Improving Ozone Simulations in the Great Lakes Region: the Role of Emissions, Chemistry, and Dry Deposition

Georgia Tech

Momei Qin,
Haofei Yu, Yongtao Hu,
Armistead Russell, Talat Odman

THE UNIVERSITY OF ALABAMA IN HUNTSVILLE

Kevin Doty,
Arastoo Pour-Biazar,
Richard McNider

EPRI

Eladio Knipping

March 20, 2019

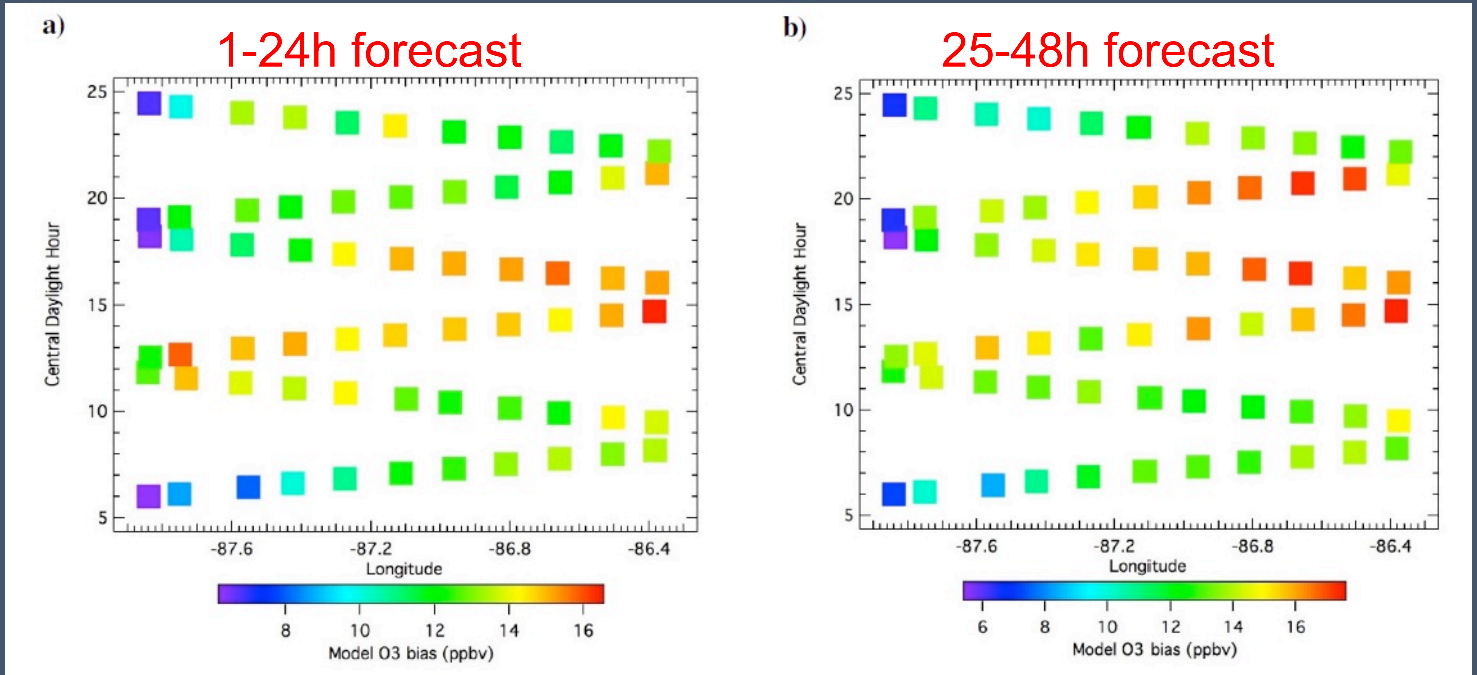
LADCO "EPRI Great Lakes Ozone Study" webinar

Outline

- Background
- WRF simulations
  - Baseline evaluation
- CMAQ simulations
  - Baseline evaluation
    - Ground observations (O_3 & NO_x)
  - Emissions
    - 50% NO_x from mobile sources
    - MEGAN vs. BEIS (cb05)
    - MEGAN vs. BEIS (cb6)
- CMAQ simulations (continued)
  - Chemistry
    - CB6 vs. CB05
  - Deposition
    - 10-fold dry deposition of O_3 over fresh water
  - Final simulation
  - Lateral boundary conditions
- Conclusions

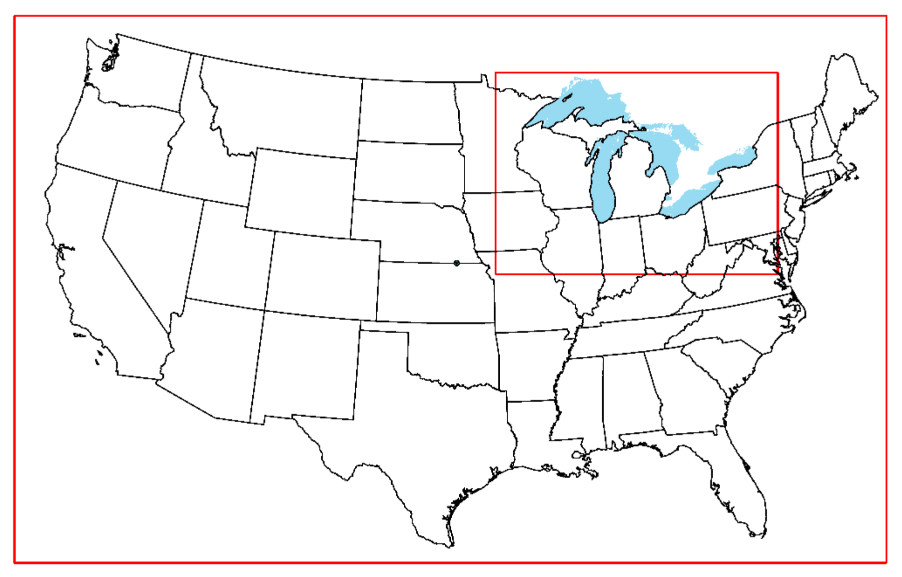
Background

- O_3 exceedance is still of concern in the Great Lakes Region
- Air quality model tends to overestimate O_3 over cooler bodies of water, e.g. over Lake Michigan



Cleary *et al.*, ACP, 2015

WRF configurations

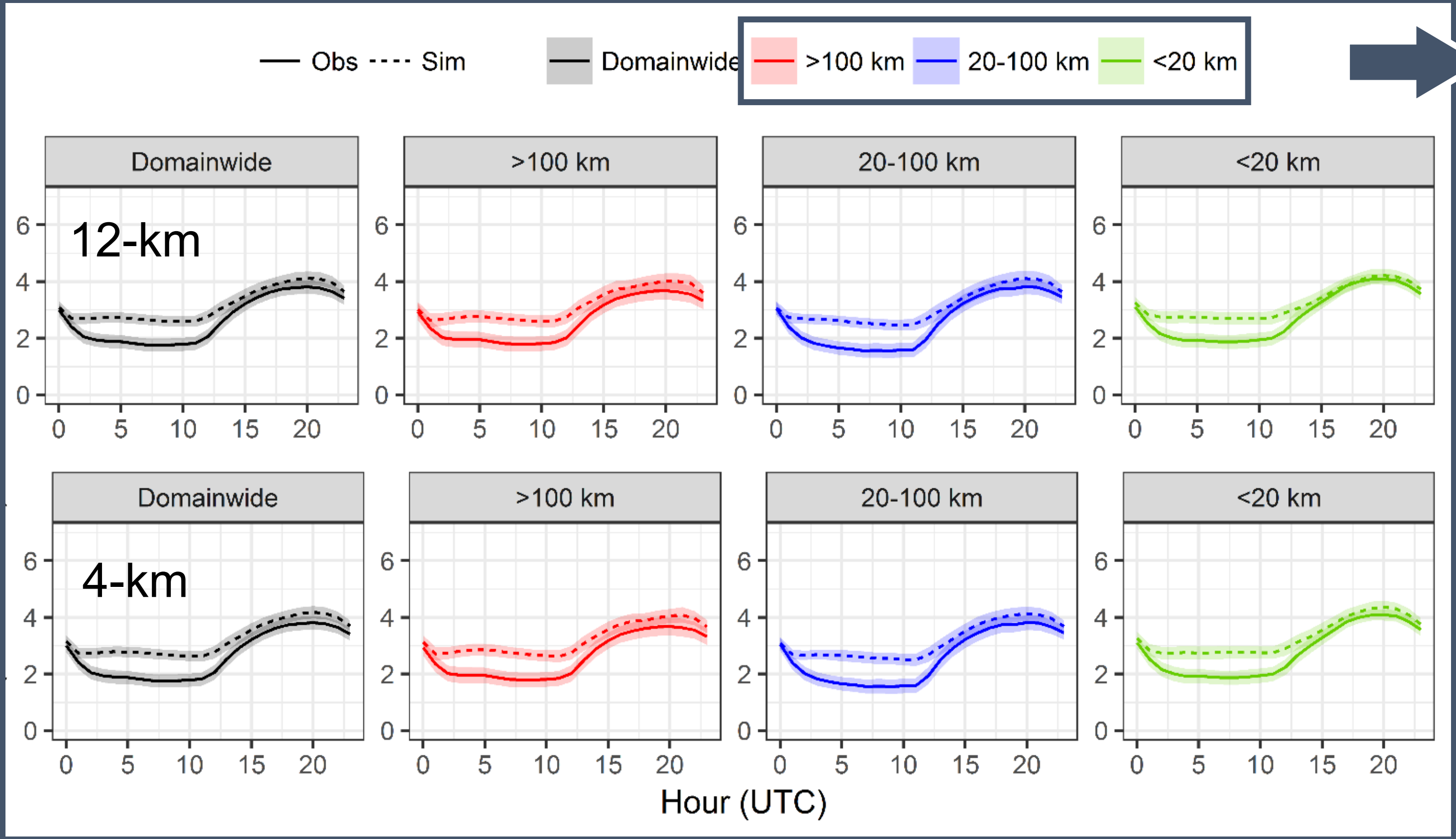


- **WRFv3.8.1**
- Jun 15th to Aug 1st, 2011
- One-way nested
  - 12-km (402×252)
  - 4-km (390×279)
- NAM-12 & NLCD 2011

