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Multi-scale Modeling of Air Quality and Greenhouse Gases over Greater Boston, Part I: Evaluation of Regional to Local Predictions Using Surface and Satellite Data

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Background and Objectives

- **Background**
  - The Intelligent Solutions to Urban Pollution for Equity and Resilience (iSUPER) Impact Engine sponsored by Northeastern University
  - Ground-level ozone (O_3) and particulate matter (PM): criteria air pollutants (CAPs); Carbon dioxide (CO_2): a greenhouse gas (GHG)
  - The Weather Research and Forecasting model coupled with Chemistry and Greenhouse Gases (WRF-Chem-GHG) simultaneously tracks CAPs and GHGs

- **Objectives**
  - Assess model capability of reproducing CAPs and GHGs, and its sensitivity to grid resolutions
  - Identify underlying reasons for model biases in typical summer and winter months to inform potential areas of model improvements
  - To provide background conditions for hyperlocal street-scale modeling (Part II)

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WRF-Chem-GHG Configuration

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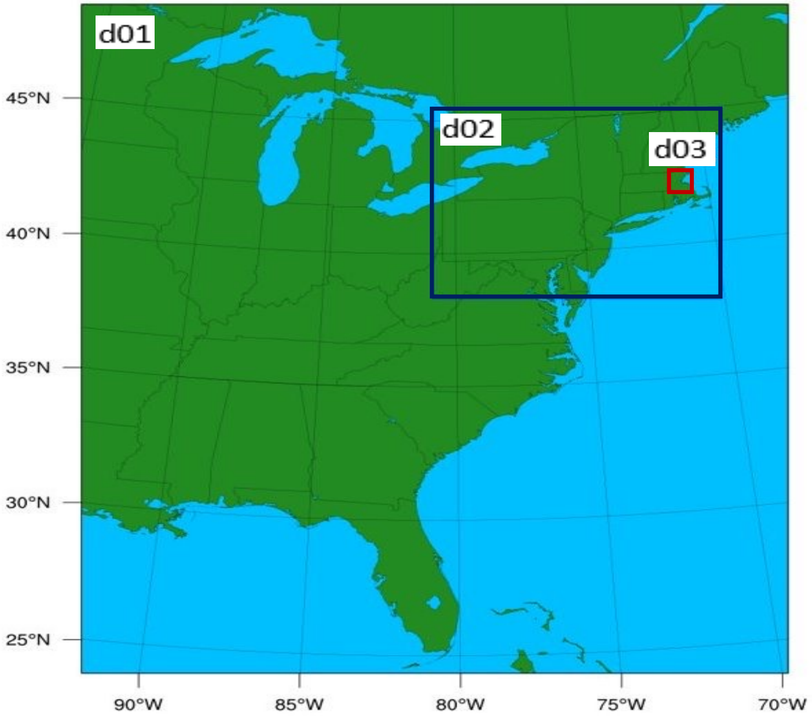

ICON/BCON: initial/boundary condition
NCEP FNL: National Center for Environmental Protection FNL (Final) Operational Global Analysis data
WACCM: The Whole Atmosphere Community Climate Model
FINN: Fire INventory from NCAR
QFED: Quick Fire Emissions Dataset
NEMO: Neighborhood Emission Mapping Operation
EDGAR: Emissions Database for Global Atmospheric Research
MEGAN: Model of Emissions of Gases and Aerosols from Nature
AER/AFWA: Atmospheric and Environmental Research Inc. and Air Force Weather Agency
VPRM: Vegetation Photosynthesis and Respiration Model

Baseline Simulation

Attribute	Configuration
Period	January and July 2023
Domains	Triple-nested: 12-km (d01), 3-km (d02), 1-km (d03)
Vertical layers	34 layers up to 100 hPa (~16 km)
ICON/BCON	NCEP FNL (Meteorology); WACCM-FINN & Carbon Tracker (Chemistry)
Anthropogenic emissions	1-km NEMO 2019 regridded to 12-, 3- and 1-km; EDGAR 2021
Online emissions	MEGAN v2 (biogenic); Gong scheme (sea-salt); AER/AFWA scheme (dust); VPRM (GHG)

Sensitivity Simulations

	Period	Simulation Design	Objectives
SEN1	Jan	Adjust emissions	Reduce $PM_{2.5}$ overpredictions
SEN2	Jul	Use WACCM-QFED	Better representation of Canadian fires

Observations for Model Evaluation

Network/Satellite	Variables	Data Frequency
Air Quality System (AQS)	O_3, $PM_{2.5}$	hourly, daily
	EC, OC, NH_4, NO_3, SO_4	daily every 3 days
AirNow	O_3, $PM_{2.5}$	hourly
PurpleAir	$PM_{2.5}$	hourly
METeorological Aerodrome Reports (METAR)	T2, RH2, WS10, WD10, PRECIP	hourly
Orbiting Carbon Observatory-3 (OCO-3)	CO_2	daily
CERES	SWDOWN, GLW	monthly
MODIS	AOD, CCN	monthly
OMI	TOR	monthly

EC: elemental carbon
OC: organic carbon
NH_4, NO_3, SO_4: ammonia, nitrate, sulfate
T2, RH2: temperature and relative humidity at 2-m height
WS10, WD10: wind speed and wind direction at 10-m height
PRECIP: precipitation
SWDOWN: downward shortwave radiation
GLW: downward longwave radiation
AOD: aerosol optical depth
CCN: cloud condensation nuclei
CF: cloud fraction
TOR: tropospheric ozone residual
CERES: the Clouds and the Earth's Radiant Energy System
MODIS: the Moderate Resolution Imaging Spectroradiometer
OMI: Ozone Monitoring Experiment

