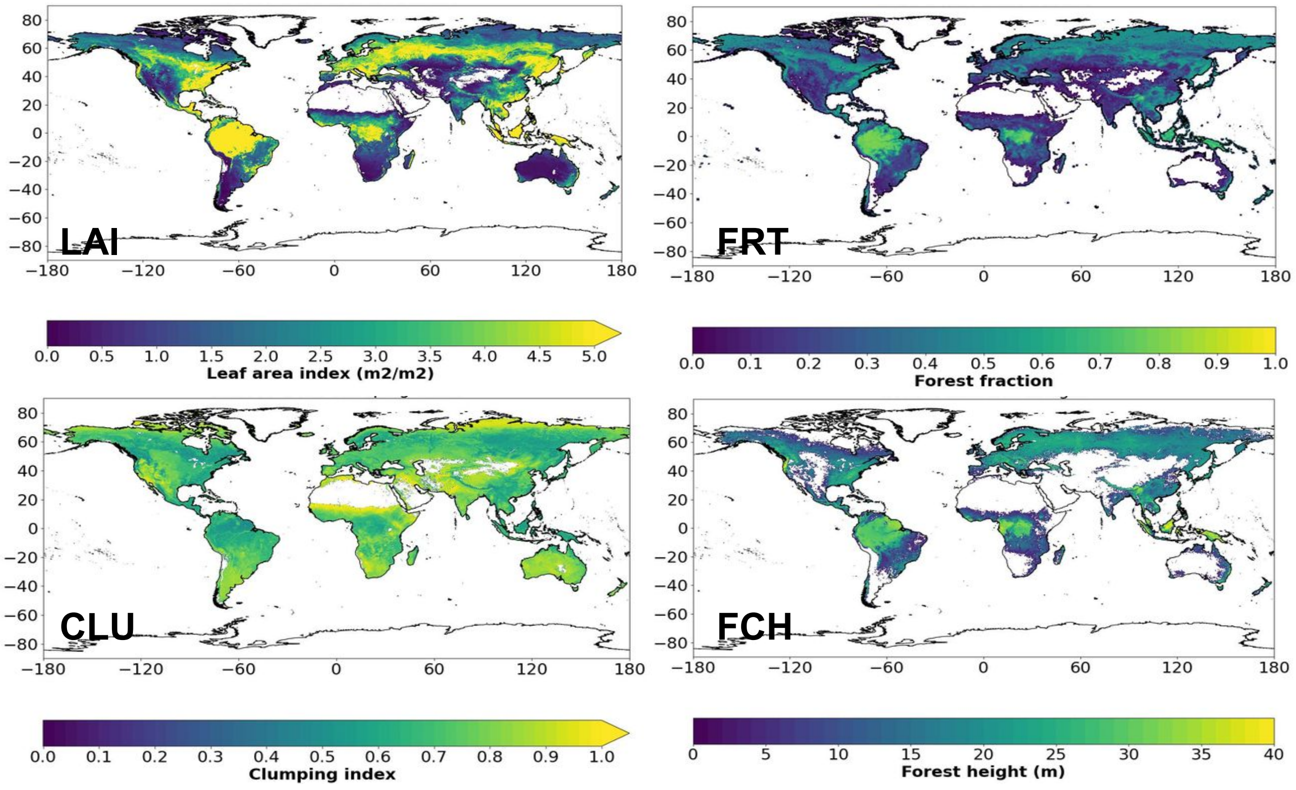
Modified turbulent diffusivity is scaled to 1st model layer and depends on variance in Eulerian vertical velocity (σ_w^2) and turbulent length scale (T_L)

$$K_{\mathrm{est}}\left(\frac{z}{h_c}\right) = \sigma_w^2\left(\frac{z}{h_c}\right) T_L\left(\frac{z}{h_c}\right),$$

$$T_L\left(\frac{z}{h_c}\right) = \frac{h_c}{u^*}\left[0.256\left(\frac{z-0.75h_c}{h_c}\right) + 0.492\exp\left(\frac{-0.256z/h_c}{0.492}\right)\right],$$

Note: Based on Makar et al. (2017), but not exact implementation.

