

# High resolution CMAQ simulations of ozone exceedance events during the Lake Michigan Ozone Study

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**Abstract:** We evaluate two high-resolution Lake Michigan air quality simulations during the 2017 Lake Michigan Ozone Study campaign. These air quality simulations employ identical chemical configurations but use different input meteorology. The “AP-XM” configuration follows EPA recommended modeling practices, whereas the “YNT\_SSNG” employs different parameterization schemes and satellite-based inputs of sea surface temperatures, green vegetative fraction, and soil moisture and temperature. Overall, we find similar performance in model simulations of hourly and daily 8-hour maximum (MDA8) ozone, with the AP-XM and YNT\_SSNG simulations showing biases of -11.42 and -13.54 ppbv, respectively during periods when the observed MDA8 was greater than 70ppbv. However, for the two monitoring sites that observed high ozone events, the AP-XM simulation better matched observations at Chiwaukee Prairie and the YNT\_SSNG simulation better matched observations at Sheboygan KA. We find differences between the two simulations are largest for column amounts of ozone precursors, particularly NO<sub>2</sub>. Across three high ozone events, the YNT\_SSNG simulation has a lower column NO<sub>2</sub> bias ( $0.17 \times 10^{15}$  molecules/cm<sup>2</sup>) compared to the AP-XM simulation ( $0.31 \times 10^{15}$  molecules/cm<sup>2</sup>). The YNT\_SSNG simulation also has an advantage in better capturing the structure of the boundary layer and lake breeze during the June 2 high ozone event, although the timing of the lake breeze is about 3 hours too early at Sheboygan. Our results are useful in informing an air quality modeling framework for the Lake Michigan area.

## 1. Introduction

Ground-level ozone has many well-documented effects on human health, including increased risk for respiratory and cardiovascular diseases, and even premature death (Di et al., 2017; Lelieveld et al., 2015; Manisalidis et al., 2020). Ozone also damages plant tissue, affecting crop health (e.g. Clifton et al., 2020; Shindell et al., 2012). Ground-level ozone is formed by photochemical reactions between nitrogen oxides (NOx) and volatile organic compounds (VOCs); major NOx sources include fuel combustion, biomass burning, soil microbes, and lightning, with anthropogenic sources dominant (Hall et al, 1996; Juncosa Calahorrano et al., 2021; Lamsal et al., 2010; Lawrence and Crutzen, 1999; Nault et al., 2017), major sources of VOCs include industrial processes and natural sources, such as trees (Guenther et al., 1995; He et al., 2019).

Since the first National Ambient Air Quality Standard (NAAQS) for ozone was released in 1979, most lakeshore counties in the states bordering Lake Michigan (Wisconsin, Illinois, Indiana, and Michigan) have been designated as being in nonattainment for surface ozone in one or more of the subsequent NAAQS revisions. These states are required by the Clean Air Act to develop State Implementation Plans (SIPs) to demonstrate strategies to bring affected areas into attainment and to mitigate the impacts of high ozone concentrations. Large decreases in local emissions of ozone precursors have steadily reduced one- and eight-hour maximum ozone concentrations across the region in recent decades (Adelman 2020). However, the implementation of stricter ozone NAAQS, along with increases in susceptible

48 populations (e.g. Daggett et al., 2000), means that additional air quality modeling assessments are necessary to help  
49 states demonstrate that they can reach attainment by the required statutory deadlines.

50  
51 The areas along the Lake Michigan shoreline are susceptible to high ozone amounts because of a combination of  
52 abundant precursor emissions and transport processes, particularly the lake breeze circulation. The relationships  
53 between area emissions and meteorology as they impact air quality along the Lake Michigan shoreline have been  
54 characterized in field campaigns (Sexton and Westberg, 1980; Dye et al., 1995; Foley et al., 2011; Stanier et al., 2021),  
55 and the meteorological component is the subject of Part 1 of this study (Otkin et al., 2023). Ozone concentrations  
56 along coastlines can be enhanced significantly when urban emissions react within the shallow, stable, marine boundary  
57 layer (Fast and Heilman, 2003). The lake breeze circulation is particularly important for enhanced ozone production  
58 over Lake Michigan where it contributes to roughly 80% of high ozone episodes observed in eastern Wisconsin  
59 (Lennartson and Schwartz, 2002; Cleary et al., 2021). Lake breeze circulations impact ozone concentrations elsewhere  
60 in the Great Lakes including southern Ontario, Michigan, and Ohio (Makar et al, 2010, He et al., 2011, Brook et al,  
61 2013, Stroud et al, 2020).