Model Evaluation Protocols

Variable	Benchmark	Reference
T2	MB within ±0.5 °C MAGE ≤ 2 °C	Tesche and Tremback (2002); Monk et al. (2019)
WS10	MB within ±0.5 m/s RMSE ≤ 2 m/s	
WD10	MB within ±10 ° MAGE ≤ 30°	
Max 8-h O_3	NMB within ±15% NME ≤ 25%	Emery et al. (2017)
24-h Avg $PM_{2.5}$	NMB within ± 30% NME ≤ 50%	
CO_2	NMB within ± 30% NME ≤ 50%	Basu et al. (2023)

MB: mean bias
MAGE: mean absolute gross error
RMSE: root mean square error
NMB: normalized mean bias
NME: normalized mean error

Meteorology: Performance Statistics

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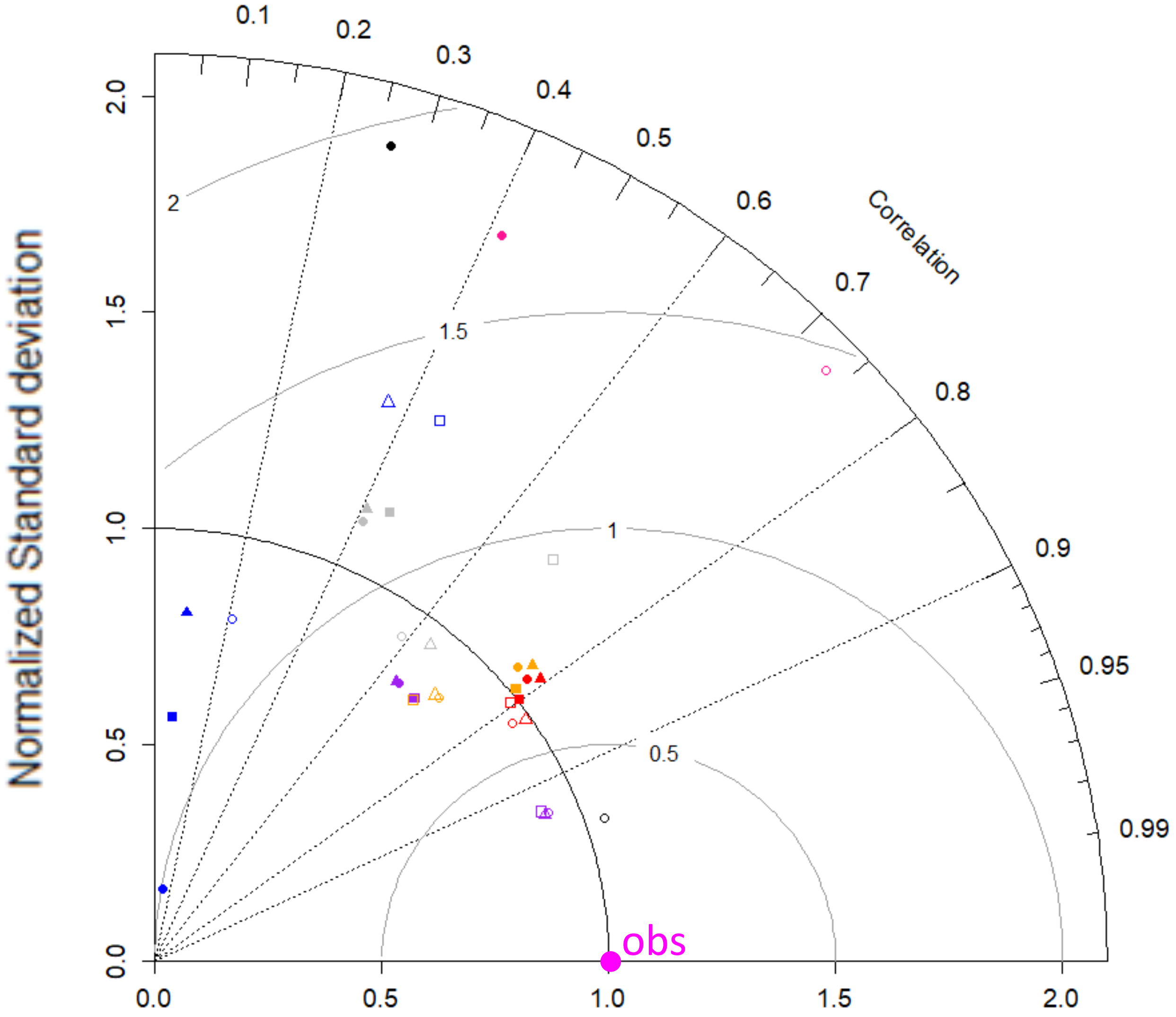
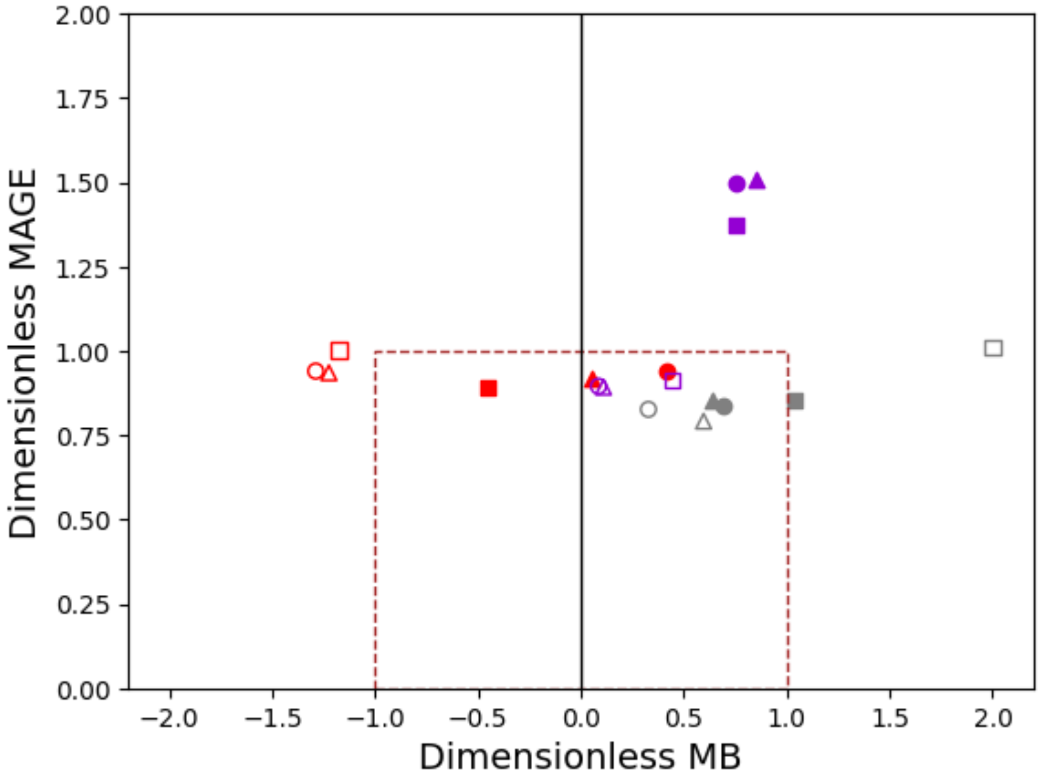