Updated 1-km Global Canopy Dataset for the UFS



Four major canopy parameters based on MODIS, VIIRS, and GEDI:

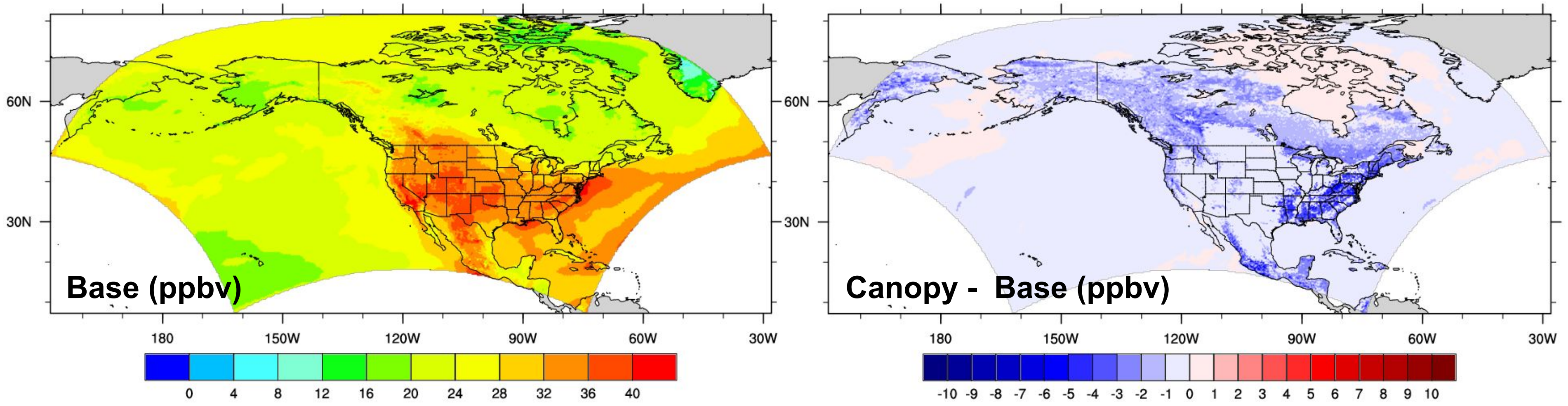
- Leaf area index (LAI)
- Canopy clumping index (CLU)
- Forest fraction (FRT)
- Forest canopy height (FCH)

canopy-app

https://github.com/noaa-oar-arl/canopy-app

Impacts of Canopy Effects on Ozone Predictions

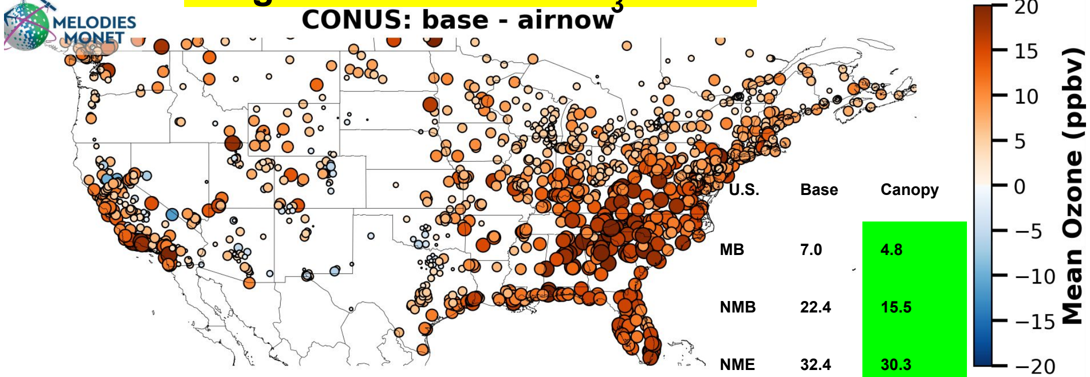
August 01 -31, 2023
Average Ozone Model Layer 1



