Evaluation of Model Simulated Ozone and its Precursors Using the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) during the Michigan-Ontario Ozone Source Experiment (MOOSE)

2023 CESM Workshop

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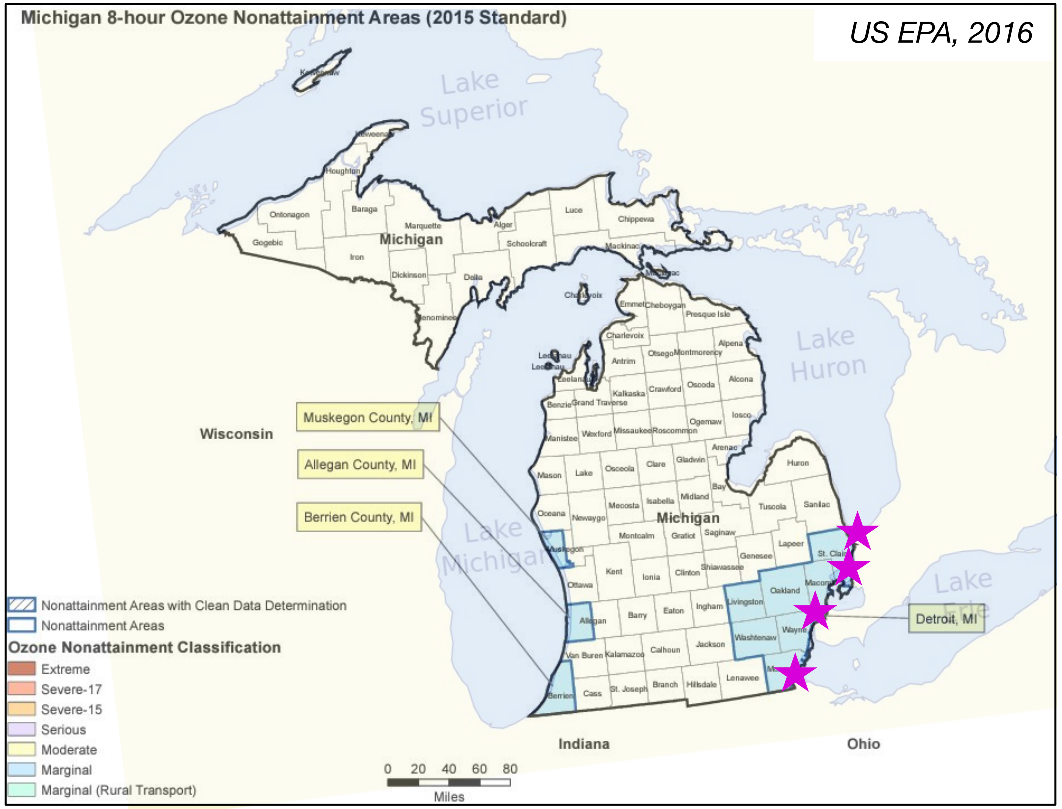
OZONE IN SEMI



- O_3 levels continue to **exceed NAAQS standards** in SEMI.
- Many **factors** are **associated with O_3 exceedance** (e.g., precursor emissions, long-range transport, meteorology, land-lake interactions).
- More detailed and innovative measurements and modeling studies are necessary for understanding O_3 production and loss in SEMI.

> MDA8 of 70 ppbv

Monroe, MI

Detroit, MI

East China, MI

Sarnia, ON

CLIMATE IN CRISIS

Black residents of Detroit brace themselves for rougher air quality conditions

Detroit's air quality is among the worst in the world because of the Canadian wildfires, exposing an already-vulnerable population to more health risks.

OBJECTIVES

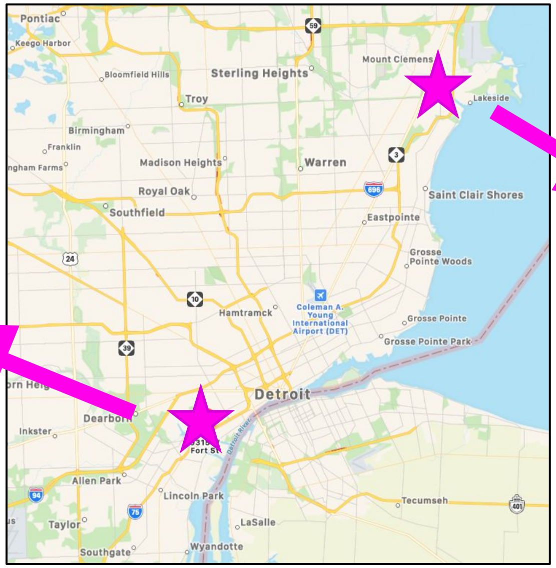
A. **Investigate the sensitivity of model simulated O_3 and its precursors to model horizontal grid resolutions in MUSICAv0.**
   1. *Create ~7 km (1/16˚) grid over Michigan.*
   2. *Implement and evaluate new grid.*

B. **Quantify the drivers of O_3 nonattainment in Southeast Michigan using optimal MUSICAv0 model grid.**
   1. *Implement diurnal cycle for NO emissions*
   2. *Identify and quantify physical and chemical drivers of O_3 production and loss in SEMI through emission sensitivity experiments.*

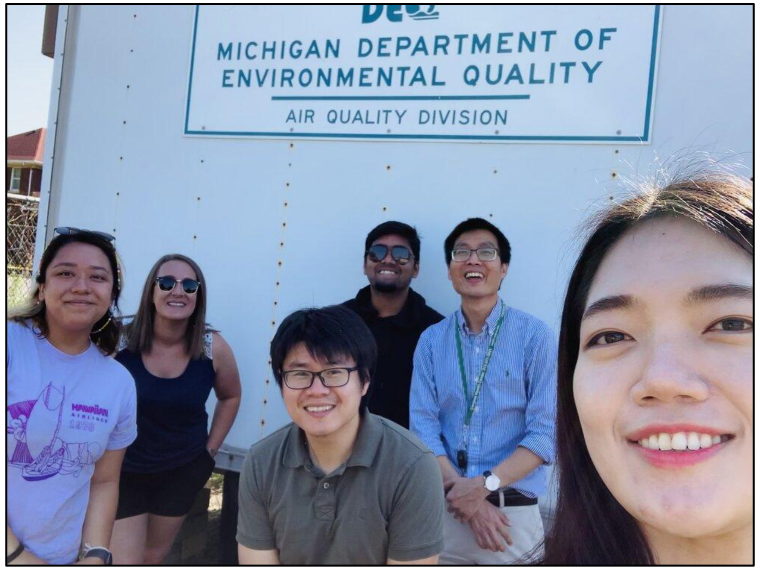
MICHIGAN-ONTARIO OZONE SOURCE EXPERIMENT (MOOSE)