	12-km	4-km
Longwave radiation	rrtmg scheme	
Shortwave radiation	rrtmg scheme	
Land surface	Pleim-Xiu LSM	
Cumulus	Kain-Fritsch scheme	
microphysics	Morrison (2 moments)	
PBL	ACM2 (Pleim) PBL	
Surface nudging	off	
Grid nudging	above the PBL	off
Soil nudging	on	on

WRF baseline evaluation

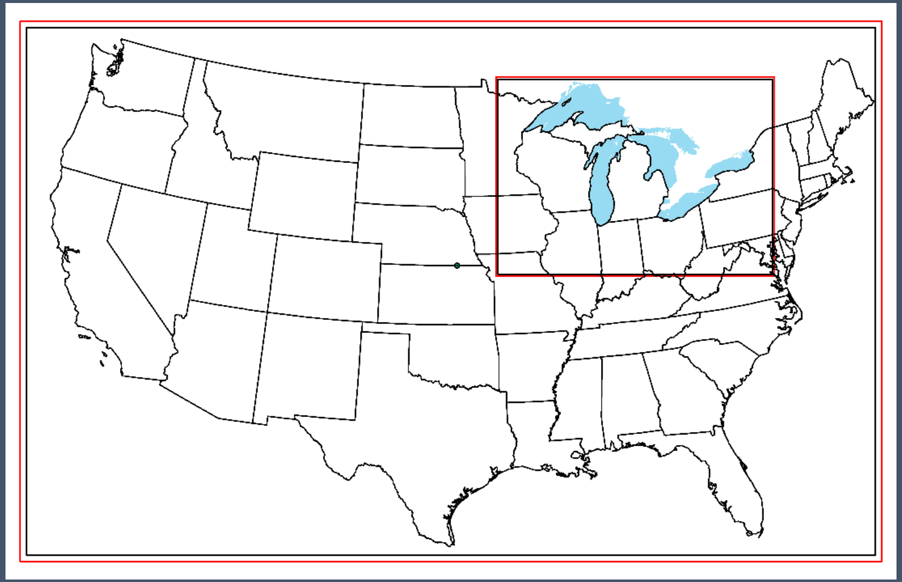
- Surface temperature, humidity
- Wind speed (m/s)



Distance from the shoreline	Type
>100km	Inland
20-100km	Buffer
<20km	Coastal

High biases occurred during the nighttime and in the early morning (19:00-8:00 CST), when wind speed is low

CMAQ configurations (baseline)



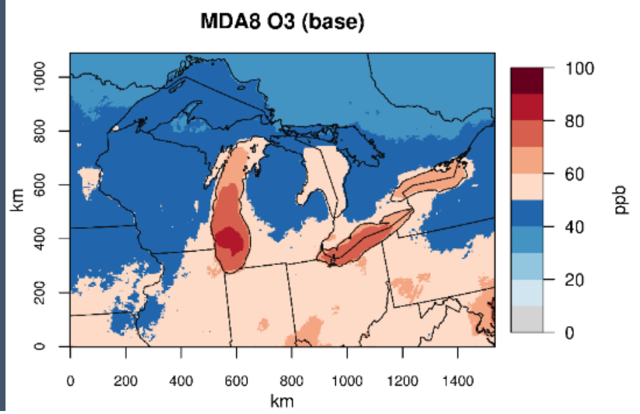
- **CMAQv5.1**
- Jun 21st to Aug 1st, 2011
- Grids
  - 12-km, 12US2 (396×246)
  - 4-km, 04GL (384×273)
  - 35 vertical layers

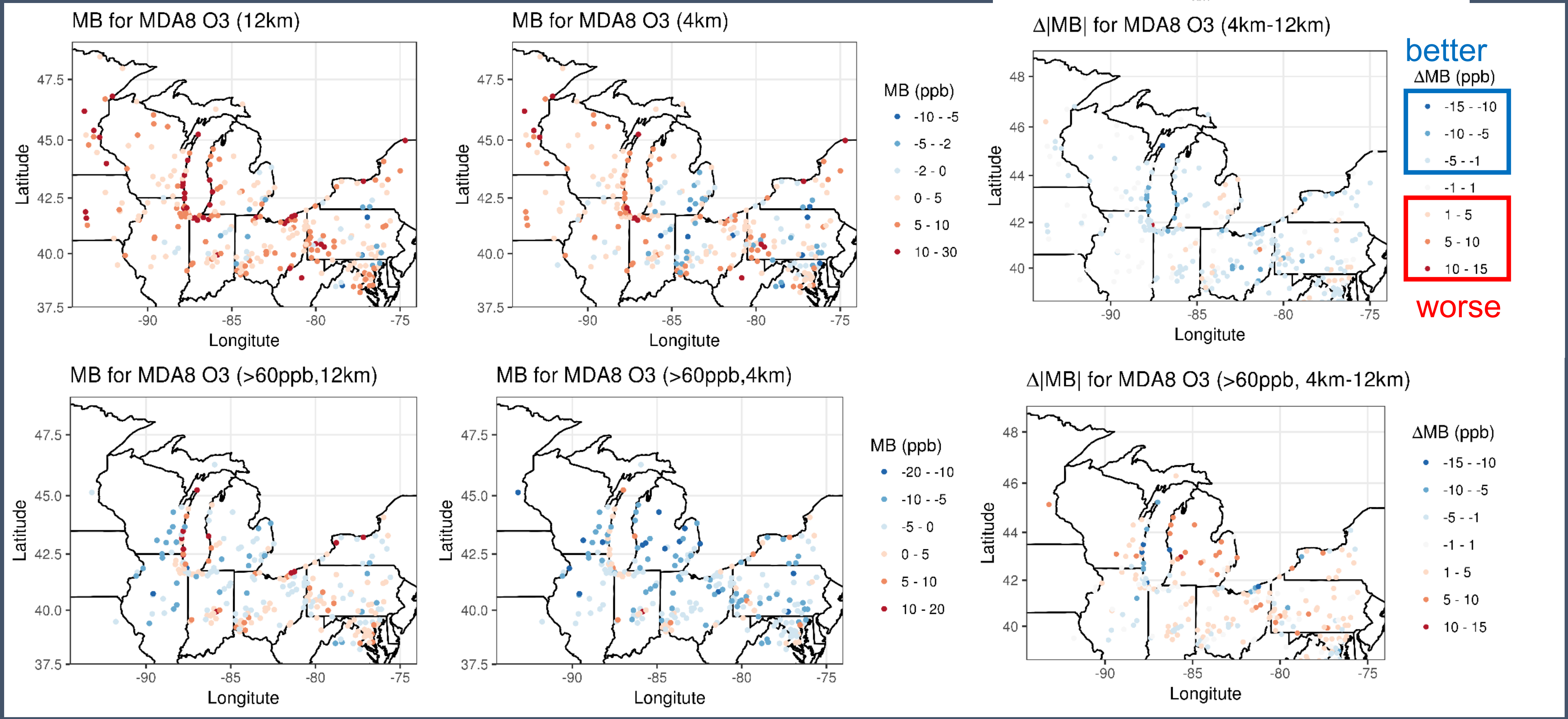
- Mechanism
  - Cb05e51, with 6th aerosol module
- Emissions
  - 2011 NEI (Version 6.2 Platform)
  - In-line calculation in CMAQ
    - ➢ Point sources & Biogenic emissions (BEIS3)
- Other options

Use inline windblown dust emissions	N
Turn on lightning NO_x	N
Use min Kz in edyintb	Y
Calculate in-line deposition velocities	Y
Ammonia bi-directional flux for in-line deposition velocity	N
Mercury bi-directional flux for in-line deposition velocity	N
Surface HONO interaction	Y

CMAQ performance (baseline)

- MDA8 O_3



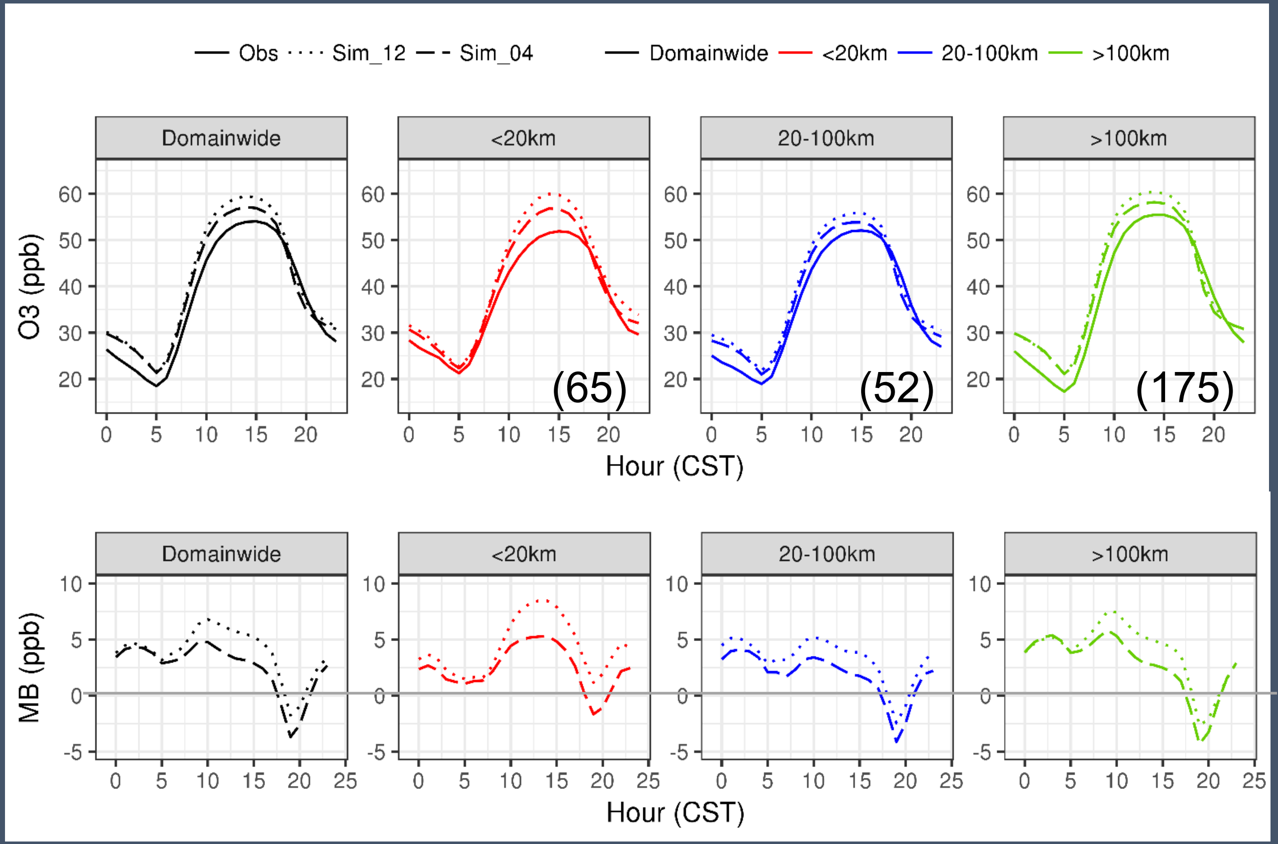


CMAQ performance (baseline)