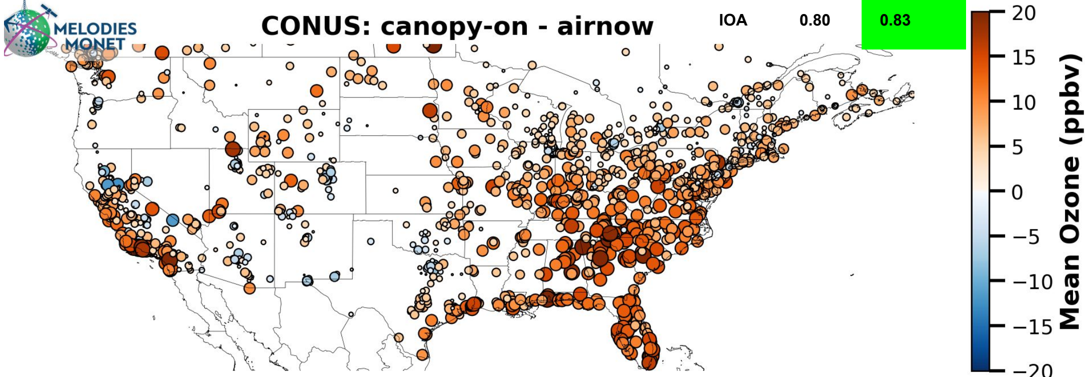
Maximum average grid cell ozone decrease of ~ - 10 ppb (-37% relative change).

Preliminary Canopy Effects on Model Performance

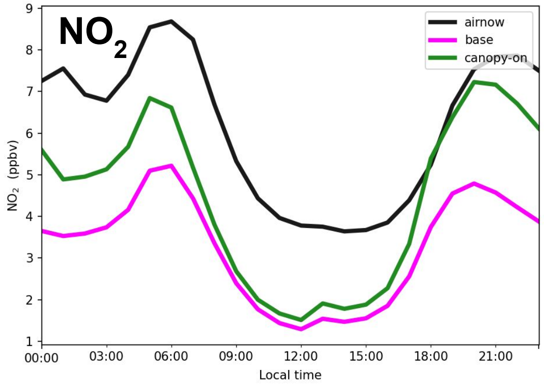
August 2023 Surface O_3 Bias

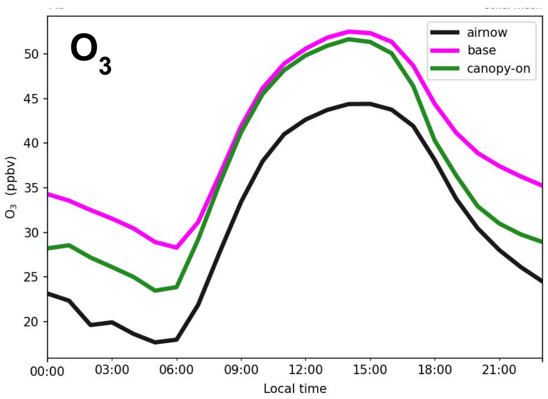


U.S.	Base	Canopy
MB	7.0	4.8
NMB	22.4	15.5
NME	32.4	30.3
IOA	0.80	0.83



August 2023 East U.S. Diurnal NO_2 and O_3





Courtesy of Dr. Zachary Moon (NOAA-ARL/ERT)