- Good performance for all variables except larger cold bias in T2 in Jan and gross error in WD10 in Jul
- Biases and gross errors for WS10 decrease with finer resolutions



Red: T2; Orange: RH2; Grey: WS10; Purple: WD10; Blue: PRECIP; Black: GLW, Pink: SWDOWN ----- dimensionless benchmark

□: 12-km; Δ: 3-km; o: 1-km; hollow markers: Jan; solid markers: Jul

Meteorology: Temporal Evaluation

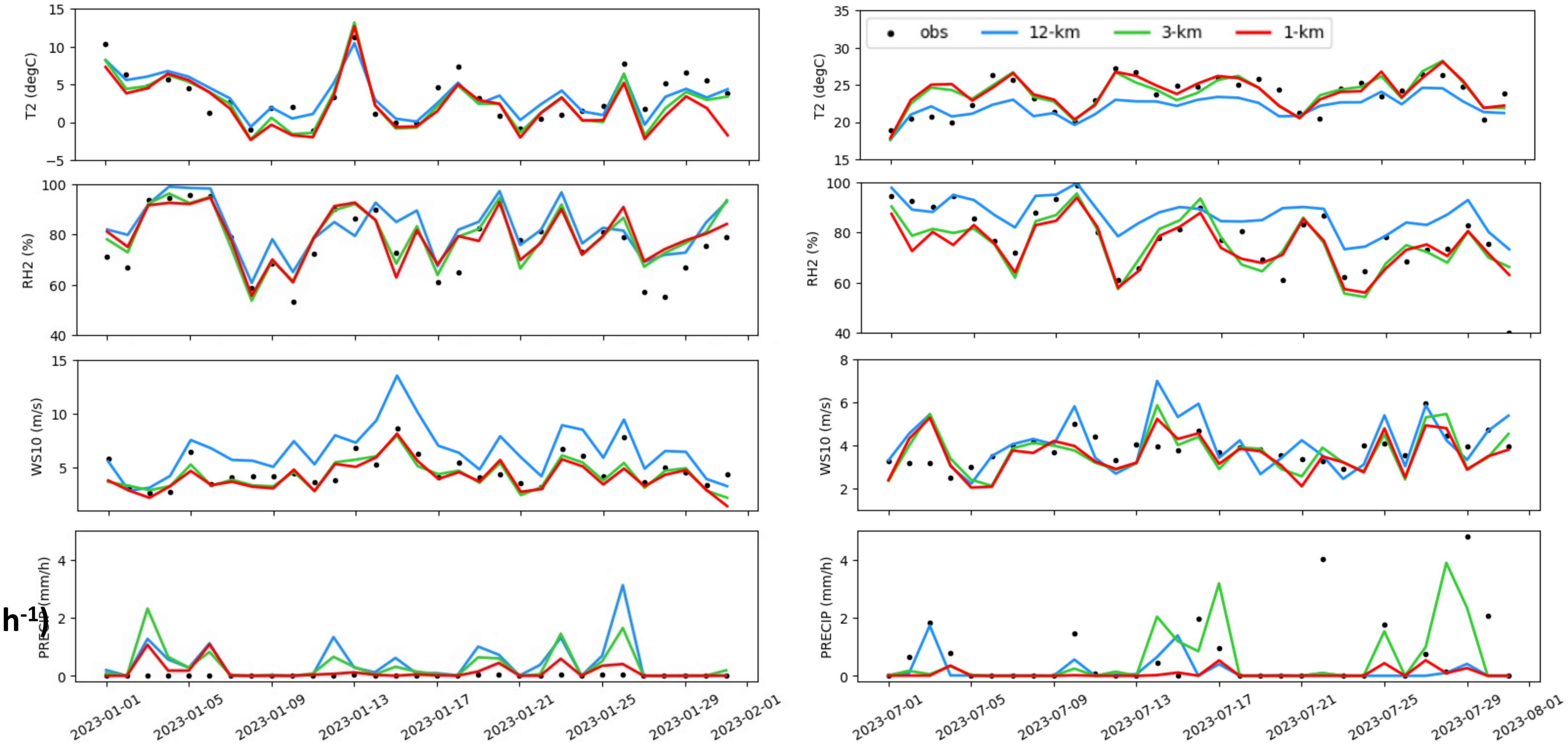
Logan International Airport 71.02°W, 42.37°N