- O_3

July Monthly Means

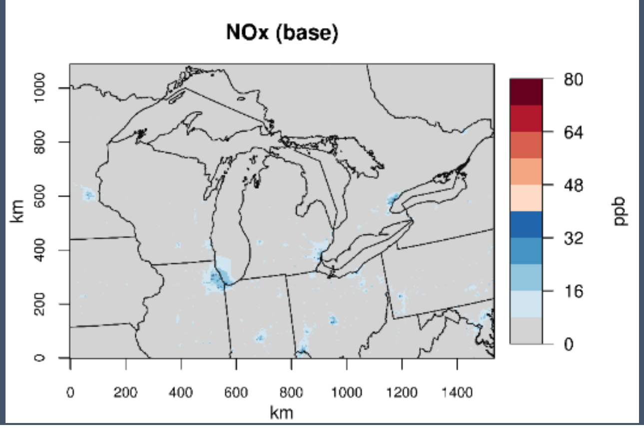
Group		<20km	20 – 100km	>100km
MDA8 O_3	Obs	51.2	50.9	54.1
	12-km	60.3	55.0	58.6
	4-km	56.6	52.5	56.4
MDA8 O_3 (>60ppb)	Obs	69.1	67.8	68.1
	12-km	71.4	65.1	68.3
	4-km	67.4	61.5	64.7

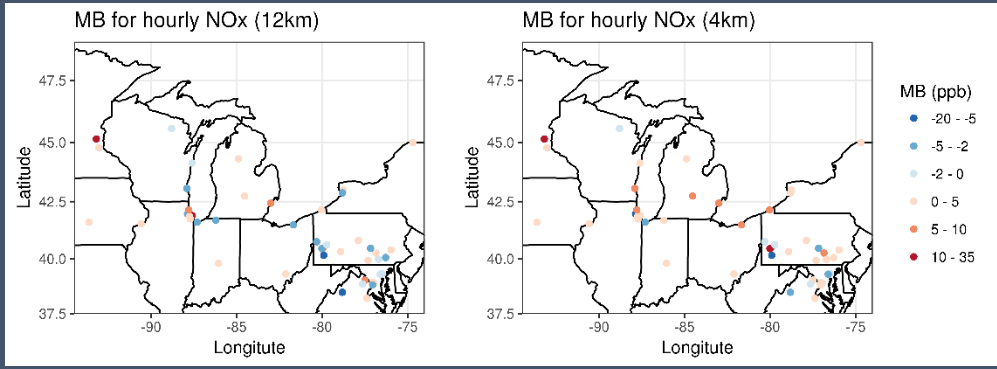


Number of sites given in parentheses

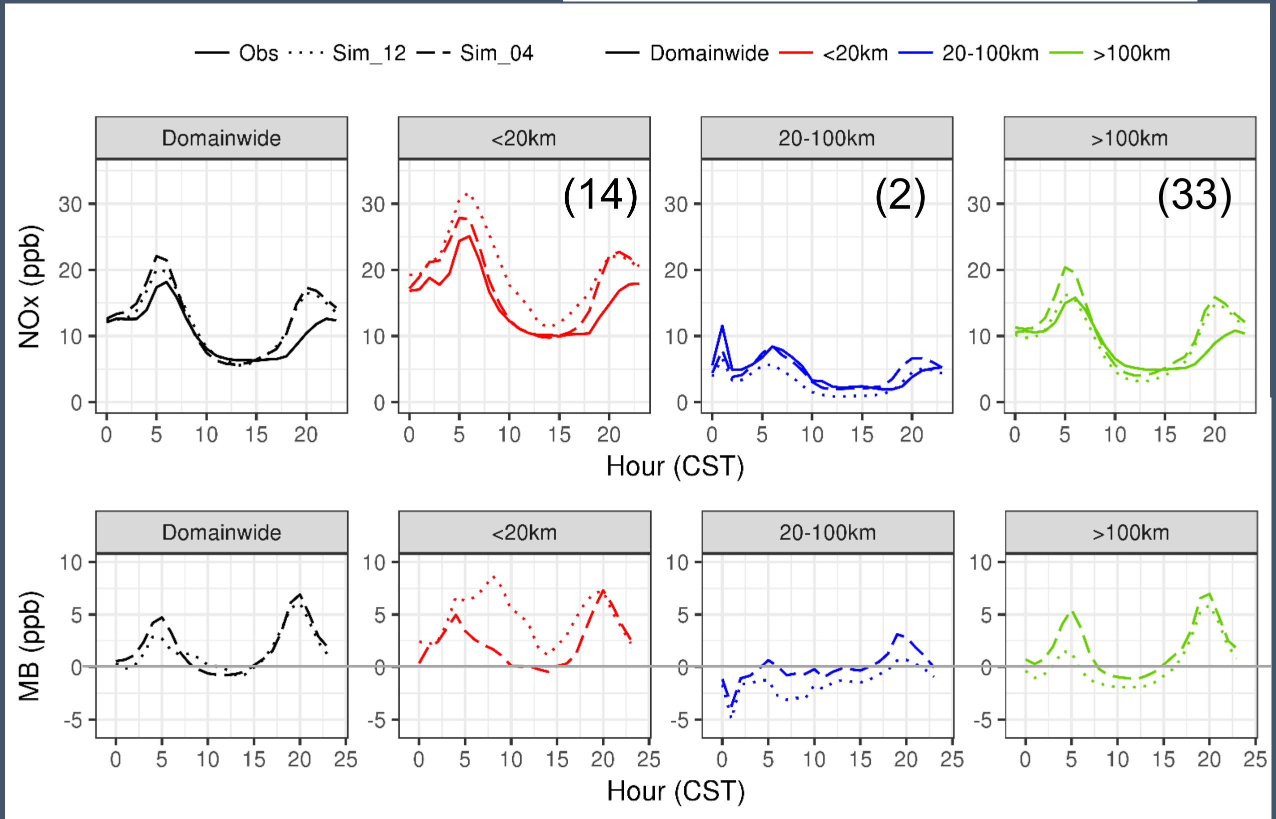
CMAQ performance (baseline)