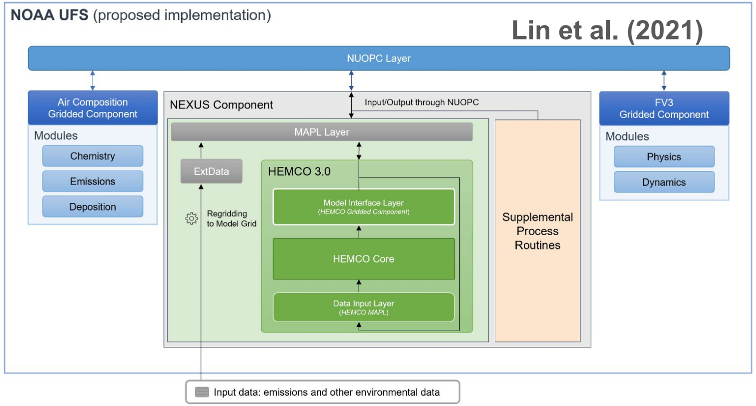
Updating Anthropogenic Emissions in UFS-AQM

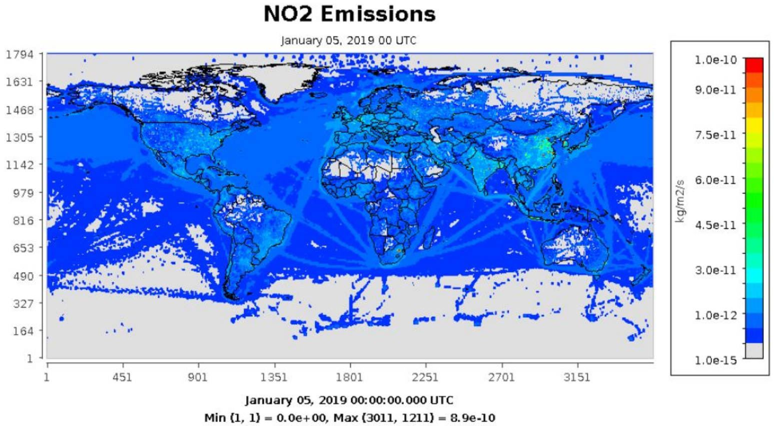
For the UFS-AQM domain, we use the **NOAA Emissions and eXchange Unified System (NEXUS)** component to online generate the following combined regional + global emissions:

- CEDSv2-2019 for all gases (SO_2 ocean only), OC, and BC (global)
- OMI-HTAP-2019 for SO_2 (land only)
- HTAPv2-2010 for PMC and $PM_{2.5}$ (global)
- NEI2016v1 all gas and aerosols (CONUS Only)

1) The current versions of NEI2016v1 and HTAPv2 are largely outdated.

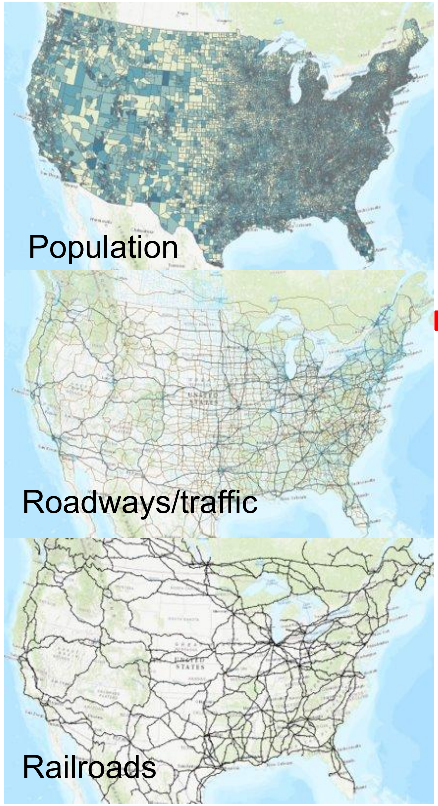
2) All global emissions are monthly and have no daily or diurnal patterns.