T2 (°C)

RH2 (%)

WS10 (m s[-1])

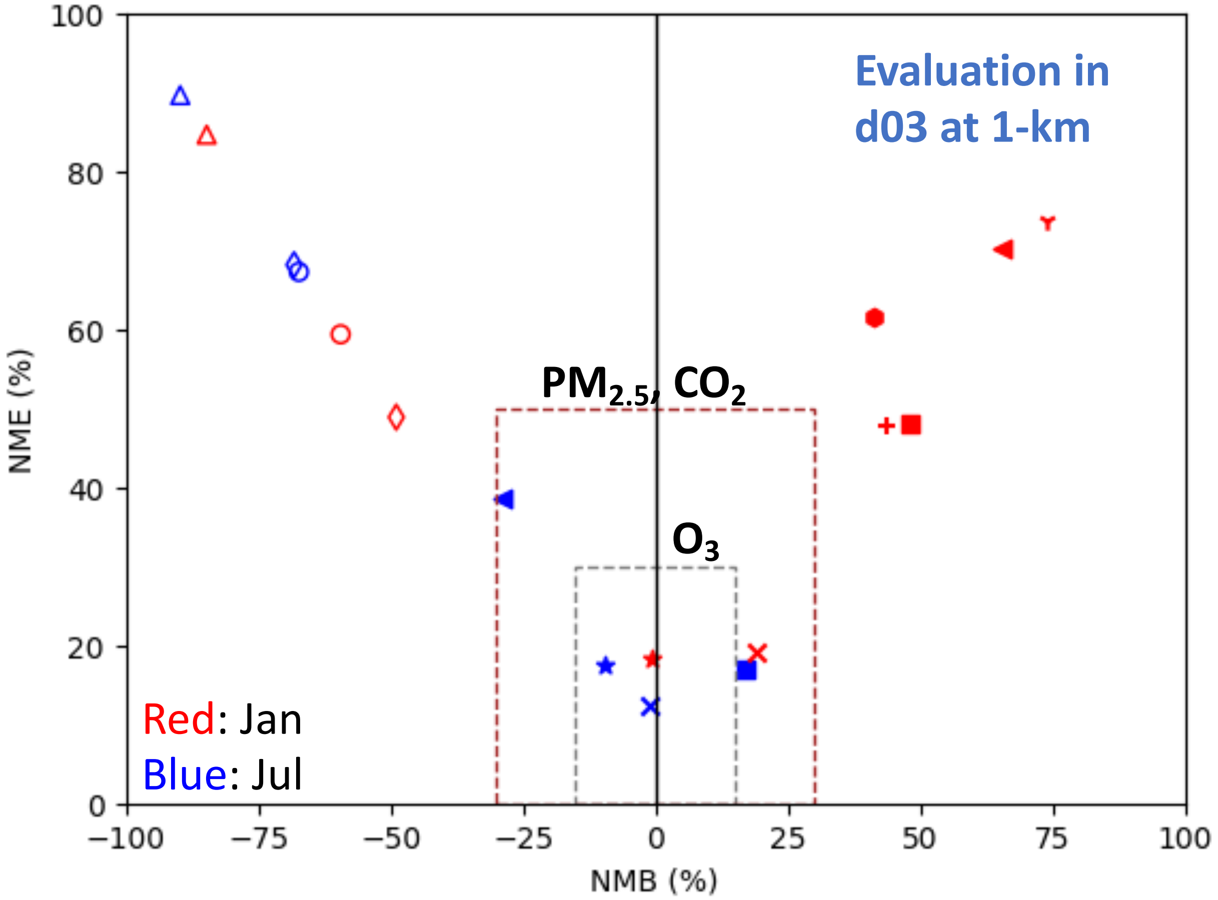
PRECIP (mm h[-1])



- Temporal trend of meteorological variables is well captured
- Better reproduction for most meteorological variables at finer resolutions

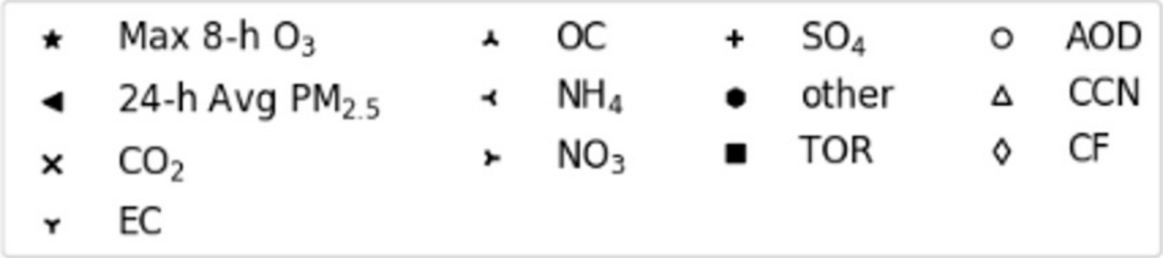
Air Quality: Performance Statistics

----- benchmark for O_3 ----- benchmark for $PM_{2.5}$ and CO_2



Outliers: OC: $\frac{215\%}{215\%}$, NH_4: $\frac{395\%}{395\%}$, NO_3: $\frac{94.9\%}{107\%}$ ($\frac{NMB}{NME}$ in Jan)