62  
63 As highlighted by Dye et al. (1995), there has been a need for a modeling framework that represents the finer scales  
64 of emissions transport and chemistry near the Lake Michigan shoreline. It is our opinion that developing emission  
65 control strategies to mitigate these coastal high ozone events requires accurate prediction of the lake breeze transport  
66 processes at scales of 1-10 km. Furthermore, these chemical transport processes cannot be accurately resolved using  
67 the 12-km resolution meteorological and chemical simulations typically used in air quality modeling for previous  
68 SIPs.

69  
70 We have developed a high-resolution, satellite-constrained meteorological modeling platform for the Midwest United  
71 States that supports the needs of the Lake Michigan Air Directors Consortium (LADCO) as they conduct detailed air  
72 quality modeling assessments for its member states. In part I of this study, Otkin et al. (2023) assessed the impact of  
73 different high-resolution surface datasets, parameterization schemes, and analysis nudging on near-surface  
74 meteorological conditions and energy fluxes relative to the model configuration and input datasets typically employed  
75 by the Environmental Protection Agency (EPA). In part II of this study, we use meteorological output obtained from  
76 two of these simulations, as input to the EPA Community Multiscale Air Quality (CMAQ) model version 5.2.1 (Byun  
77 and Schere, 2006; Nolte et al., 2015) model simulations to assess the impact of these model changes on ozone forecasts  
78 in the Lake Michigan region. The remainder of this paper is organized as follows: Section 2 contains a description of  
79 the CMAQ model configurations and observational data used for evaluation; results are presented in Section 3, with  
80 discussion and conclusions provided in Section 4.

## 81 2. Methods

82 In this work, we compare two CMAQ simulations, one with baseline meteorology, and the other with meteorology  
83 from our optimized WRF configuration, as detailed in Part I (Otkin et al., 2023). Both sets of meteorological  
84 simulations employ a triple-nested domain configuration containing 12-, 4-, and 1.33333 (1.3)-km resolution grids,  
85 respectively (Figure 1 in Otkin et al., 2023), constrained to 6-hourly, 0.25-degree GFS Final analyses and using  
86 RRTMG longwave and shortwave radiation (Iacono et al. 2008; Mlawer et al. 1997) on all three domains, the Kain-  
87 Fritsch cumulus scheme (Kain 2004) on the outer two domains, and explicit convection on the innermost domain.  
88 Both simulations have the same vertical resolution throughout, with 6 model layers below 200m, 4 model layers below  
89 100m, and the lowest three layers at ~9, 27, and 55m above ground level. The AP-XM simulation employs the  
90 Morrison microphysics (Morrison et al. 2005), ACM2 PBL (Pleim 2007), and the Pleim-Xu LSM (Gilliam and Pleim  
91 2010; Xiu and Pleim, 2001) parameterization schemes, which are the same schemes used within CMAQ and is  
92 therefore considered our baseline meteorological simulation. Our optimized meteorological modeling platform uses  
93 the YSU PBL (Hong et al. 2006), Noah LSM (Chen and Dudhia, 2001; Ek et al. 2003), and Thompson microphysics  
94 (Thompson et al. 2008, 2016) schemes, constrained by high-resolution (1km) soil moisture and temperature analyses  
95 (Case 2016; Case and Zavodsky 2018; Blankenship et al. 2018) from the Short-term Prediction Research and  
96 Transition Center (SPoRT), daily high resolution (1.3 km) Great Lakes surface temperatures (Schwab 1992) from the  
97 Great Lakes Surface Environmental Analysis (GLSEA), and high resolution (4 km) Green Vegetation Fraction (GVF)  
98 from the Visible Infrared Imaging Radiometer Suite (VIIRS; Vargas et al. 2015) in place of monthly GVF  
99 climatologies. This optimized configuration is hereafter referred to as the YNT\_SSNM. Otkin et al. (2023) found that  
100 the AP-XM configuration generally produced more accurate meteorological analyses on the 12-km domain, but its