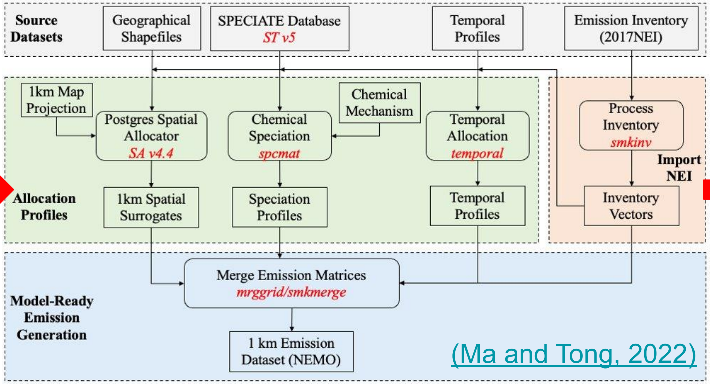


Use of a High Resolution 1-km Emissions Dataset

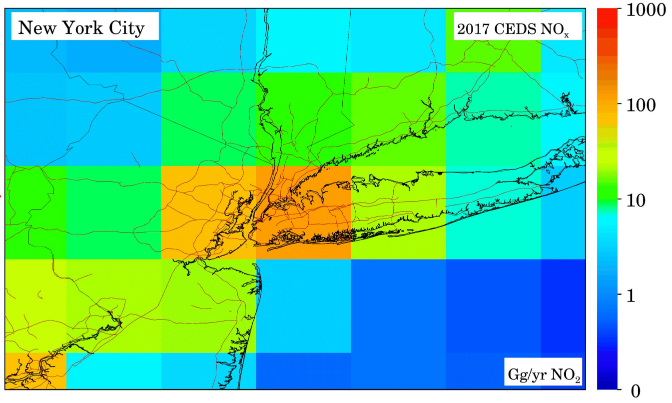
Geographical Information



Neighborhood Emission Mapping Operation (NEMO) from George Mason University



High Resolution 1-km Emissions for 2019

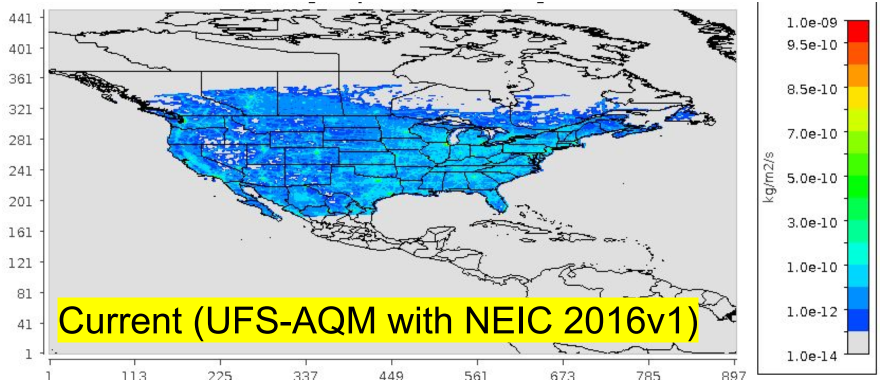


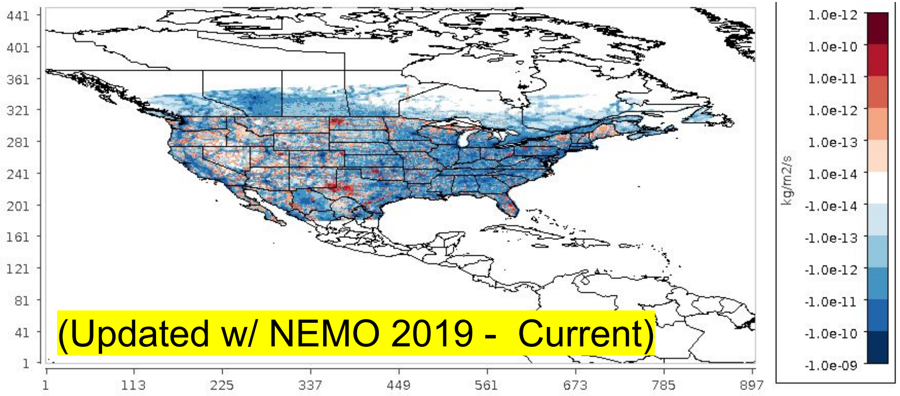
A total of 108 spatial surrogates were prepared and applied over 9 anthropogenic emissions sectors, with the base emissions inventory based on the U.S. EPA National Emissions Inventory (NEI) for 2017 → with sector updates to the 2019 modeling platform.