- Good performance for Max 8-h O_3 and CO_2 and marginal performance for 24-h Avg $PM_{2.5}$ in Jul
- Overpredicted $PM_{2.5}$ compositions in Jan and underpredicted cloud variables in both months



** Observational data for $PM_{2.5}$ compositions is not yet available for Jul

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Air Quality: Spatial Evaluation in Jan

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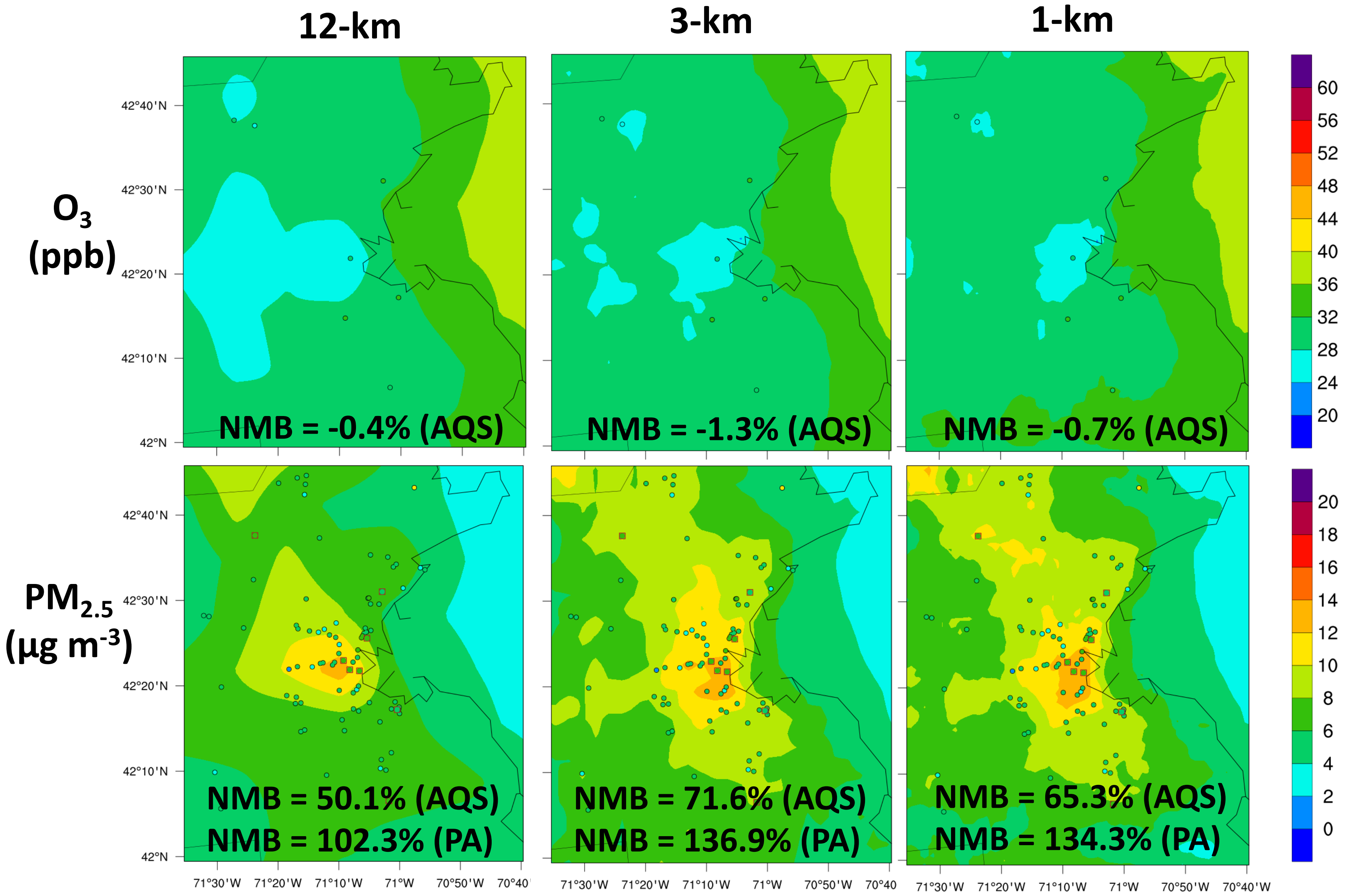
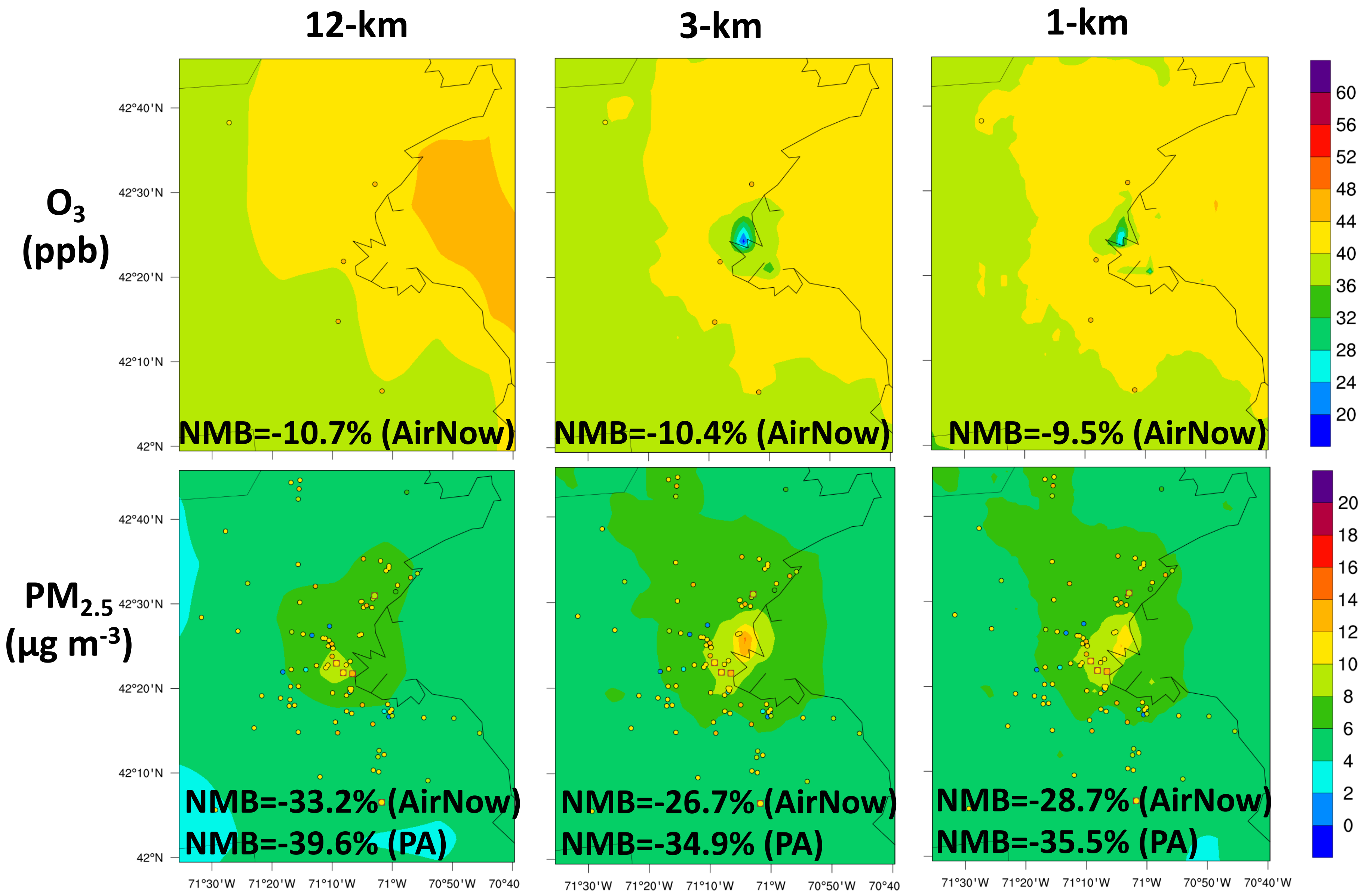