101 accuracy decreased with finer model grid resolution. In contrast, the YNT\_SSNG statistics showed consistent  
102 reductions in root-mean-square error (RMSE) for 2-m temperature, 2-m water vapor mixing ratio, and 10-m wind  
103 speed relative to the AP-XM as the model resolution increased from 12 km to 1.3 km. We note that differences in  
104 near surface wind speed and GVF will also impact deposition velocities in the CMAQ simulations.

105  
106 Each CMAQ simulation is run with the same configuration and anthropogenic emissions. Using CMAQv5.2.1  
107 (Appel et al., 2017; US EPA, 2018), our configuration includes "AERO6" aerosol chemistry, the Carbon Bond 6  
108 chemical mechanism revision 3 (CB6r3; Emery et al., 2015; Luecken et al., 2019), and in-line photolysis. CMAQ  
109 was run with 39 vertical layers with a top of approximately 100 hPa, thus using all available layers from our WRF  
110 simulations. As with our WRF simulations, we ran CMAQ on three domains: one using 12 km by 12 km horizontal  
111 resolution over the continental U.S. (396 x 246 grid points), one using 4 km by 4 km horizontal resolution over the  
112 upper Midwest (447 x 423 grid points), and one using 1.3 km by 1.3 km horizontal resolution over Lake Michigan  
113 and nearby areas (245 x 506 grid points). The 12 km CMAQ simulations employ lateral boundary conditions (LBC)  
114 from the global Real-time Air Quality Modeling System (RAQMS) model (Pierce et al., 2007), which includes  
115 assimilation of ozone retrievals from the Microwave Limb Sounder (MLS) and Ozone Monitoring Instrument (OMI)  
116 on the NASA Aura satellite and assimilation of aerosol optical depth (AOD) from the Moderate Resolution Imaging  
117 Spectroradiometer (MODIS) on the NASA Terra and Aqua satellites. Utilizing RAQMS LBC for CMAQ  
118 continental scale simulations has been shown to significantly increase upper tropospheric ozone and improve daily  
119 maximum surface O<sub>3</sub> concentrations (Song et al, 2008) and improve agreement with OMI tropospheric ozone  
120 column (Lee et al, 2012) relative to fixed LBC. The 4-km and 1.3-km simulations employ lateral boundary  
121 conditions from the respective parent grid.

122  
123 Anthropogenic emissions for the 12 km domain were taken from the 2016 National Emissions Inventory Collaborative  
124 (NEIC, 2019), version 1. Anthropogenic emissions for the 4 km and 1.3 km domains were taken from the 2017  
125 National Emissions Inventory, version 1 (US EPA, 2021; Adams, 2020), where emissions on the 4 km domain were  
126 provided by the EPA (Kirk Baker, personal communication), and then interpolated and downscaled by 1/9<sup>th</sup> for use  
127 on the 1.3 km domain. We acknowledge that the use of downscaled 4km emissions will degrade the performance of  
128 the 1.3km simulations, but generating 1.3km area emissions from the Sparse Matrix Operator Kernel Emissions  
129 (SMOKE) programs was beyond the scope of this project. Biogenic emissions were calculated in-line using the  
130 Biogenic Emission Inventory System (BEIS) with the Biogenic Emissions Landuse Database, version 3 (BELD3;  
131 Carlton and Baker, 2011). Meteorologically-sensitive input for biogenic emissions calculations (such as frost dates)  
132 were generated separately for each set of CMAQ simulations using (SMOKE programs. As biogenic emissions are  
133 calculated in-line, they vary among our configurations with differing input meteorology and GVF.