Use of NEXUS model to process the updated GMU 1-km 2019 emissions.

Example Nitric Oxide (NO) Emissions Updates

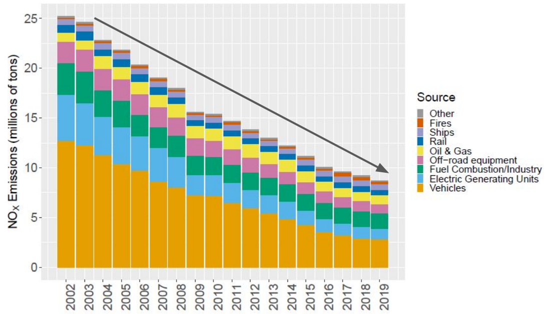
January 5: NO Emissions





January 5: Total NO Emissions differences (mt)

Red = Total Increase Blue = Total Decrease	**Current UFS-AQM (mt)**	**Updated NEMO (mt)**	**Percent Difference (%)**
East	431	276	-36
West	192	114	-40
CONUS	624	390	-37



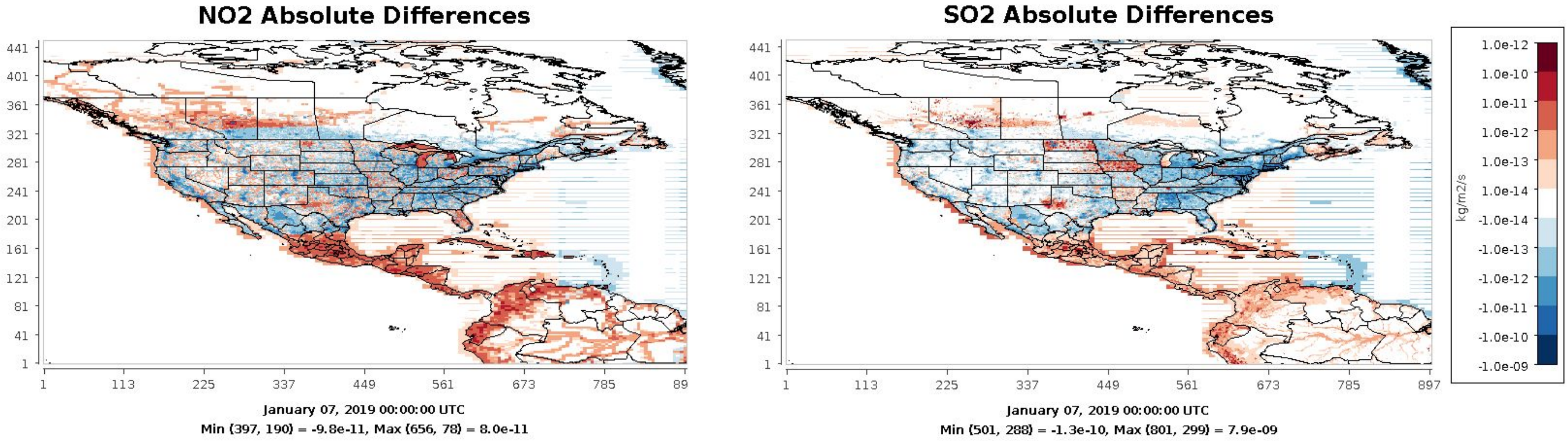
Annual total U.S. anthropogenic NO_X emissions from the U.S. EPA EQUATES dataset.

Example NO_2 and SO_2 Emissions Updates in UFS-AQM

Full emissions updates include more recent regional and global inventories and the use of CAMS-TEMPO for improved temporal profiles for regions outside of CONUS.

