Improving Ozone Simulations in the Great Lakes Region: Sensitivity to Emissions and Chemistry

Momei Qin[1,*], M. Talat Odman[1], Haofei Yu[1,2], Yongtao Hu[1], Armistead G. Russell[1], Arastoo Pour-Biazar[3], Richard T. McNider[3], and Eladio Knipping[4]

1. Georgia Institute of Technology 2. University of Central Florida 3. University of Alabama at Huntsville 4. Electric Power Research Institute * Now at U.S. Environmental Protection Agency

Background

- Exceedances of ozone (O_3) standards in spite of many years of emissions controls in the Great Lakes Region
- Complex interactions between meteorology (heavily influenced by the presence of the Great Lakes) and emissions from the surrounding large cities (e.g., Chicago)
- It is challenging to fully capture the O_3 dynamics in the region
  - The Community Multiscale Air Quality (CMAQ) model presented positive biases of O_3 (up to 16 ppb) over the water compared to ferry observations (Cleary et al., 2015)

Methodology

Model configurations

- CMAQv5.1 (WRFv3.8.1)
- July 2011
- One-way nested (12 & 4km)
- Base, 4 sensitivity tests and final simulation
- Mechanism (base)
  Cb05e51, with 6th aerosol module
- Emissions (base)
  2011 NEI (Version 6.2 Platform)
  Inline: point sources & BEIS

Fig.1 Modeling domains

Table 1 The base/final simulations and four sensitivity tests

NO.	Case	Biogenic emissions	Mobile NO_x emissions	Chemical mechanism
0	Base	BEIS	100%	CB05
1	Megan	**MEGAN**	100%	CB05
2	0.5NO_x	BEIS	**50%**	CB05
3	CB6	BEIS	100%	**CB6**
4	CB6_megan	**MEGAN**	100%	**CB6**
5	Final	**MEGAN**	**70%**	**CB6**

Results and discussions

Base simulation

Elevated MDA8 O_3 refers to MDA8 O_3 above 60 ppb

- Higher MDA8 O_3 over water than on land
- Compared to measurements on land
  - In general, MDA8 O_3 was overestimated, while elevated MDA8 O_3 (>60ppb) was underestimated (Table 2)
  - Higher positive biases for MDA8 O_3 and lower negative biases for elevated MDA8 O_3 at coastal sites (<20km from shoreline) (Table 2)
  - O_3 diurnal trend: more biased around noon and in the early morning (Fig. 3)
  - NO_x diurnal trend: the biases reached their maxima at about 5:00 and 20:00 CST (Fig. 3)

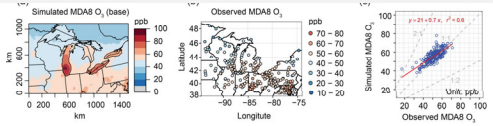


Fig. 2 (a) Simulated MDA8 O_3 in the base case, and (b) Observed MDA8 O_3 at the AQS sites in the Great Lakes Region. (c) Scatter plot of the simulations against observations.

Results and discussions

Table 2 Model performance on MDA8 O_3 without and with a cutoff of 60 ppb in the base and final simulation.

Site	Case	MDA8 O_3 (no cutoff) # of pairs	MB (ppb)	ME (ppb)	MNB (%)	MNE (%)	r^2	MDA8 O_3 (>60 ppb) # of pairs	MB (ppb)	ME (ppb)	MNB (%)	MNE (%)	r^2
Coastal (<20km)	Base	1946	6.3	10.5	16.7	23.2	0.4	555	0.0	10.0	0.4	14.6	0.1
	Final		4.5	10.0	13.6	22.3	0.3		-2.9	10.7	-3.8	15.4	0.1
Buffer (20-100km)	Base	1559	1.8	7.1	6.8	15.4	0.5	382	-5.6	8.2	-8.0	12.0	0.1
	Final		0.0	7.3	3.6	15.4	0.4		-8.7	10.1	-12.5	14.8	0.1
Inland (>100km)	Base	5113	2.4	7.5	7.4	15.6	0.4	1633	-2.8	7.5	-4.0	11.1	0.2
	Final		0.1	7.4	3.1	15.1	0.4		-5.7	8.8	-8.3	12.9	0.2
All	Base	8618	3.2	8.1	9.4	17.3	0.4	2570	-2.6	8.2	-3.6	12.0	0.2
	Final		1.1	8.0	5.6	16.8	0.4		-5.6	9.4	-8.0	13.7	0.2

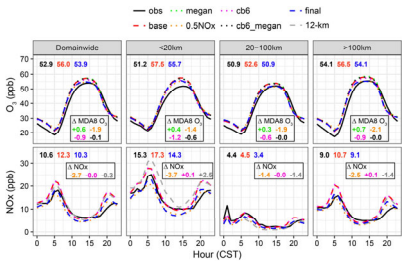


Fig. 3 Diurnal trends of O_3 (top) and NO_x averaged across the domain (Domainwide), at coastal, buffer and inland sites. Monthly means from observations (black), simulations in the base (red) and final (blue) are shown at the top of each panel. Changes in MDA8 O_3 and NO_x in each sensitivity run with respect to the base case are shown in small boxes.