- NO_x



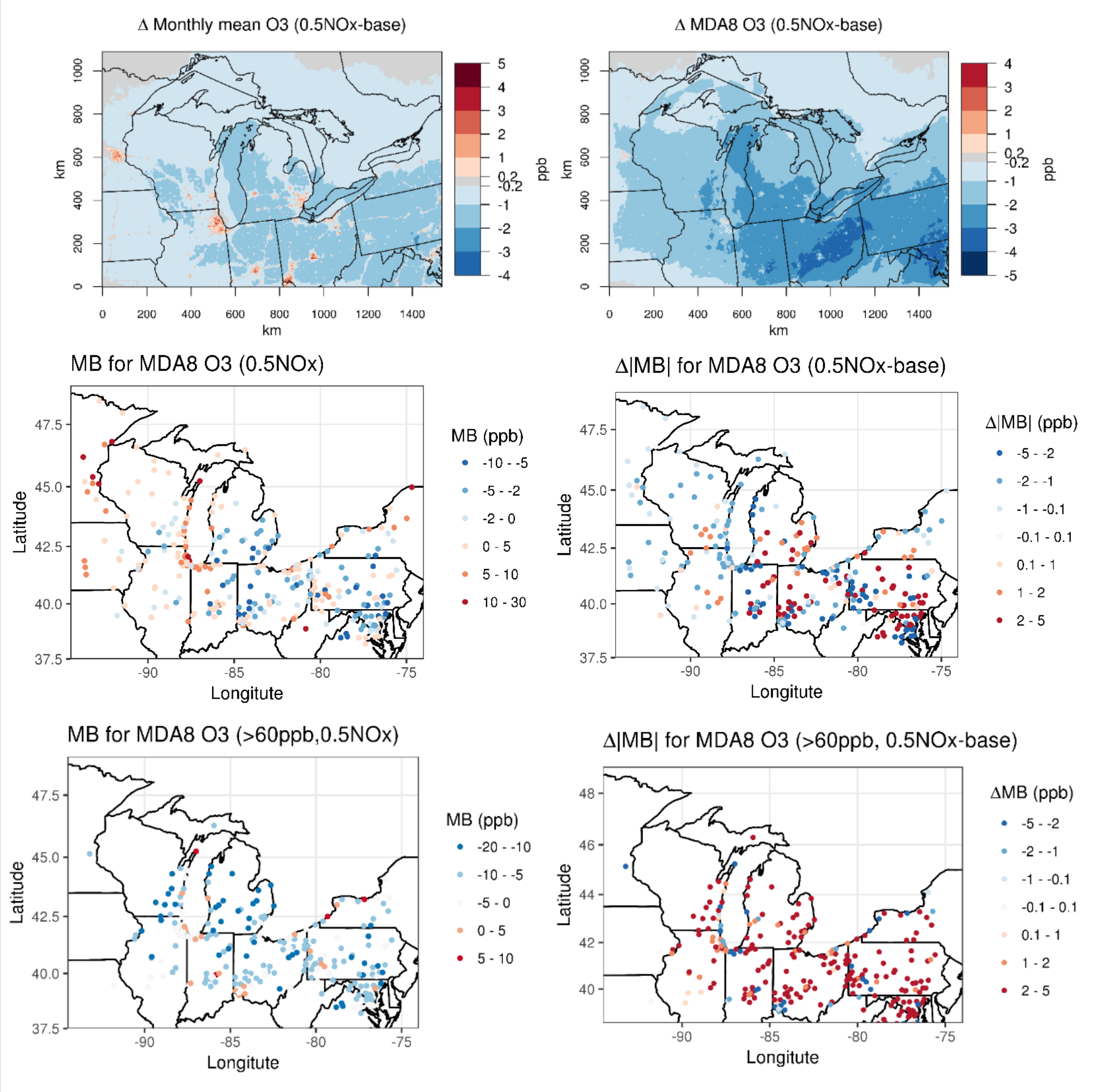


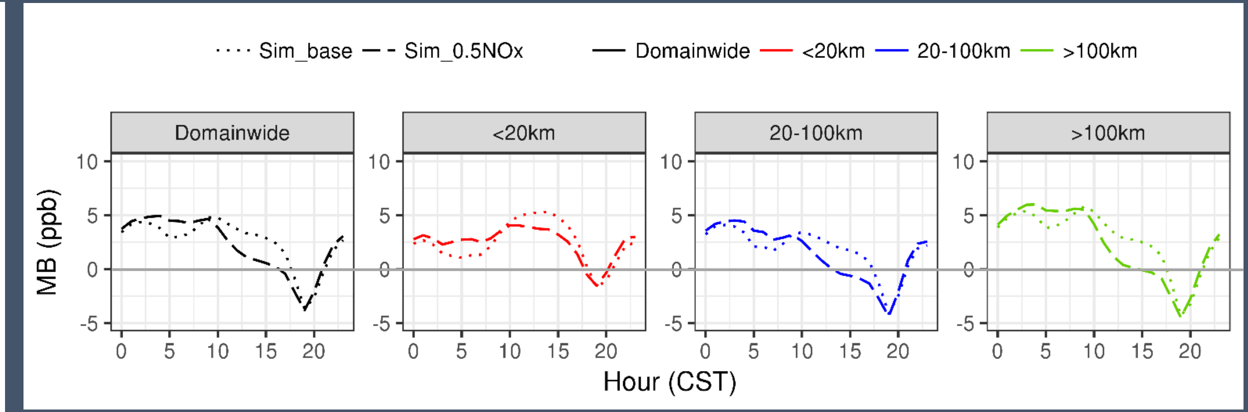
Group		<20km	20 – 100km	>100km
NO_x	Obs	15.3	4.4	9.0
	12-km	20.0	3.1	9.3
	4-km	17.5	4.5	10.7



Number of sites given in parentheses

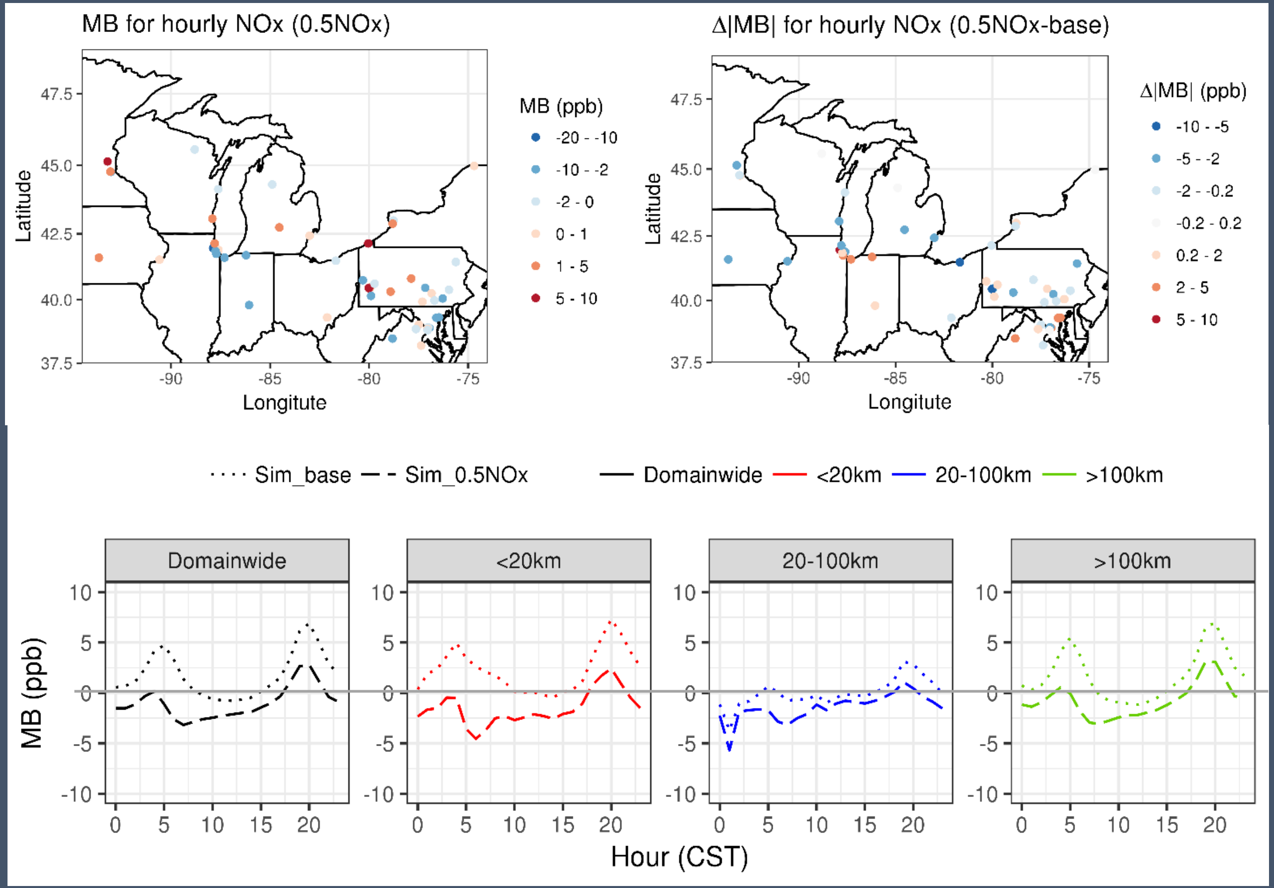
50% NO_x emissions from mobile sources： O_3 performance





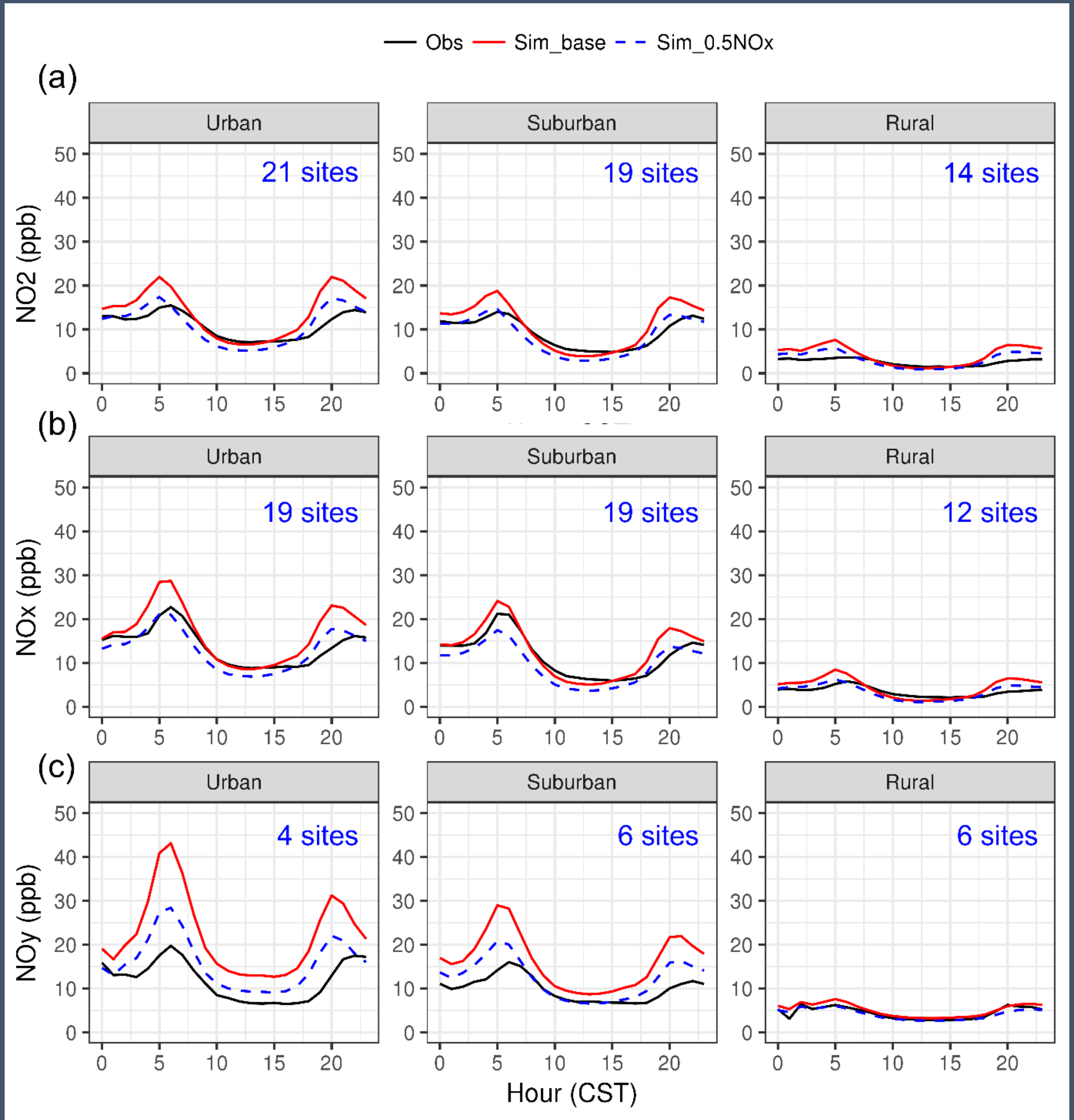
Group		<20km	20 – 100km	>100km
MDA8 O_3	Obs	51.2	50.9	54.1
	Base	56.6	52.5	56.4
	0.5NO_x	55.2	50.6	54.3
MDA8 O_3 (>60ppb)	Obs	69.1	67.8	68.1
	Base	67.4	61.5	64.7
	0.5NO_x	65.1	58.7	61.8

50% NO_x emissions from mobile sources: NO_x performance



	Group	<20km	20 – 100km	>100km
NO_x	Obs	15.3	4.4	9.0
	Base	17.5	4.5	10.7
	$0.5NO_x$	13.8	3.1	8.2