- O_3 magnitude is well captured
- High localized emission in urban center leads to higher $PM_{2.5}$ at finer grid resolutions

PA: PurpleAir

Air Quality: Spatial Evaluation in Jul



- Better performance for O_3 at finer grid resolution
- Underpredicted $PM_{2.5}$ due in part to chemical BCON
- 1-km is not fine enough to capture sub-grid variability

PA: PurpleAir

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Air Quality: Spatial Evaluation in Jul

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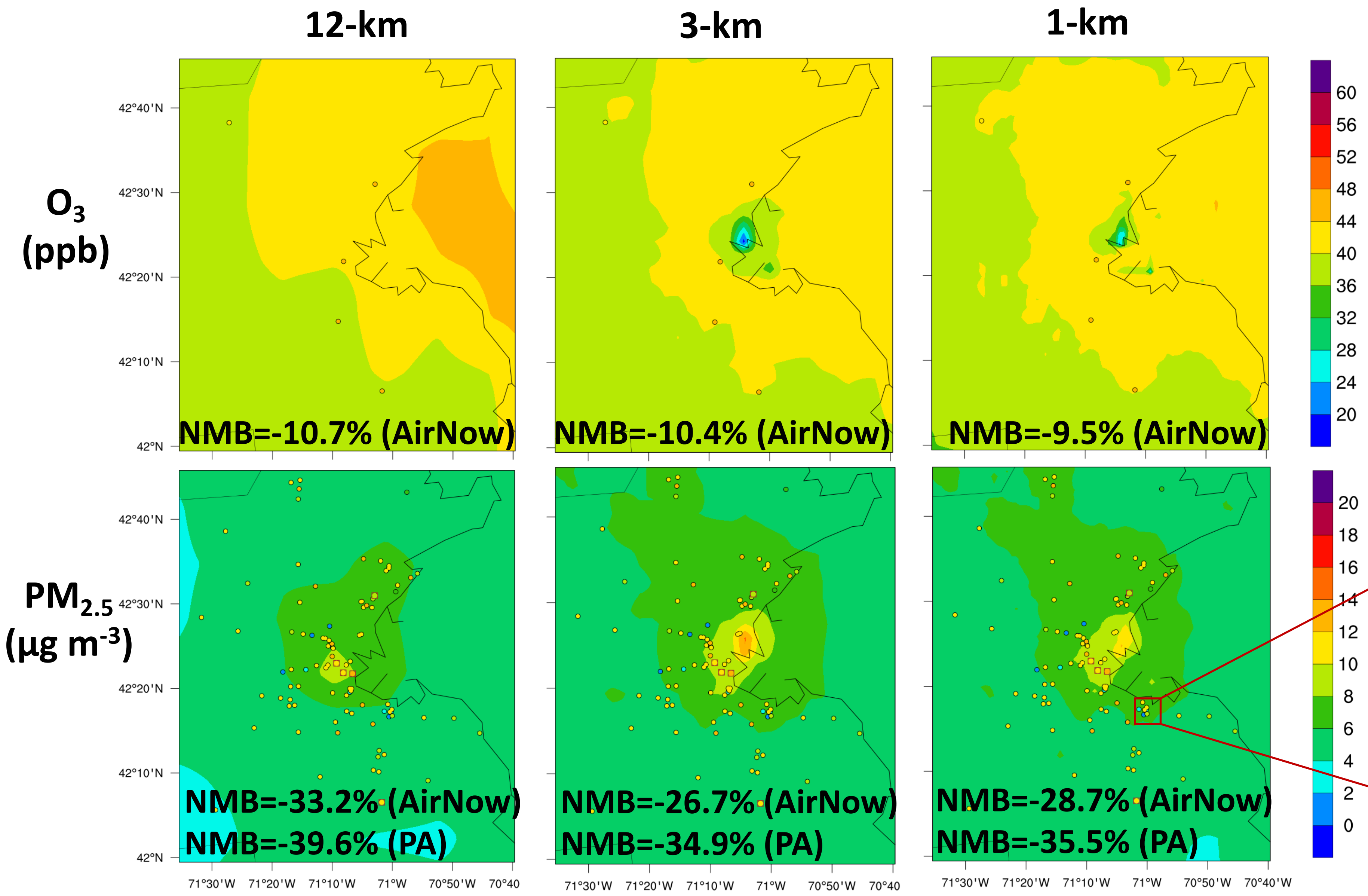