- Led by Michigan Department of Environment, Great Lakes, and Energy (EGLE), with participants from universities, federal agencies, and Environment Climate Change Canada.
- Seeks to define potential attainment strategies in SEMI region and better understand what contributes to excess O_3.
- **Phase I: May 24 – June 30, 2021**
- Phase II: June 6-28, 2022
- Varied, High-Resolution Measurements
  - Aircraft (NASA G-III), Mobile Lab (Aerodyne), Stationary

SW Detroit



New Haven

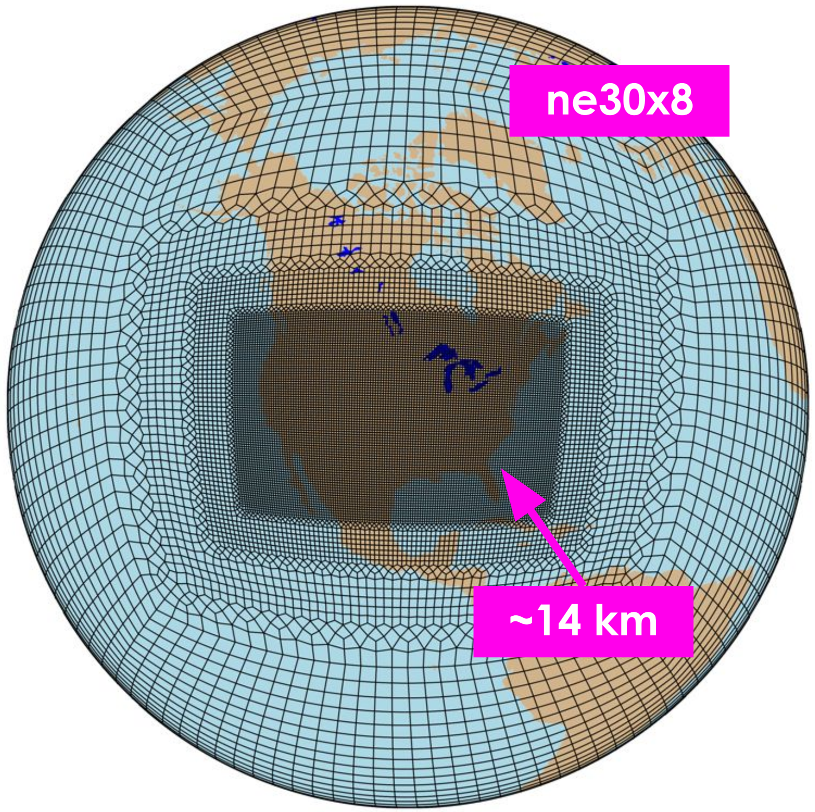


From left to right: Noribeth Mariscal, Erin Browne, Jiajue Chai, Debatosh Partha, Yaoxian Huang, Heejeong Kim

MUSICAv0

MUlti-Scale Infrastructure for Chemistry & Aerosols, Version 0

- Configuration of CESM/CAM-Chem
- Uses Spectral Element (SE) Dynamical Core
- Regional Refinement (RR)
- Described in *Pfister et al (2020)*
- Default Resolution:
    - ~14 km Latitude x ~14 km Longitude (1/8˚) over CONUS
    - 32 Vertical Layers (~40 km Model Top)