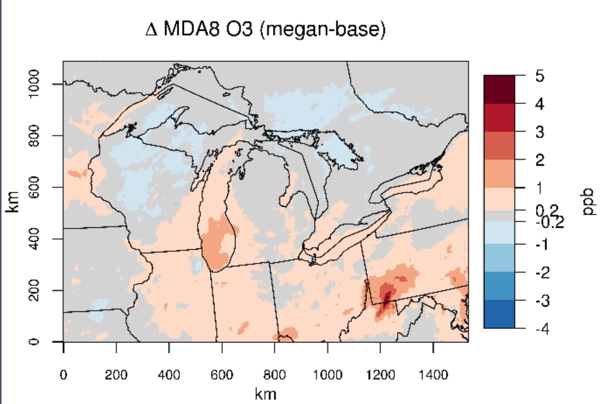
50% NO_x emissions from mobile sources: NO_x performance

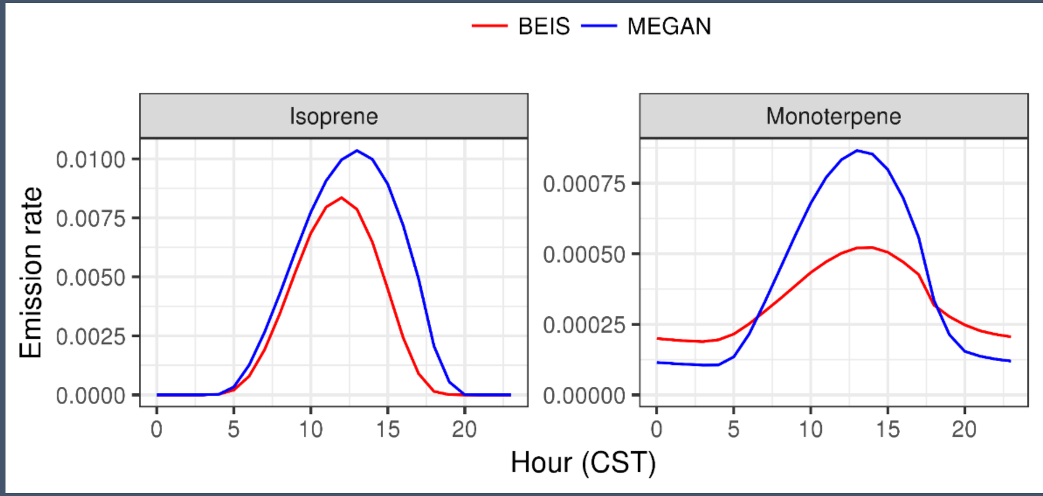


With 50% reduction of NO_x emissions from mobile sources

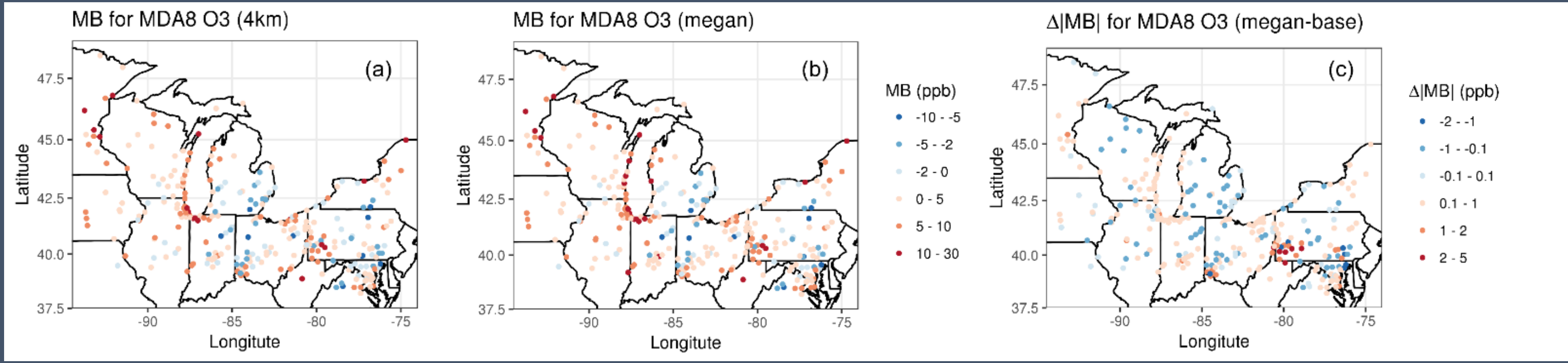
- Better agreement of NO_2, NO_x and NO_y with the observations around sunrise/sunset
- Daytime NO_2 and NO_x tended to be underestimated at urban and suburban sites
- Overestimation of NO_y remained

MEGAN vs. BEIS (cb05)

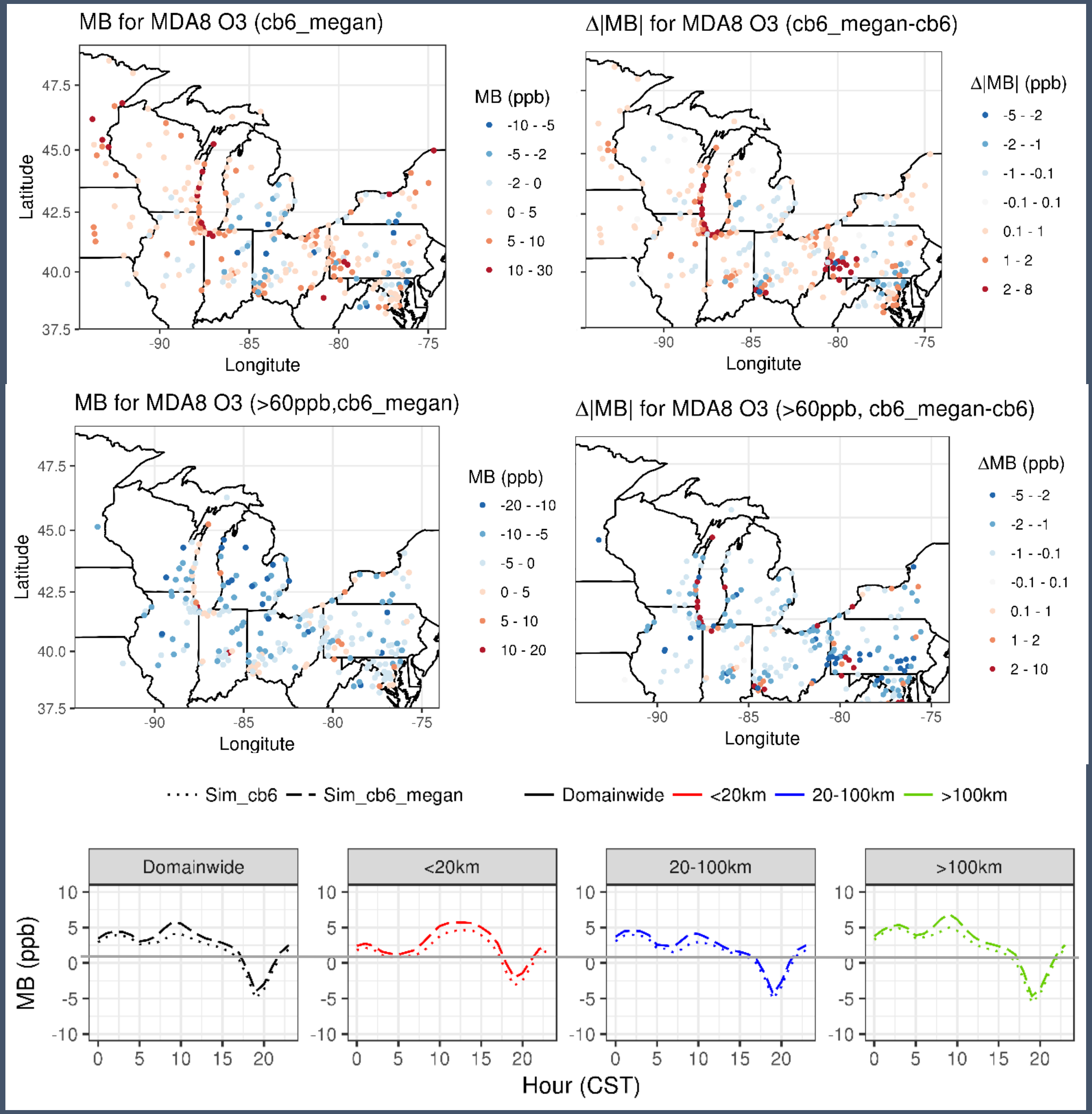


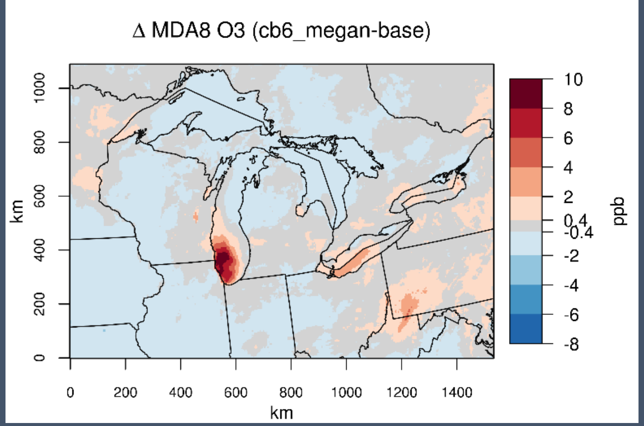


- MEGAN yielded higher emissions of isoprene and monoterpene
- Positive biases of MDA8 O_3 along the Lake Michigan shore and in the urban areas in Pennsylvania, Ohio and Indiana were larger



MEGAN vs. BEIS (cb6)