Sensitivity runs (Part 2)

- 50% reduction in emissions from mobile sources (Continued)
  - A distinct impact on peak O_3 concentrations, particularly in buffer/inland areas (containing more rural sites; Fig. 3)
  - Better agreement of simulated NO_x with the observations over the period from 22:00 to 7:00 CST (Fig. 3)
- CB6 instead of CB05
  - The difference reached its maximum (~ 4 ppb) over southern Lake Michigan (Fig. 4)

Sensitivity runs (Part 1)

- MEGAN instead of BEIS
  - Higher emissions with spatial differences in some locations
  - Little changes (± 1 ppb) over a large portion of the domain for MDA8 O_3 (Fig. 4)
- 50% reduction in emissions from mobile sources
  - Domain-wide decrease for MDA8 O_3 (1-4ppb; Fig. 4)
  - Decreases in high biases for MDA8 O_3, e.g. along the lakes (Fig. 5)
  - More biased in locations where MDA8 O_3 was biased low in the base case, which is also the case for elevated MDA8 O_3 (Fig. 5)

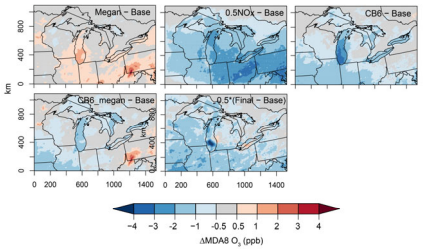
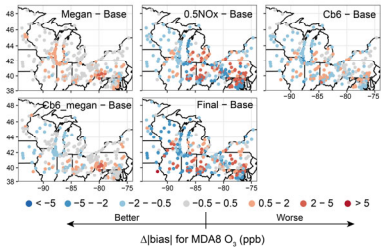


Fig. 4 Changes in MDA8 O_3 for each sensitivity run with respect to the base case. Note that the bottom right panel displays half of the changes in the final simulation.



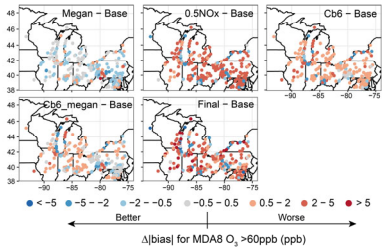


Fig. 5 Changes in absolute mean bias (MB) for MDA8 O_3, without (left) and with a cutoff of 60ppb (right) in each sensitivity run compared to the base case.

Results and discussions

Sensitivity runs (Part 3)

- CB6 instead of CB05 (Continued)
  - Changes in biases of the simulation with CB6 compared to the base case were mixed across the domain, with worse performance for elevated MDA8 O_3 (Fig. 4)
  - Similar to the effect of reducing NO_x emissions while less significant (Fig. 5)
- CB6 & MEGAN instead of CB05 & BEIS
  - O_3 on land was mostly unchanged compared to the base case

Final simulation

- Compared to the base case
  - Significant decrease of O_3, i.e., ~10 ppb over southern Lake Michigan, along with 4-6 ppb in a large part of the southern domain (Fig. 4)
  - ~60% of the sites within the domain showed improvements in simulated MDA8 O_3 and NO_x, except low biases being larger for elevated MDA8 O_3 (Fig. 5)
  - Overall MB decreased from 3.2 to 1.1 ppb for MDA8 O_3, while underestimation of elevated MDA8 O_3 remained (-5.6 ppb compared to -2.6 ppb)

Conclusions

- The base simulation overestimated MDA8 O_3 in the Great Lakes Region (e.g., by ~6 ppb at coastal sites) while elevated MDA8 O_3 (i.e., >60ppb) was biased low
- Using CB6 or 50% reduction of NO_x emissions from mobile sources led to substantial domain-wide decreases in O_3 from the base case (improvements of MDA8 O_3 along the Lake Michigan shoreline, but elevated MDA8 O_3 was more biased)
- Using MEGAN instead of BEIS had minor impacts on O_3
- Using CB6 combined with MEGAN and a 30% reduction of mobile NO_x emissions led to the best performance of MDA8 O_3 and NO_x as well (not the case for elevated MDA8 O_3)

Acknowledgements

This research was funded by the Electric Power Research Institute grant number 10005953 and the National Aeronautics and Space Administration (NASA) Applied Sciences Program grant number NNX16AQ29G.

References

Cleary, P., Fuhrman, N., Schulz, L., Schafer, J., Fillingham, J., Bootsma, H., McQueen, J., Tang, Y., Langel, T., McKeen, S., 2015. Ozone distributions over southern Lake Michigan: comparisons between ferry-based observations, shoreline-based DOAS observations and model forecasts. Atmospheric Chemistry and Physics 15, 5109-5122.