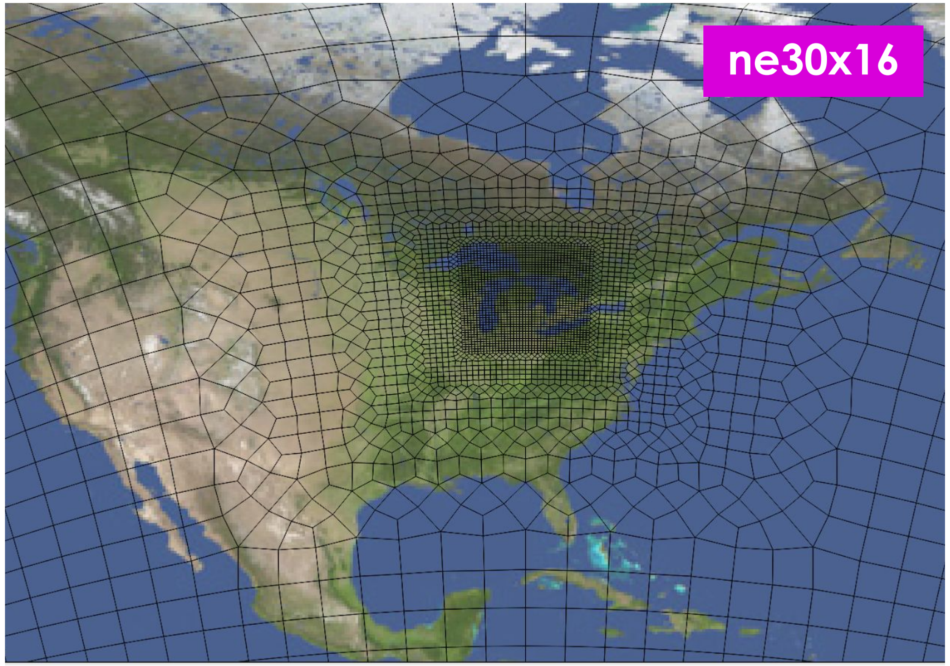


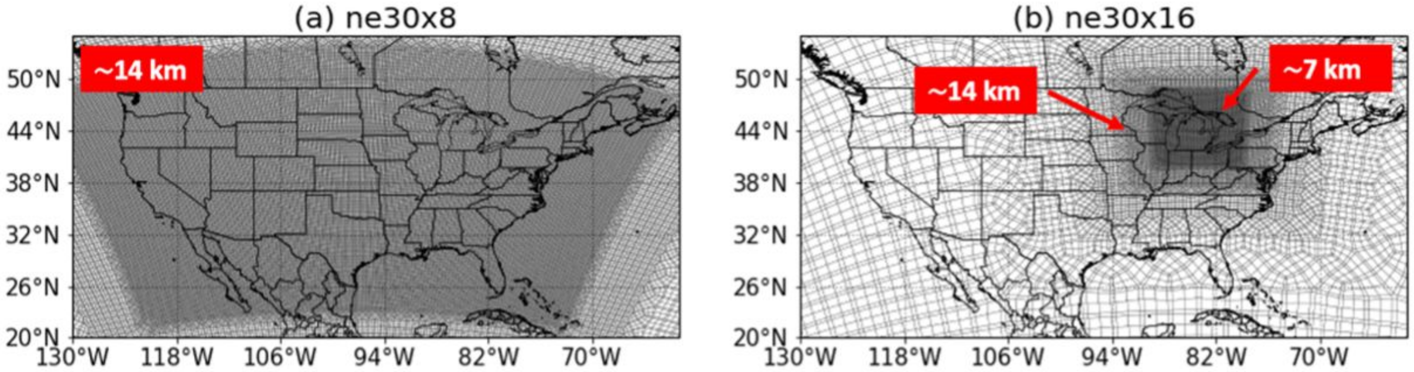
Model Configuration:
→ April-August 2021
→ Initial Conditions based on SE 1˚ CAM-Chem Run
→ NASA MERRA-2 (Resolution: 0.625˚ x 0.5˚ every 3 hours)
→ MOZART-TS2
→ CAMS-GLOB-ANTv5.1, CAMS-GLOB-AIRv2.1, QFED, MEGANv2.1

GRID SETUP

Regional Refinement over Michigan

- *Community Mesh Generation Toolkit*
- ne30x8 CONUS → **ne30x16 MICH**
- ~7 km Latitude x ~7 km Longitude over Michigan
- Smooth transition (halo) between resolutions to mitigate potential errors
- Time Step: 3.75 mins