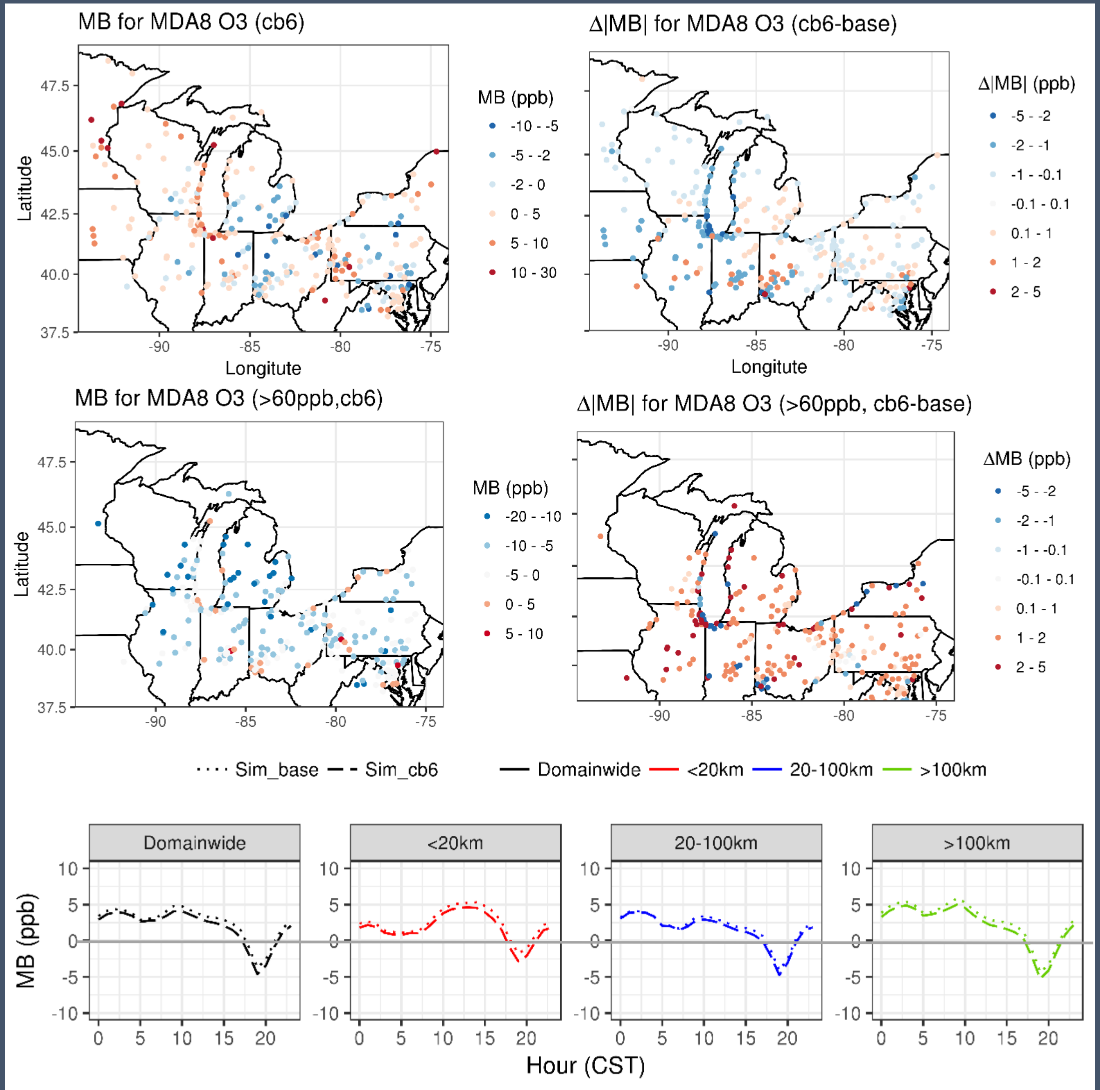


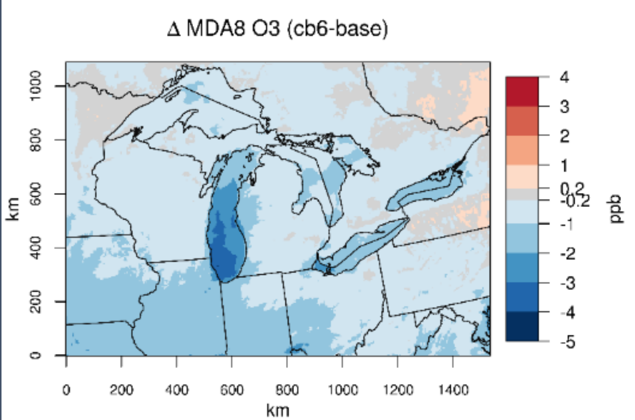


Group		<20km	20 – 100km	>100km
MDA8 O_3	Obs	51.2	50.9	54.1
	Base	56.6	52.5	56.4
	CB6	55.4	51.9	55.5
	CB6_megan	56.9	52.6	56.5
MDA8 O_3 (>60ppb)	Obs	69.1	67.8	68.1
	Base	67.4	61.5	64.7
	CB6	64.9	60.0	63.3
	CB6_megan	67.1	61.1	64.8

- ✓ Base: cb05 + BEIS
- ✓ CB6: cb6 + BEIS

CB6 vs. CB05 (both with BEIS)

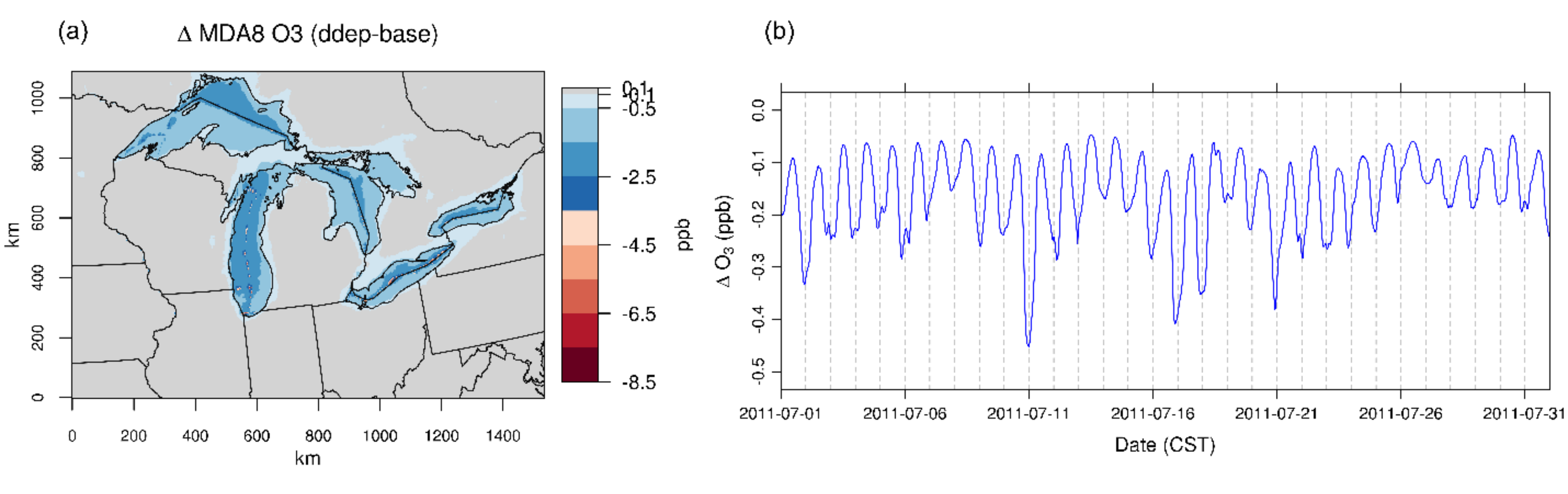




Group		<20km	20 – 100km	>100km
MDA8 O_3	Obs	51.2	50.9	54.1
	Base	56.6	52.5	56.4
	CB6	55.4	51.9	55.5
MDA8 O_3 (>60ppb)	Obs	69.1	67.8	68.1
	Base	67.4	61.5	64.7
	CB6	64.9	60.0	63.3
NO_x	Obs	15.3	4.4	9.0
	Base	17.5	4.5	10.7
	CB6	17.6	4.5	10.8

Dry deposition

- **Increase dry deposition of O_3 over fresh water by a factor of ten**

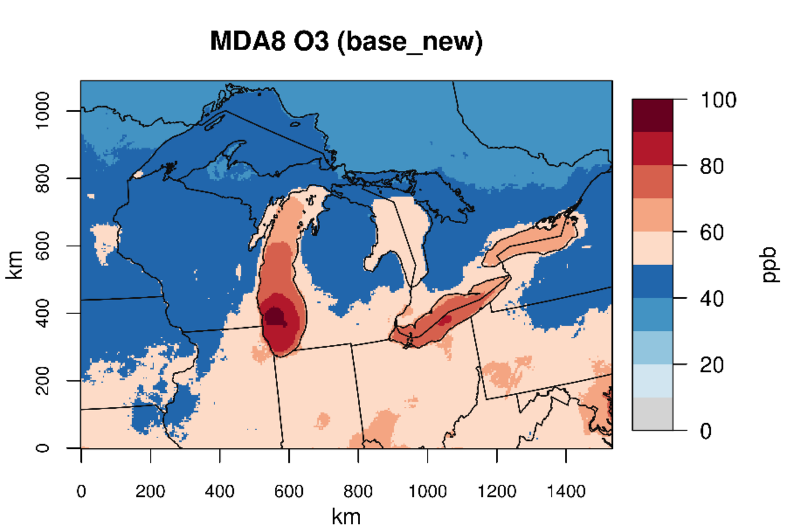


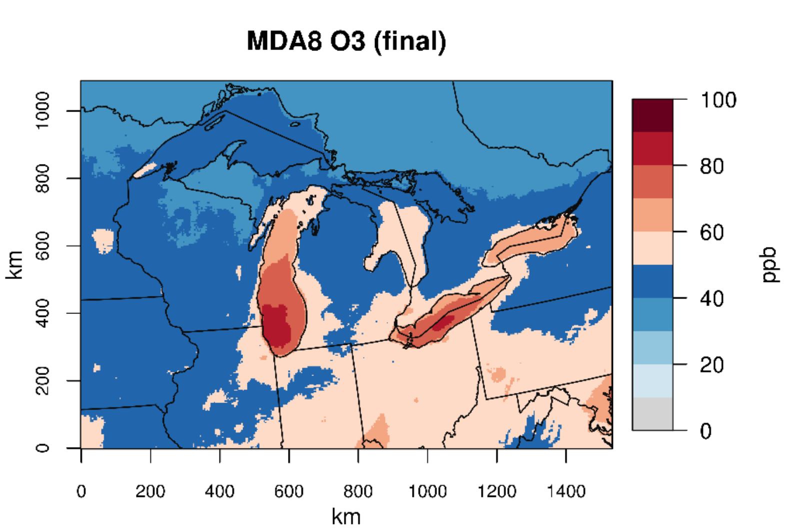
- Reductions of MDA8 O_3 in the range 0.5-2.5 ppb over the lakes
- Negligible influence on surface O_3 over coastal areas