134  
135 We focus on the innermost, 1.3 km domain surrounding Lake Michigan, during the 2017 Lake Michigan Ozone Study  
136 (LMOS) field campaign (Stanier et al., 2021) which occurred from 22 May –22 June 2017. Our chemical evaluation  
137 focuses on ozone and three of its precursors, nitrogen dioxide, formaldehyde and isoprene, in the surface layer and in  
138 the atmospheric column. We employ ozone observations from the Air Quality System (AQS) monitoring network,  
139 using the Atmospheric Model Evaluation Tool (AMET) developed by the EPA. We also utilize nitrogen dioxide (NO<sub>2</sub>)  
140 and formaldehyde (HCHO) in situ observations from an EPA trailer that was deployed at Sheboygan, WI, and NO<sub>2</sub>  
141 and isoprene measurements from the LMOS Zion supersite (Stanier et al, 2021). In situ O<sub>3</sub> and wind observations at  
142 select monitors that were submitted to the LMOS data repository (<https://asdc.larc.nasa.gov/soot/power-user/LMOS/2017>). For column evaluation, we employ observations of column NO<sub>2</sub> and HCHO from the  
143 Geostationary Trace Gas Aerosol Sensor Optimization (GeoTASO; Leitch et al., 2014) instrument taken during LMOS  
144 (Judd et al., 2019).

### 146 3. Results

147 Our model comparison is organized by three time periods. We first evaluate model performance of the AP-XM and  
148 YNT\_SSNG simulations over the entire LMOS period, based on the ozone precursors of NO<sub>2</sub>, HCHO, and isoprene  
149 as well as daily 8-h maximum ozone. Used in the NAAQS for ozone, maximum 8-hour ozone amounts are calculated  
150 as a rolling 8-h average for each day, starting for the period of 7 am to 3 pm local standard time (LST), and ending  
151 with the period of 11 pm to 7 am LST the following day. However, 8-h maximum ozone is strongly influenced by  
152 days with low and moderate ozone concentrations. Though only 5.9% (112) of the 8-hour maximum ozone periods

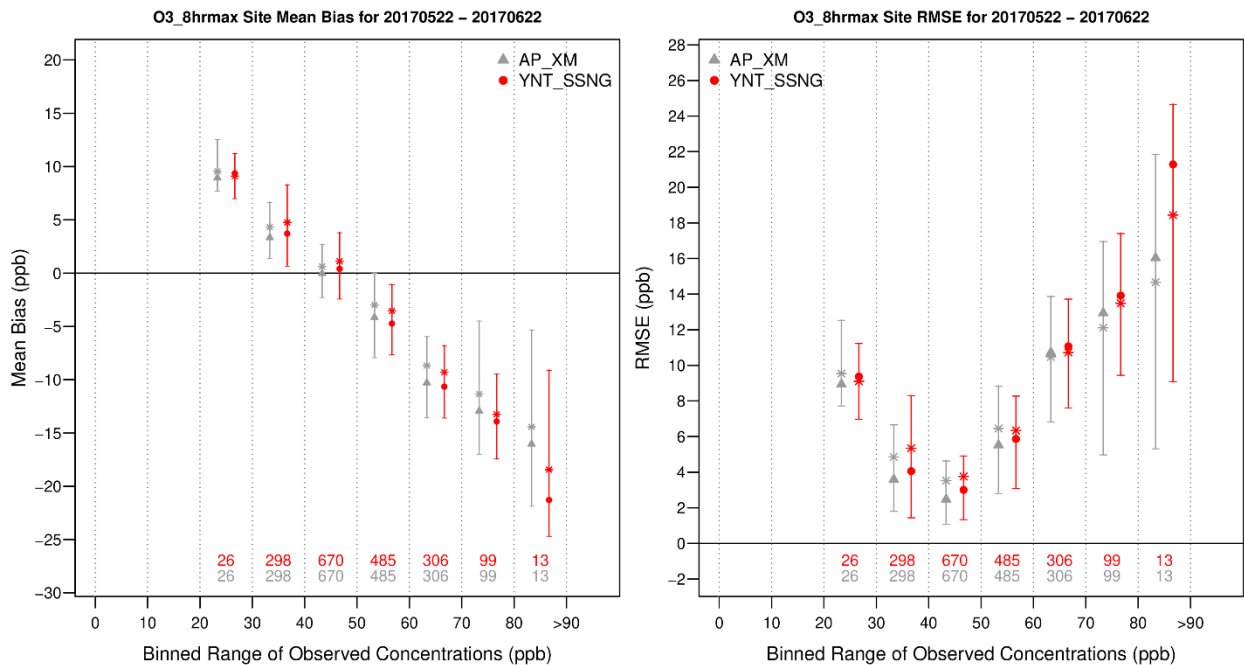
153 within the 1.3 km domain were above the NAAQS threshold for ozone (70 ppbv) during LMOS (see Fig. 1), it is these  
 154 higher 8-h maximum ozone values that are most relevant to SIP modeling.  
 155