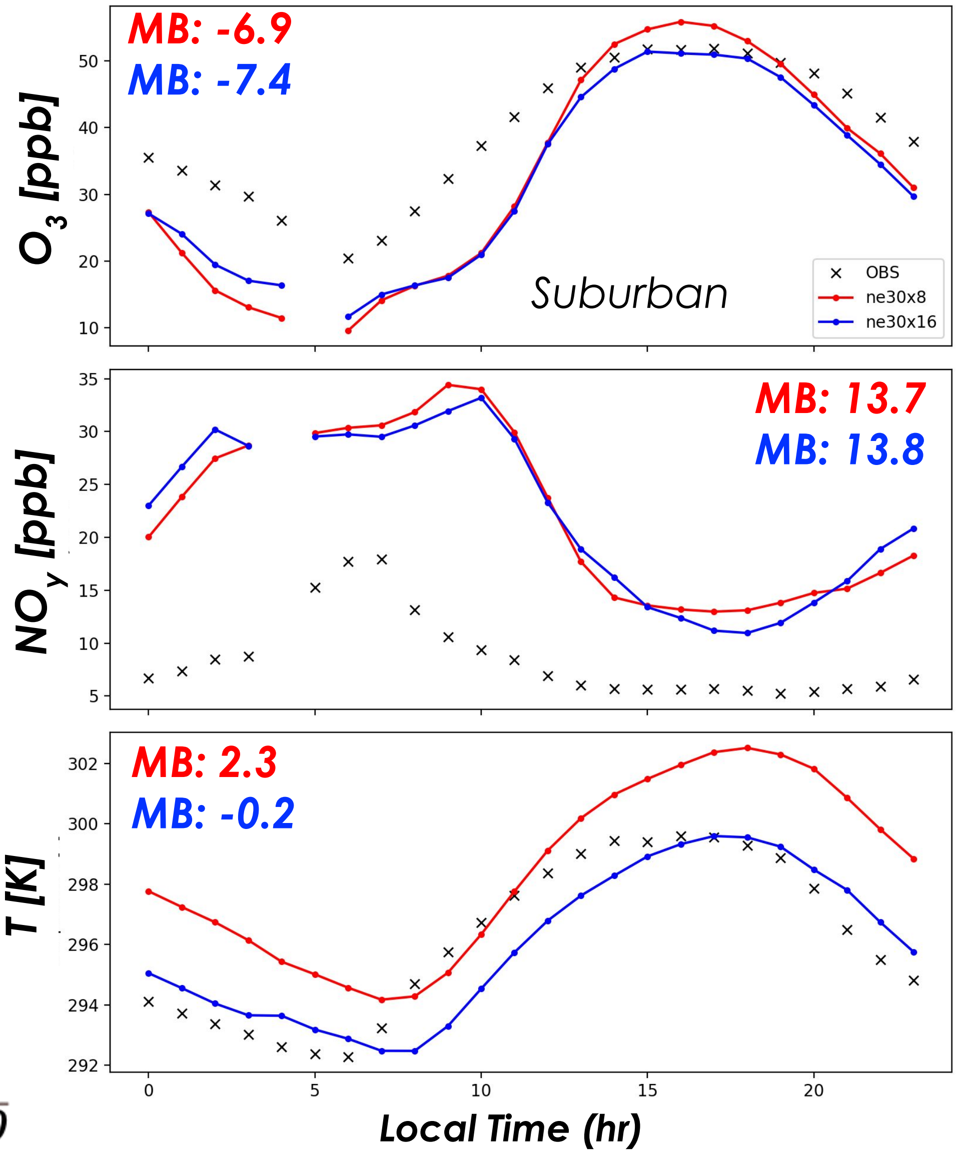




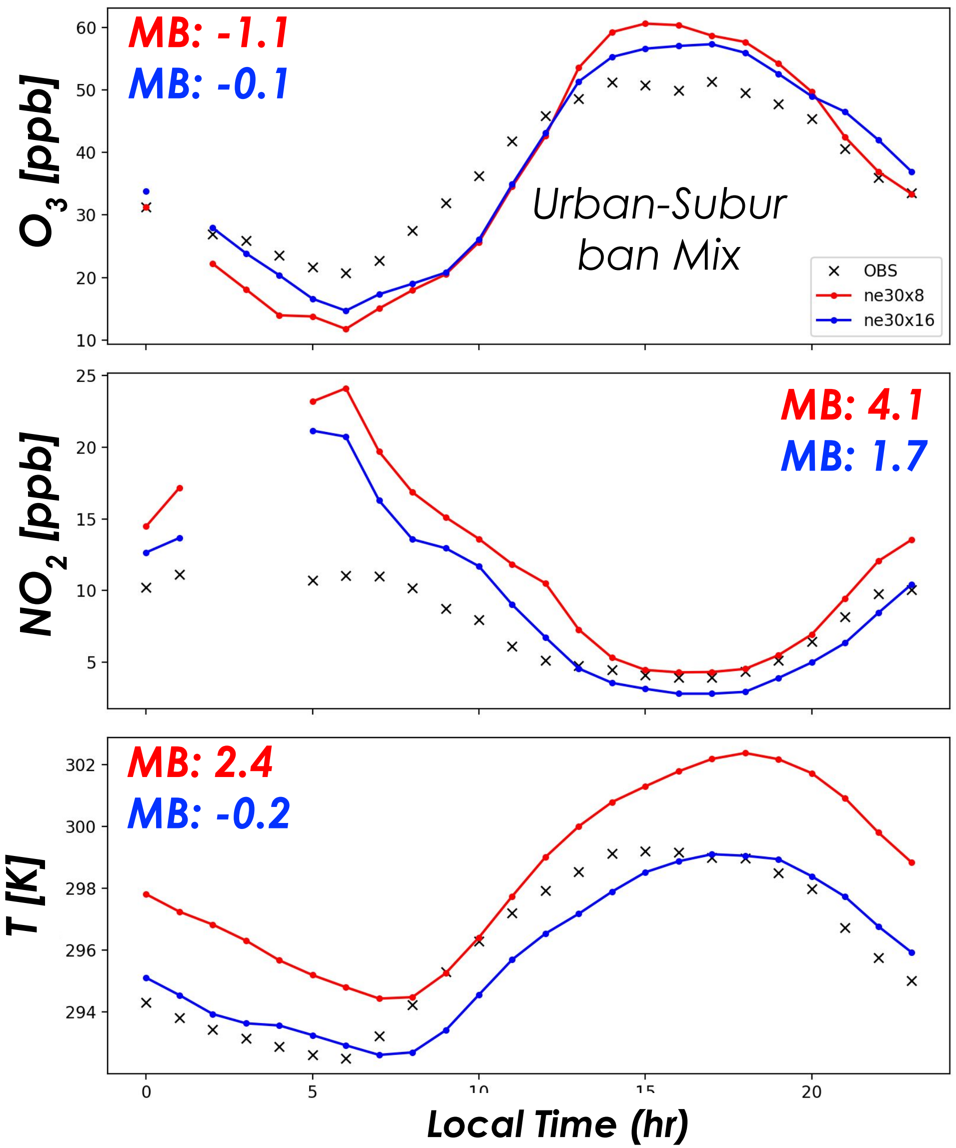
~28,000 core-hr/sim-month **~18,000 core-hr/sim-month**

COMPARISON WITH SEMI STATIONARY SITE

Allen Park [062021]



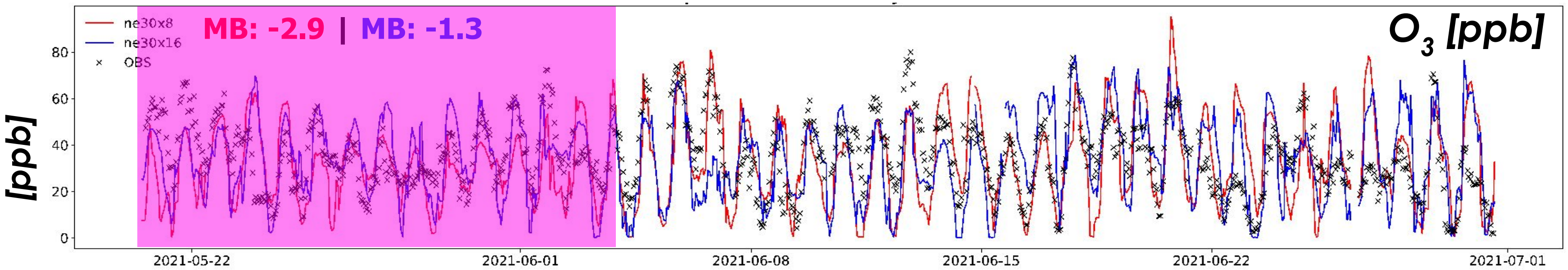
Detroit – E 7 Mile [062021]