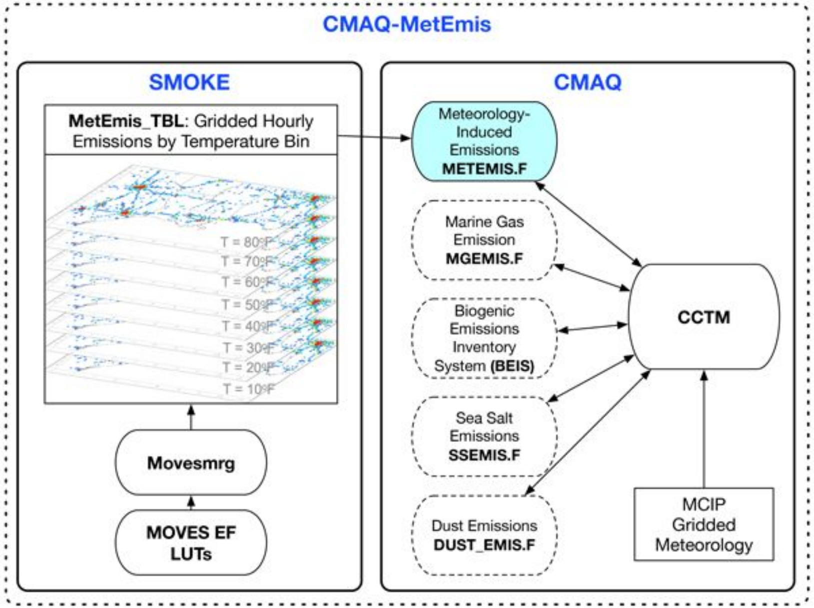
- NEI2016v1 → GMU/NEMO 1-km NEI2019 (Inside CONUS only)
- HTAPv2 2010 → HTAPv3 2018 (Outside CONUS)
- Global No Diurnal for major gas emissions → CAMS-TEMPO gridded weights (outside CONUS)

Emissions Changes (Updated - Current)

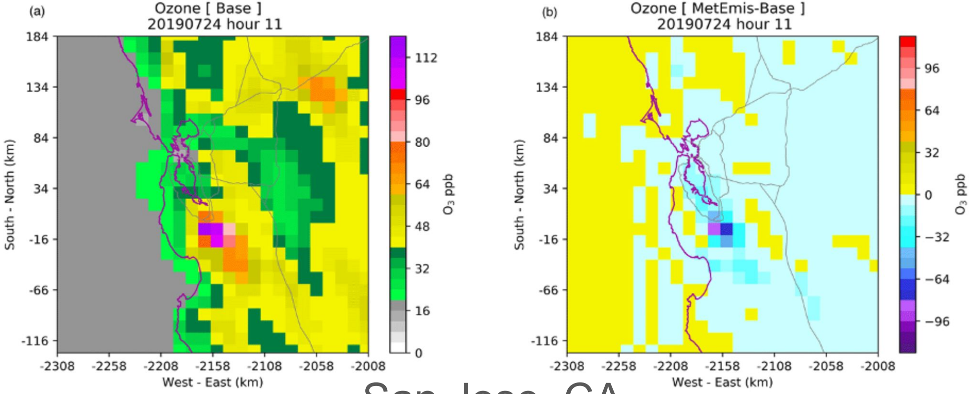


Incorporating Weather-Dependent Emissions in UFS-AQM

Dynamic Meteorology-induced Emissions Coupler (MetEmis) development in the Community Multiscale Air Quality (CMAQ) model (Baek et al., 2023)



Hourly ozone differences (MetEmis-Base)



San Jose, CA

"Dynamically estimate weather-induced hourly gridded on-road mobile emissions in the UFS-AQM."

Progress and Future of the UFS-AQM

- Further evaluate CMAQv5.4 update and tests and hopeful future transition.
- Update and improve diagnostics (e.g. fluxes, dry deposition, process analysis) to better understand AQM scientifically → Comprehensive evaluation paper.
- Updating vegetative in-canopy codes and canopy inputs → evaluate impacts.
- Integrate updated anthropogenic emissions and thoroughly test and evaluate impacts for the future of UFS-AQM predictions.