156 To evaluate the simulations more precisely, we then evaluate the high ozone days as identified by the two coastal AQS  
 157 monitors that tend to show the highest ozone concentrations. High ozone days with extensive observations during  
 158 LMOS 2017 include: 2–4 June, 9–12 June, and 14–16 June (Abdi-Oskouei et al., 2020) and are referred to as events  
 159 A, B, and C, respectively. Finally, we evaluate model performance over the broader western Lake Michigan shoreline  
 160 area during the only ozone exceedance event on 2 June.

### 161 3.1 Model performance over the entire LMOS period

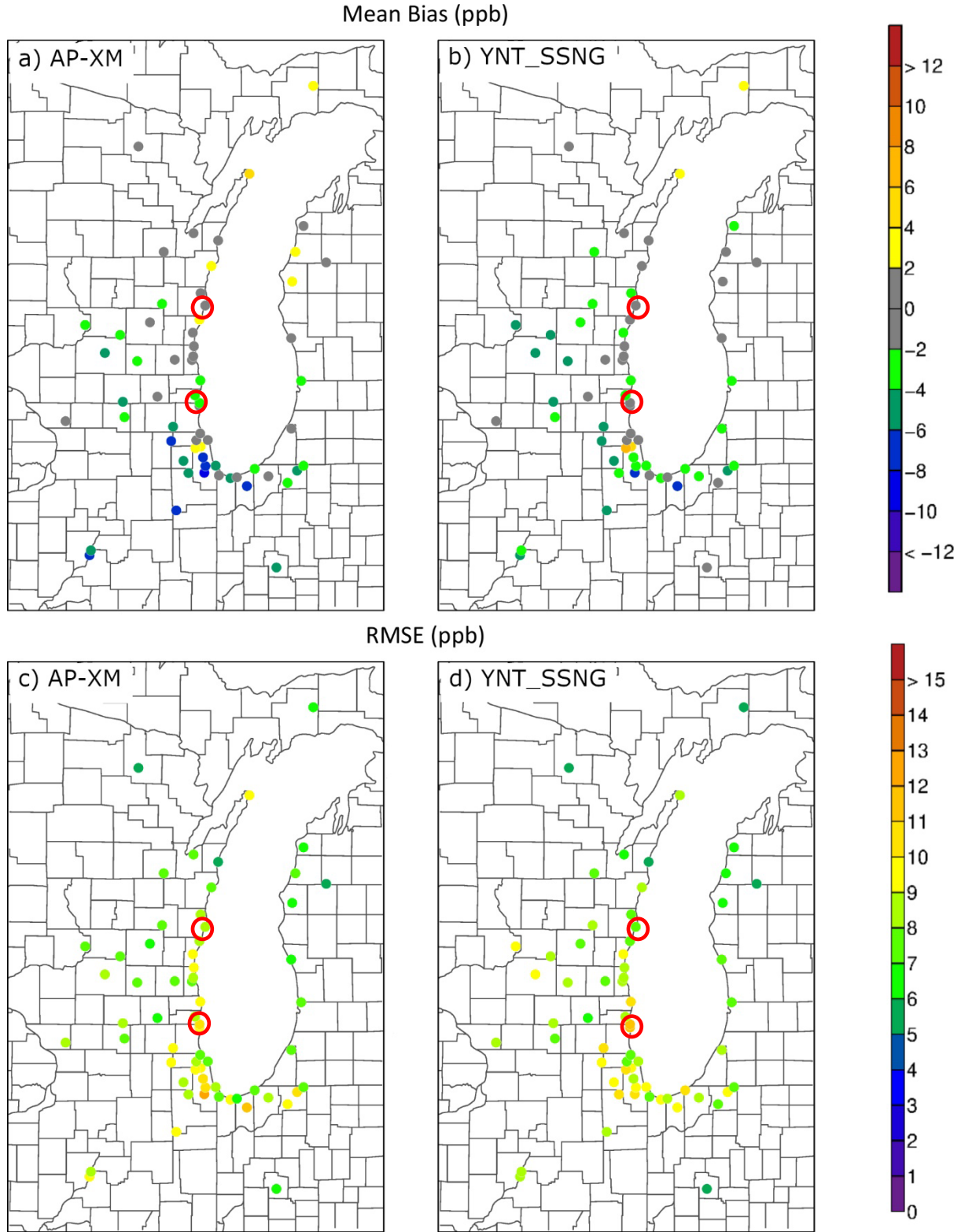
#### 162 3.1.1 8-hour maximum ozone

163 Figure 1 shows binned whisker plots of 8-h maximum ozone bias and RMSE at 10 ppb intervals for the 1.3km  
 164 simulations for all sites within the 1.3km domain. Systematic high biases for lower ozone concentrations (< ~40 ppbv)  
 165 and a low bias for higher ozone concentrations (> 50 ppbv) are evident in both simulations. The YNT\_SSNG and AP-  
 166 XM simulations show similar biases and RMSE for 8-h maximum ozone concentrations between 40-80 ppbv, but the  
 167 AP-XM shows significantly lower biases and RMSE in the 80-90 ppbv bin. Figure 2 shows the geographical  
 168 distribution of 8-h maximum ozone bias and RMSE for the 1.3km AP-XM and YNT\_SSNG for all AQS sites within  
 169 the 1.3km domain. Overall biases are largely negative, reflecting underestimates of 8-h maximum ozone at the AQS  
 170 sites. When compared on a site-by-site basis, the biases and RMSE in 8-h maximum ozone are generally smaller by  
 171 more than 2 ppbv in the YNT\_SSNG simulation with the exception of two AQS sites in North Chicago where the  