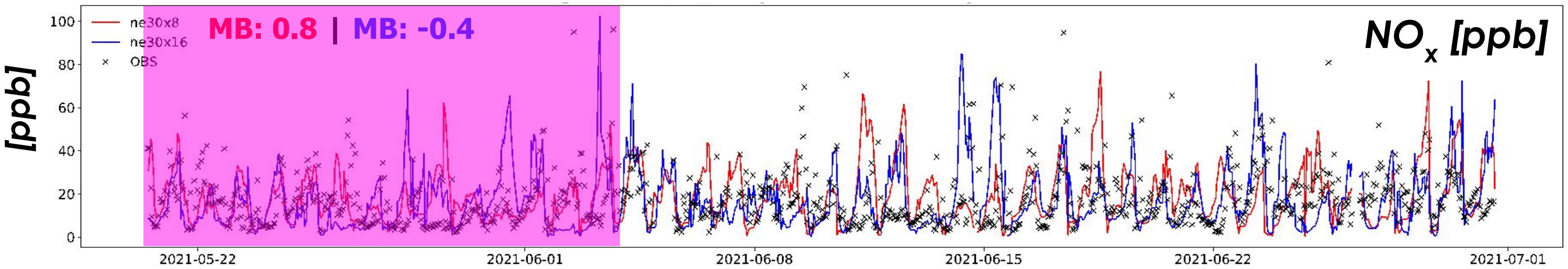
$MB = \bar{M} - \bar{O}$

COMPARISON WITH AML

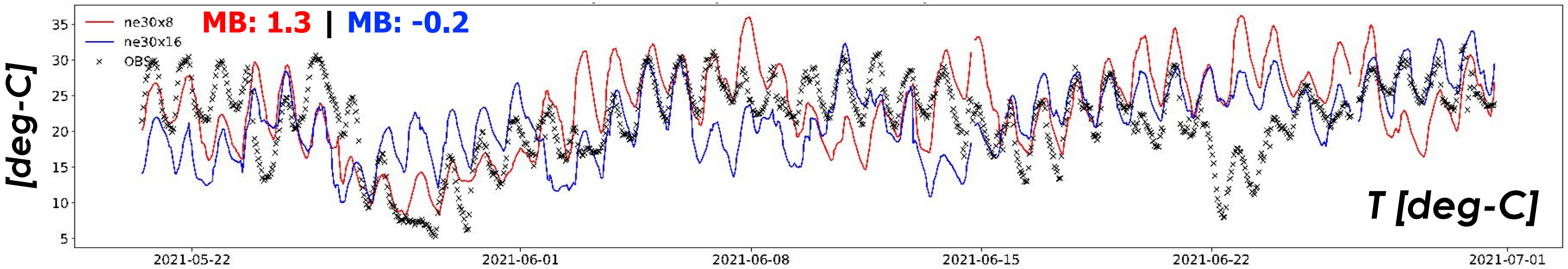
MUSICAv0 Ozone (O_3) Compared to MOOSE Aerodyne Mobile Lab Observations



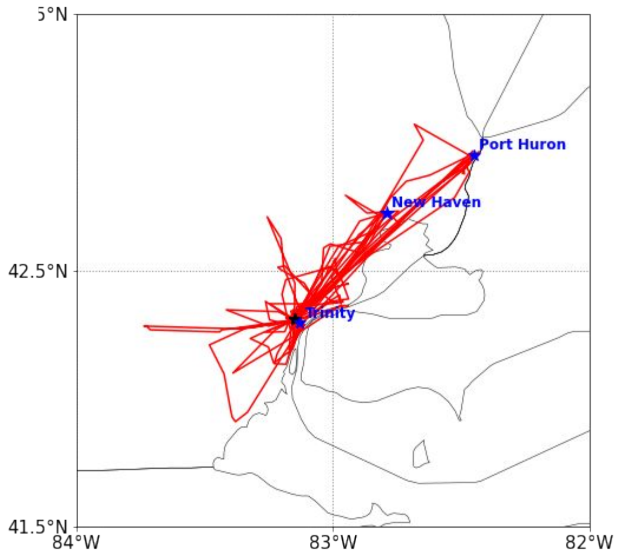
MUSICAv0 Nitrogen Oxide (NO_x) Compared to MOOSE Aerodyne Mobile Lab Observations



MUSICAv0 Temperature Compared to MOOSE Aerodyne Mobile Lab Observations



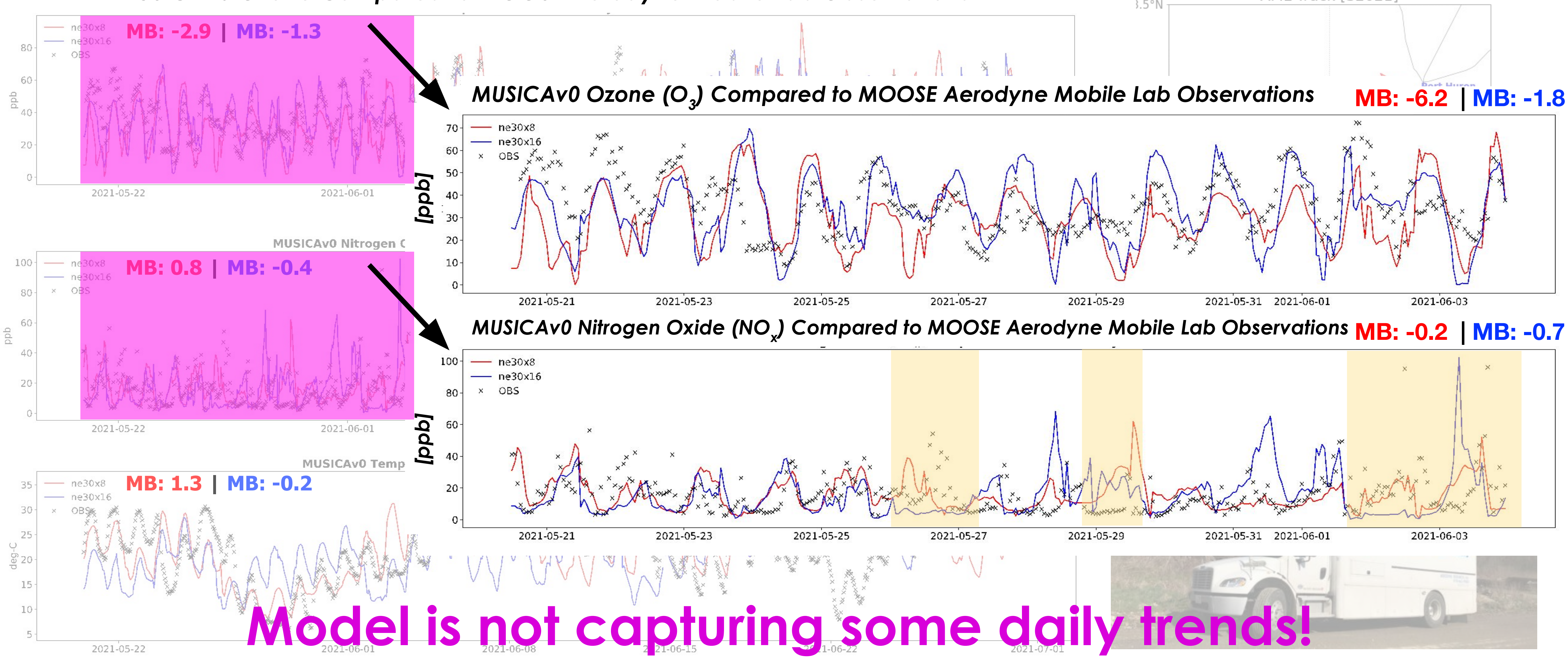
AML Track [S2021]