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PA: PurpleAir

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Air Quality: Temporal Evaluation

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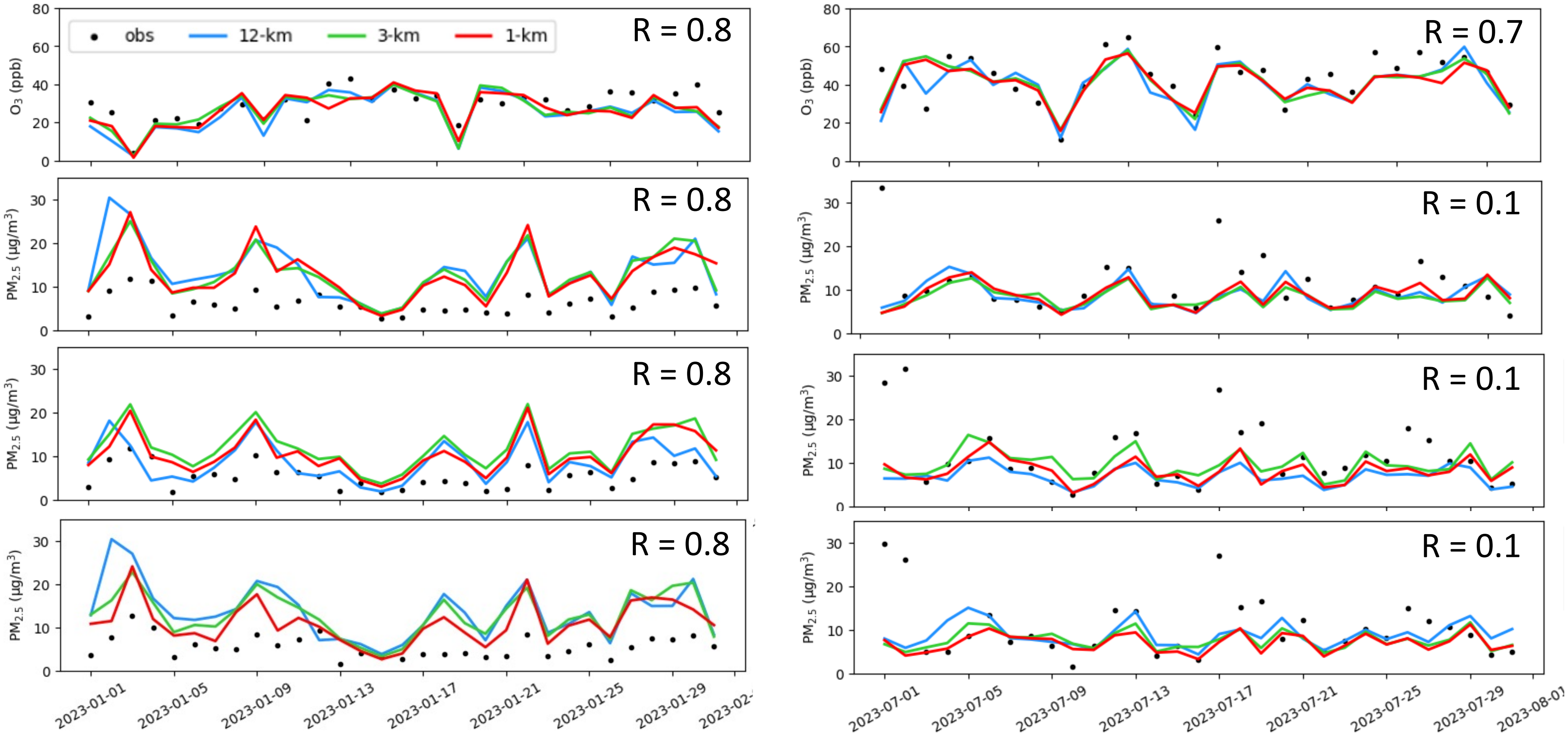
	Jan	Jul

Roxbury (AQS) — O_3 (ppb); $PM_{2.5}$ (μg m^{-3})