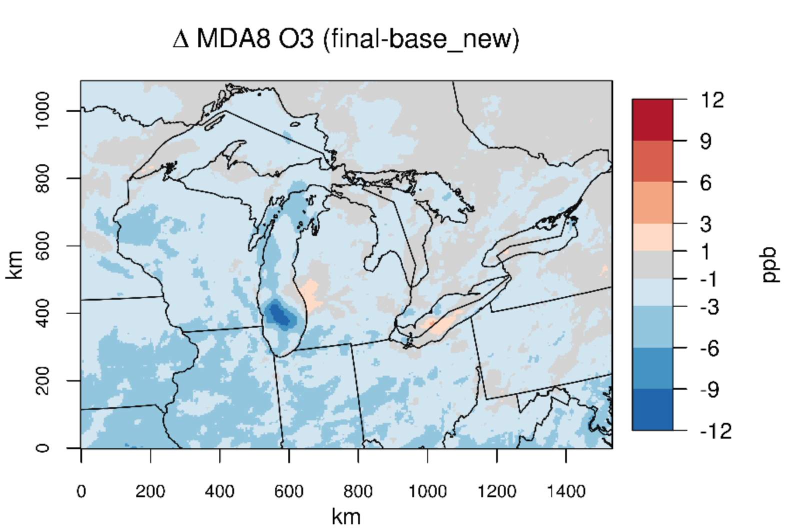
Final simulation (12 km & 4 km)

- **Meteorology**
  - Nudging above 2 km instead of above the PBL
- **Emissions**
  - Biogenic emissions from MEGAN
  - 30% reduction of NO_x emissions from mobile sources
  - Updated emissions from sectors including afdust, othafdust, onroad using new meteorology
- **Mechanism**
  - Cb6 instead of cb05