$$MB = \bar{M} - \bar{O}$$

COMPARISON WITH AML

MUSICAv0 Ozone Compared to MOOSE Aerodyne Mobile Lab Observations

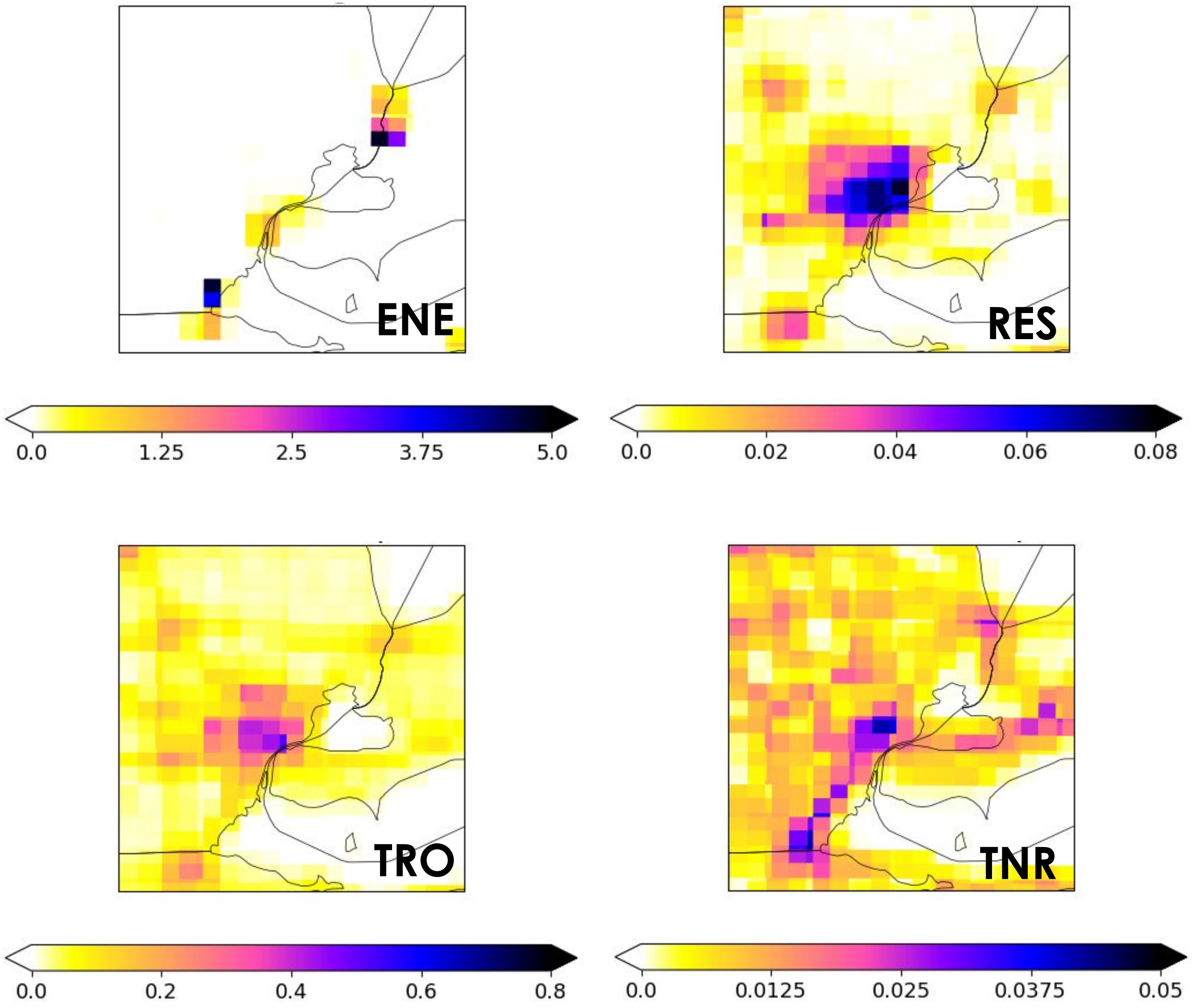


Model is not capturing some daily trends!

$$MB = \bar{M} - \bar{O}$$

IMPLEMENTATION OF DIURNAL CYCLE FOR NO

CAMSv5.1 NO Emissions in e^{12} molecules cm^{-2} s^{-1}



	MICH [kt]	SEMI [kt]	SEMI/MICH
AGS	0.46	0.04	9.0%
AWB	0.10	0.01	10.8%
ENE	9.44	2.86	**30.3%**
RES	1.03	0.48	**47.1%**
TNR	1.99	0.36	**18.1%**
TRO	15.13	3.50	**23.2%**

- Important in evaluating model uncertainties
- Diurnal variations for anthropogenic emissions are NOT considered in CESM2.
- Heavily influences regions with many anthropogenic sources.