Chelsea (PurpleAir) — $PM_{2.5}$ (μg m^{-3})

Brookline (PurpleAir) — $PM_{2.5}$ (μg m^{-3})

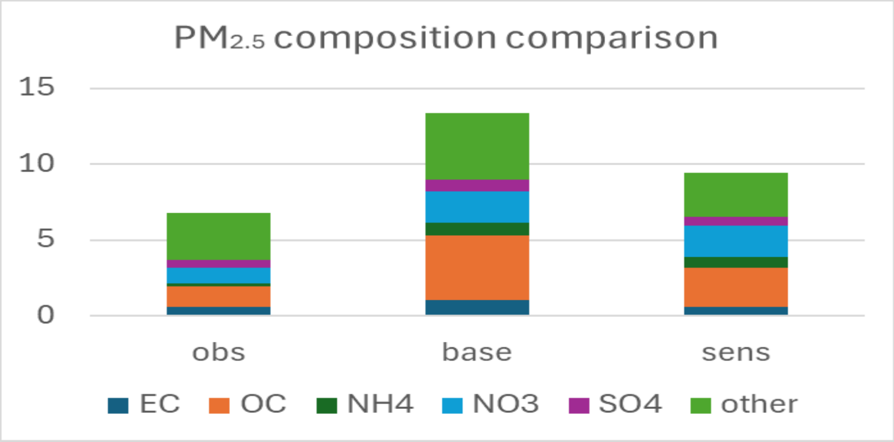


- O_3 temporal trend and magnitude are well captured
- $PM_{2.5}$ is overpredicted in Jan but well captured in Jul except Canadian wildfire days

R: correlation coefficient

Sensitivity Simulations

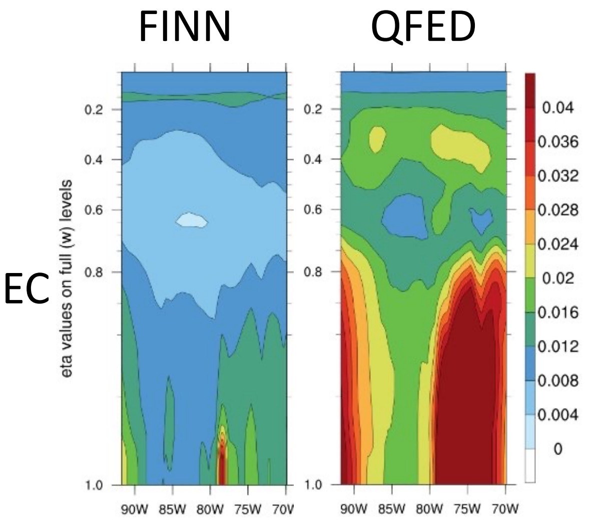
SEN1: Emission Adjustment

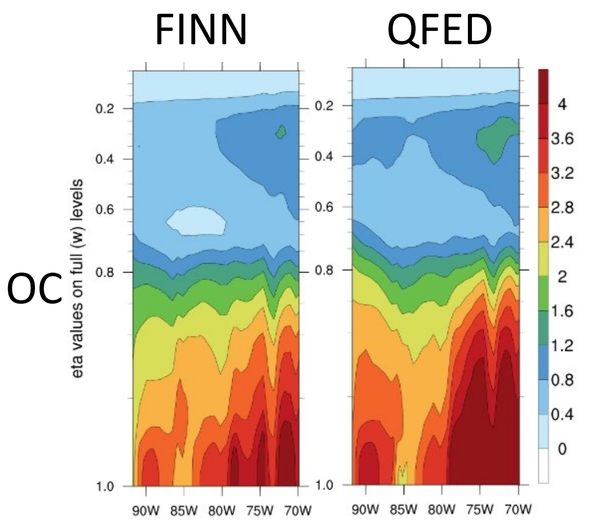


		EC	OC	NH_4	NO_3	SO_4	other	$PM_{2.5}$
MB	BASE	0.5	2.9	0.7	1.0	0.2	1.3	7.0
	SEN1	0.0	1.2	0.7	1.0	0.0	-0.2	2.6
NMB	BASE	73.9	215	397	94.9	43.7	41.2	102
	SEN1	-1.2	89.0	352	93.4	7.9	-7.2	38.0
NME	BASE	73.9	215	397	107	47.7	61.5	106
	SEN1	2.2	89.0	352	106	37.2	29.7	43.5

- Reducing primary $PM_{2.5}$ emissions reduces overpredictions in EC, OC, unknown $PM_{2.5}$ and sulfate
- Linear response of EC, OC and unknown $PM_{2.5}$

SEN2: WACCM-QFED





		O_3	$PM_{2.5}$
NMB (%)	BASE	-5.2	-32.6
	SEN2	-4.2	-30.6
NME (%)	BASE	16.9	47.3
	SEN2	16.6	45.0

- WACCM-QFED has higher wildfire-induced $PM_{2.5}$
- WACCM-QFED slightly improves O_3 and $PM_{2.5}$

Summary and Future Work

- WRF-Chem-GHG reproduces well T2 in Jul and WD10 in Jan, and RH2 and WS10 in both months, but shows large cold bias in T2 in Jan and gross error in WD10 in Jul
- WRF-Chem-GHG performs well for O_3 and CO_2. $PM_{2.5}$ is overpredicted in Jan and underpredicted on Canadian wildfire days in Jul
- WRF-Chem-GHG performs better for most meteorological variables and O_3 at finer grid resolutions
- **Future work:** Further improve model performance by improving meteorological and chemical inputs and model representations.

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