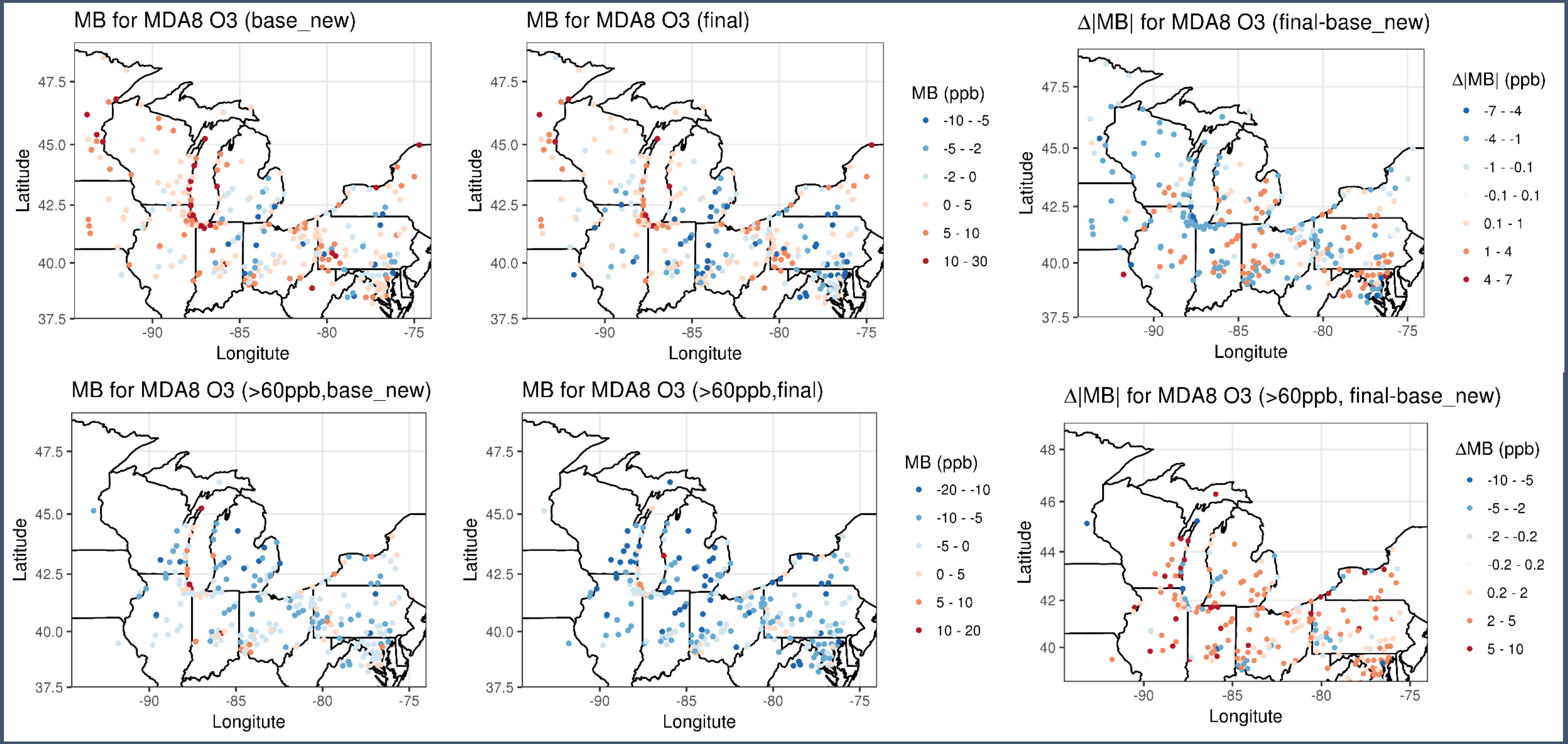
Final simulation: O_3 performance





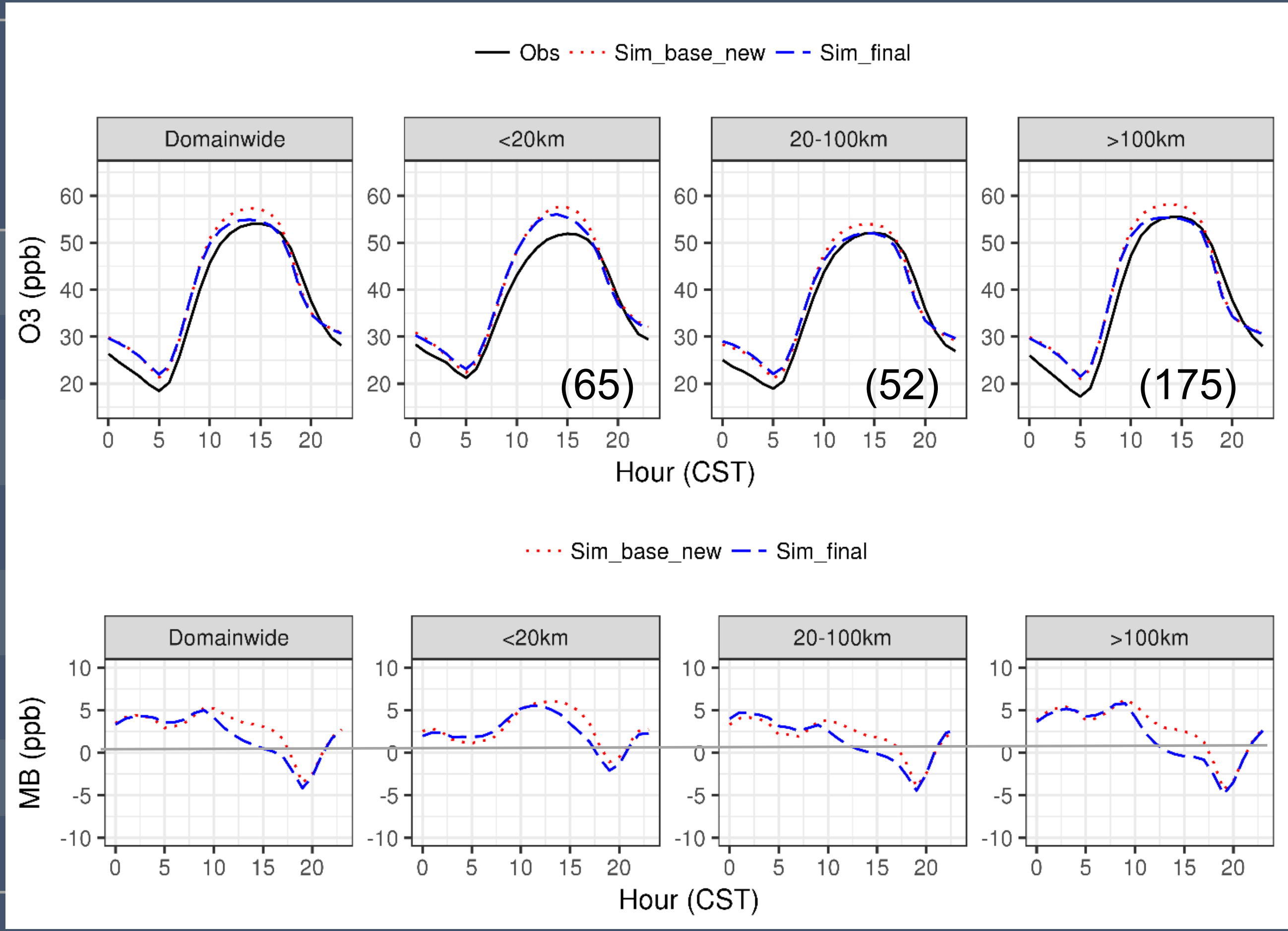


Final simulation: O_3 performance



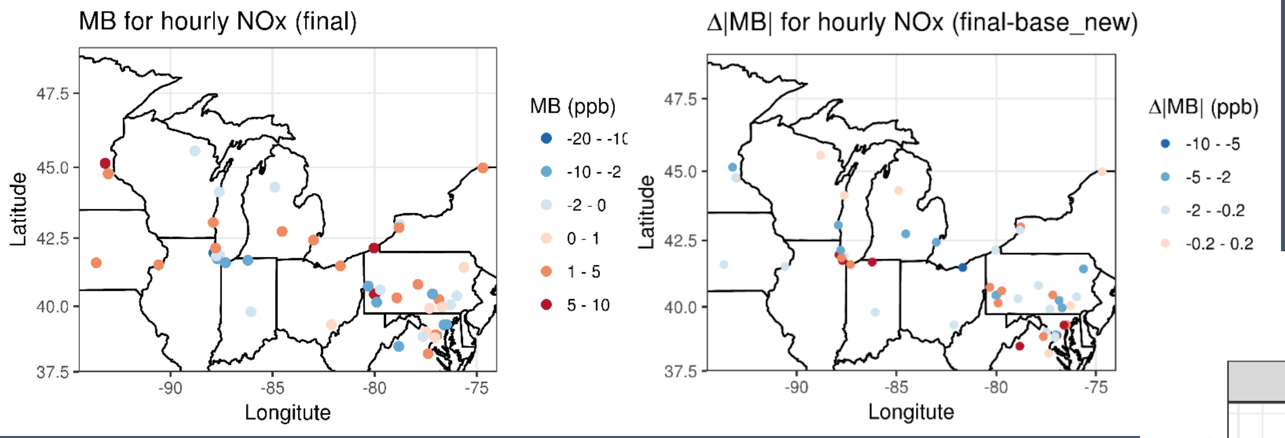
Final simulation: O_3 performance

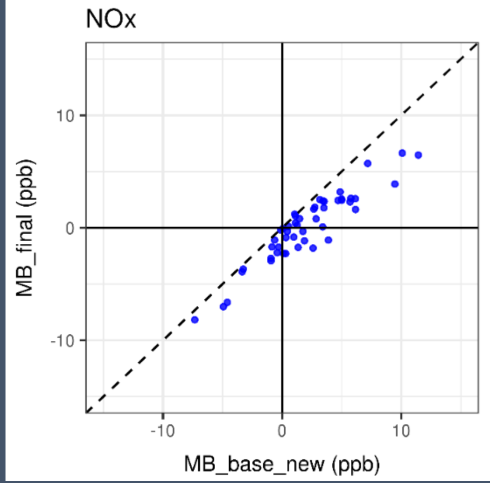
Group		<20km	20 – 100km	>100km
MDA8 O_3	Obs	51.2	50.9	54.1
	Base_new	57.5	52.7	56.5
	Cb6_megan	56.9	52.6	56.5
	Final	55.7	50.9	54.1
MDA8 O_3 (>60ppb)	Obs	69.1	67.8	68.1
	Base_new	68.8	61.9	64.9
	Cb6_megan	67.1	61.1	64.8
	Final	65.7	58.6	62.0



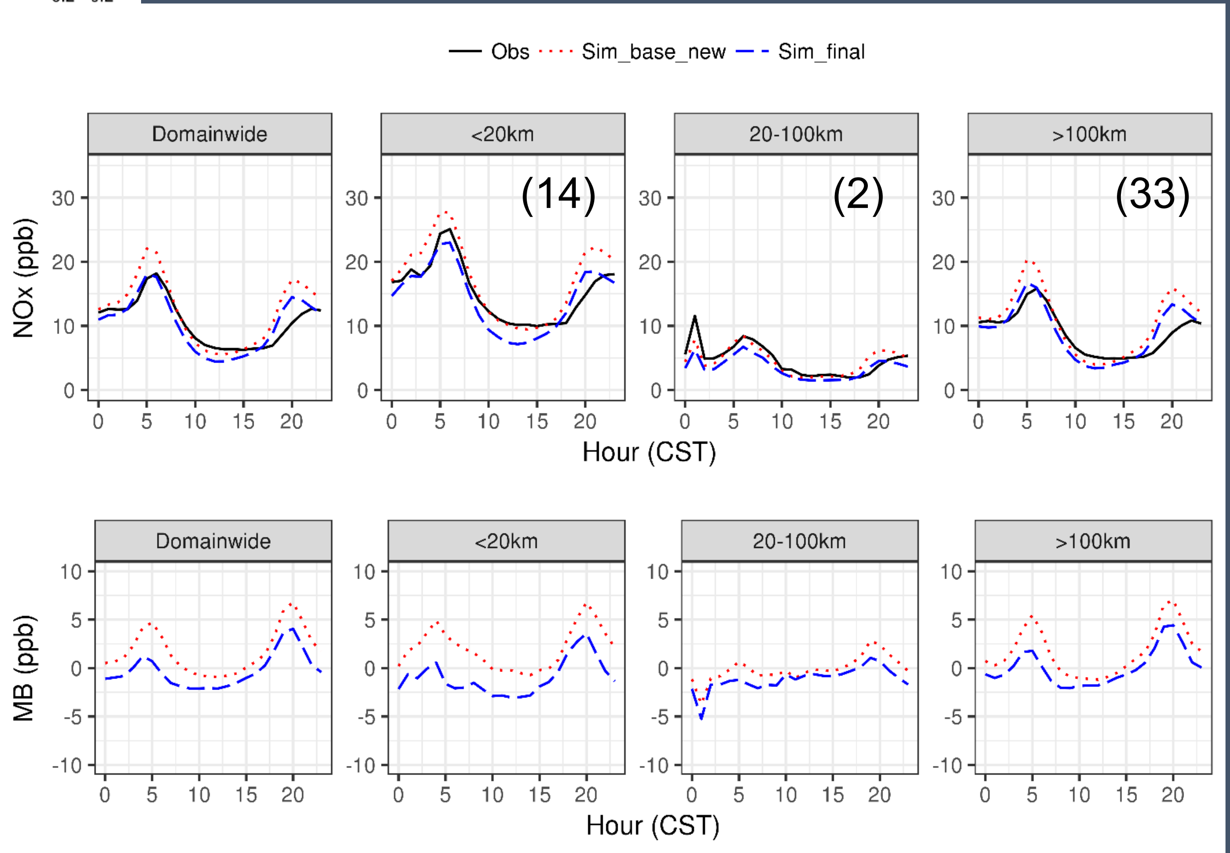
- ✓ Cb06_megan vs. base_new (cb05 + BEIS)
- ✓ Final (30% NOx reduction + nudging above 2km) vs. Cb06_megan

Final simulation: NO_x performance



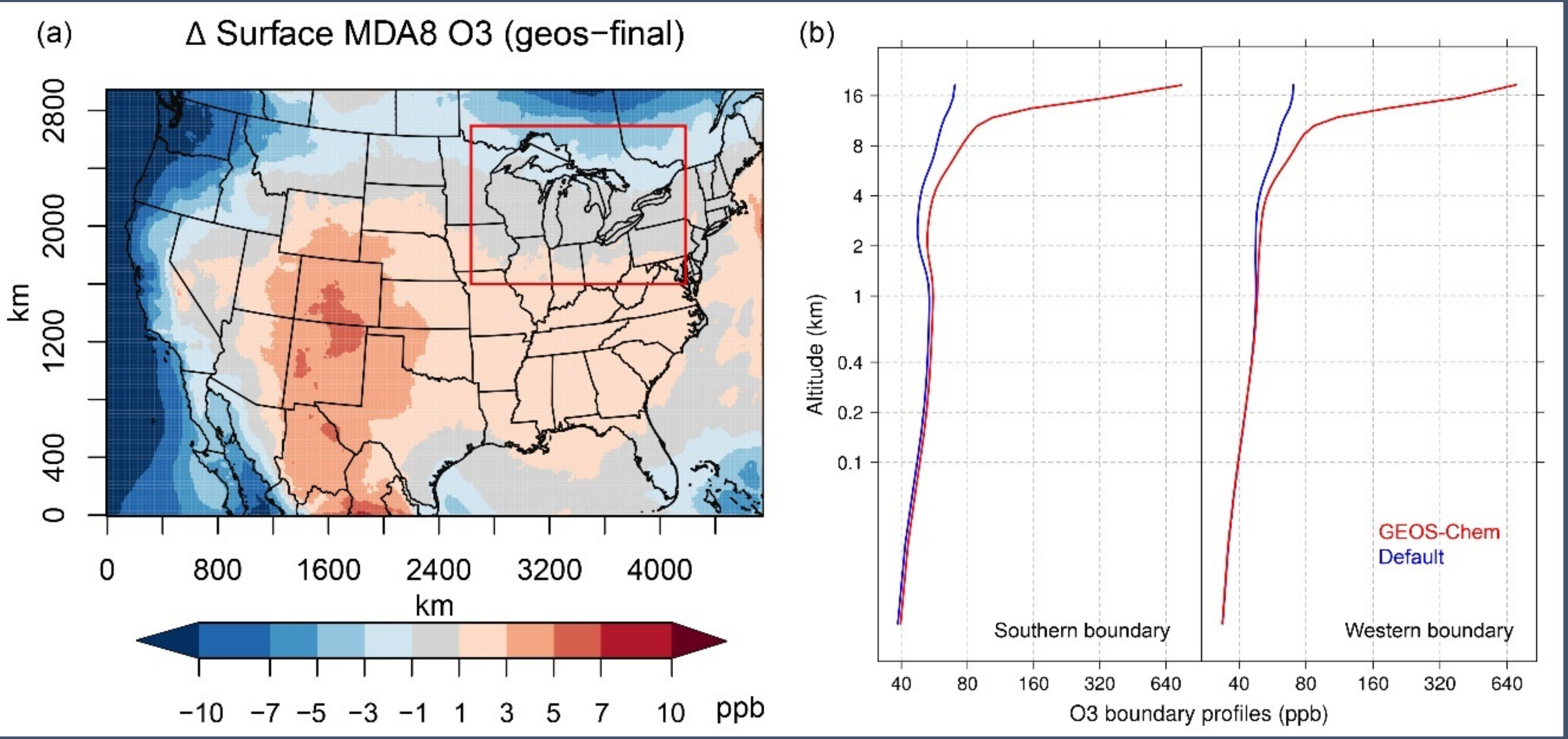


Group		<20km	20 – 100km	>100km
NO_x	Obs	15.3	4.4	9.0
	Base_new	17.3	4.5	10.7
	$0.5NO_x$	13.8	3.1	8.2
	Final	14.3	3.4	9.1



GEOS-Chem vs. Default Boundary Conditions

- Lateral boundary conditions do not affect surface O_3 in the Midwest in July 2011.



Conclusions

Baseline

- Higher MDA8 O_3 simulation against observation
  - ~10% in the coastal areas and 5% in the inland areas
  - After midnight and in the afternoon
- Elevated MDA8 O_3 (larger than 60ppb) was biased low
- NO_x was biased high by 15-20%, especially around sunrise/sunset

Sensitivity tests

- Reduction of NO_x emissions from mobile sources or using CB6 instead of CB05
  - Lower MDA8 O_3 compared to the baseline
  - High biases near the lake significantly decreased
  - Negative biases of MDA8 O_3 > 60ppb became larger
- Using MEGAN instead of BEIS or increasing O_3 dry deposition over fresh water did not improve O_3 simulation

Conclusions

Final Simulation

- 30% of mobile NO_x; MEGAN; cb6; nudging above ~2km
  - Well captured MDA8 O_3 over the domain except coastal area, leading to better agreement with the observations compared to the baseline
  - Lower biases for elevated O_3 (worse than the baseline)
  - Closer to the observations for NO_x

odman@gatech.edu