ON-GOING & FUTURE WORK

- Complete **MUSICAv0 runs with diurnal cycle for NO emissions** for the ne30x8 CONUS and ne30x16 Michigan grids
  - Regrid emission files to include sectors
  - Add in diurnal information files
  - Evaluate runs with MOOSE Phase I campaign datasets

- Run suite of sensitivity experiments to **quantify contribution of emission from various sectors and long-range transport** on O_3 in SEMI.

- Combine MUSICAv0 with an exposure model to **study impacts of O_3 nonattainment on human health** in SEMI.

Case	Grid Name	Resolution (km)	Setup
1	ne30x16	~7	Control
2	ne30x16	~7	TRO*-OFF
3	ne30x16	~7	ENE*-OFF
4	ne30x16	~7	OTH*-OFF
5	ne30x16	~7	ALL*-OFF

ACKNOWLEDGEMENTS

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- **Tara Yacovitch**, **Brian Lerner**, and **Francesca Majluf** of Aerodyne Research, Inc. and the rest of the **MOOSE Science Teams** for the campaign datasets used in this study.

thank you!

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questions?

backup slides.

MODEL CONFIGURATION

- April-August 2021
  - April used as a spin up
- Initial conditions based on SE 1˚ CAM-Chem run
- NASA MERRA-2 (Resolution: 0.625˚ x 0.5˚ every 3 hours)
  - Meteorological nudging not applied to Michigan [41˚N, 272.5˚W]
- **MOZART-TS2**
  - Comprehensive representation of tropospheric and stratospheric chemistry with updated gas-phase chemistry for isoprene and terpene species
  - **MAM4**: Spatial distribution of aerosols
  - **VBS-SOA**: secondary organic aerosols separation
- **Emissions**
  - CAMS-GLOB-ANTv5.1 (Anthropogenic)
  - CAMS-GLOB-AIRv2.1 (Aircraft)
  - QFED (Biomass Burning)
  - MEGANv2.1 (Biogenic)

EMISSIONS

Anthropogenic and biomass burning emissions are generated offline and regridded to corresponding resolution.

- **Copernicus Atmosphere Monitoring Service Version 5.1 (CAMS-GLOB-ANTv5.1)**
  - Global anthropogenic emissions based on monthly emissions from EDGARv5 and CEDSv2
  - Resolution: 0.1° x 0.1°
  - Sectors: ENE, RCO, TRO, TNR, FEF, IND, SLV, AGR, MMA, SHP, SWD
- **CAMS-GLOB-AIRv2.1**
  - Aircraft emissions
  - Resolution: 0.5° x 0.5°

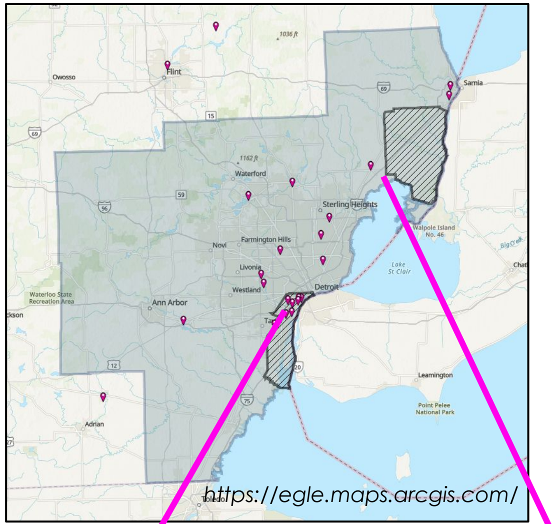
Copernicus Europe's eyes on Earth

Atmosphere Monitoring

STATIONARY MEASUREMENTS

Site Name	Coordinates	Description[1]	Types of Measurements[2]
Allen Park	42.22˚N, 276.8˚W	Suburban	O_3, NO_y, T, WS, WD
E 7 Mile	42.43˚N, 277.0˚W	Urban Suburban Mix	O_3, NO_2, T, WS, WD
New Haven	42.73˚N, 277.21˚W	Coastal	O_3, T, WS, WD
Oak Park	42.47˚N, 276.82˚W	Suburban	O_3, T, WS, WD
Port Huron	42.95˚N, 277.55˚W	Downwind	O_3, T, WS, WD
Trinity St Marks[3]	42.3˚N, 276.87˚W	Urban	O_3, CO, NO, NO_2, WS, WD
Ypsilanti	42.24˚N, 276.4˚W	Suburban	O_3, T, WS, WD

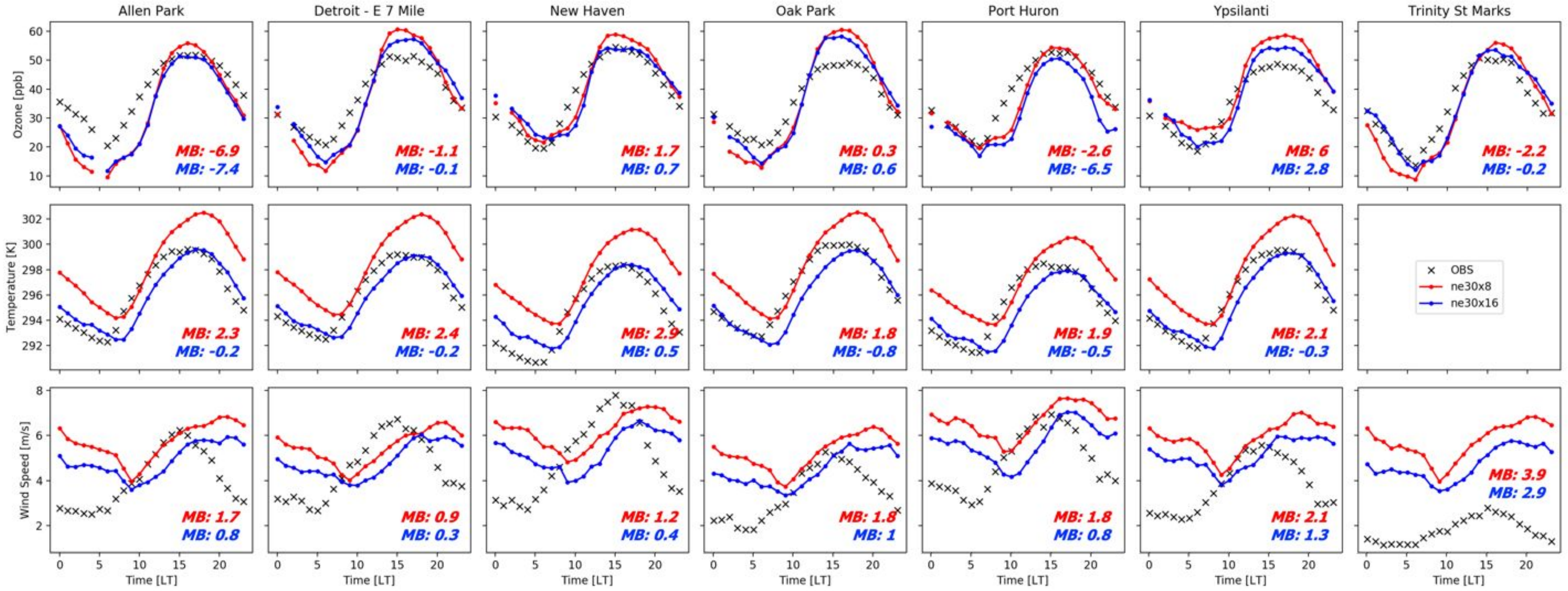
[1]Description of where the site is located.
[2]O_3 = Ozone; NO = Nitric Oxide; NO_2 = Nitrogen Dioxide; NO_y = sum of NO_x and all other reactive nitrogen; T = Temperature; WD = Wind Direction; WS = Wind Speed; CO = Carbon Monoxide.
[3]The Trinity St Marks site contains measurements of CO, NO_2, WS, and WD collected from MASN, as well as measurements of O_3, NO, and NO_2 from Chai et al., 2023, *In Preparation*.



Trinity St. Marks

New Haven

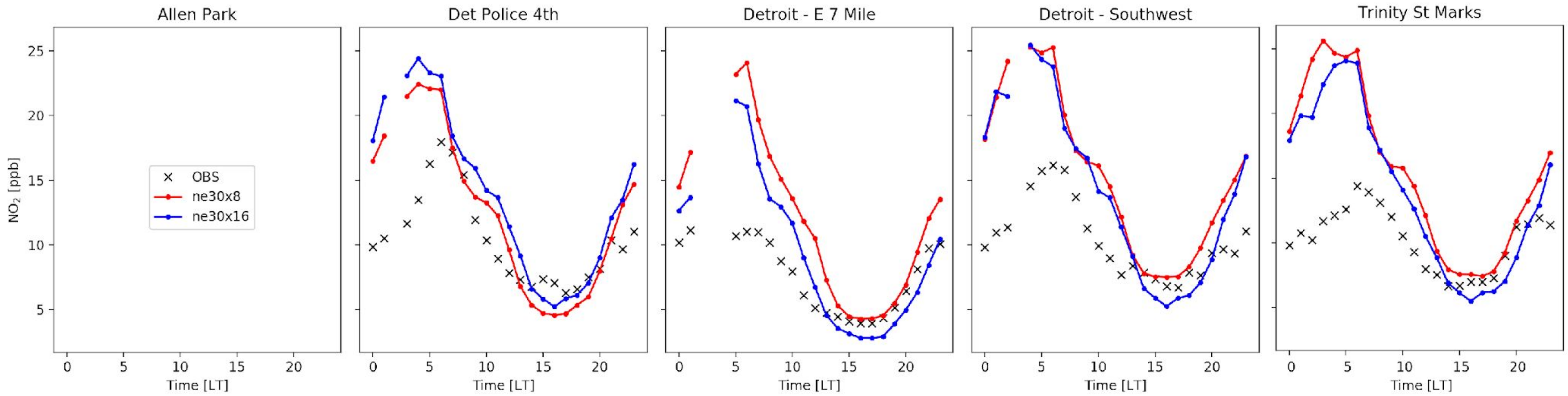
COMPARISON WITH SEMI STATIONARY SITE



Suburban	*Urban-Suburban Mix*	*Coastal*	*Suburban*	*Downwind*	*Suburban*	*Urban*

$$MB = \bar{M} - \bar{O}$$

COMPARISON WITH SEMI STATIONARY SITE



Urban *Urban-Suburban Mix* *Urban* *Urban*

SENSITIVITY EXPERIEMENTS

- Run suite of sensitivity experiments to **quantify contribution of emission from various sectors and long-range transport** on O_3 in SEMI.

Table 1: *Anthropogenic emission totals for May and June 2021 based on the CAMS-GLOB-ANTv5.1 emission inventory for Michigan and Southeast Michigan.*

Species	Molecular Weight [g/mol]	Michigan [Gg]	Southeast Michigan [Gg]
CO	28	201.6	59
NO	30	34.3	**10**
SO_2	64	19.4	6.5
C_2H_6	30	1.2	0.3
C_3H_8	44	1.1	0.5
HCHO	30	0.7	0.2
BENZENE	78	0.8	**0.3**
TOLUENE	92	3.3	**1.6**
XYLENES	106	6.1	**3**
BIGALK*	72	9.8	3.3
BIGENE*	56	1.1	0.4

*BIGALK represents lumped alkanes of C>3 (i.e., butanes, C_4H_{10}, and larger); BIGENE represents lumped alkenes of C>3 (i.e., butenes and larger) (Emmons et al., 2020).

Case	Grid Name	Resolution (km)	Setup
1	ne30x16	~7	Control
2	ne30x16	~7	TRA*-OFF
3	ne30x16	~7	IND*-OFF
4	ne30x16	~7	OTH*-OFF
5	ne30x16	~7	ALL*-OFF

Help identify the impact on O_3 from different emission sectors, in order to better determine how to reach O_3 attainment in SEMI.

CAMSv5.1 NO Emissions in e^{12} molecules cm^{-2} s^{-1}