 172 YNT\_SSNG simulations shows overestimates of 4-8 ppbv in 8-h maximum ozone. This may be due to the use a more  
 173 realistic, and lower (relative to climatology) Green Vegetation Fraction (see Figure 2 in Otkin et al, 2023) in the  
 174 YNT\_SSNG simulation which would tend to reduce ozone deposition velocities and increase ozone concentrations  
 175 (Ran et al, 2016).  
 176  
 177



178  
 179 **Figure 1. Whisker plots showing the bias (left) and RMSE (right) for binned 8-h maximum ozone concentrations from the**  
 180 **AP-XM (gray) and YNT\_SSNG (red) CMAQ simulations using hourly data within the 1.3km domain during the LMOS**  
 181 **period of record from 22 May 2017 to 22 June 2017. Triangles and circles represent the conditional distribution medians,**  
 182 **stars represent distribution means, and lines and whiskers represent the Q1 to Q3 ranges.**

183



185  
 186 **Figure 2. Geographical distribution of bias (upper panels) and RMSE (lower panels) for binned 8-h maximum ozone**  
 187 **concentrations from the AP-XM (left) and YNT\_SSNG (right) 1.3km CMAQ simulations using hourly data from all**  
 188 **stations in the 1.3 km resolution inner during the LMOS period of record from 22 May 2017 to 22 June 2017. Bias and**

189 RMSE (ppbv) at each site are indicated by the color bar. Two AQS monitors, Sheboygan KA to the north and Chiwaukee  
190 Prairie along the Wisconsin-Illinois border are indicated by the red circles.

191

### 192 3.1.2 Evaluation with Sheboygan WI ground-based NO<sub>2</sub> and HCHO measurements

193 During LMOS, the EPA deployed instruments measuring in-situ NO<sub>2</sub> and HCHO in Sheboygan, WI to characterize  
194 ozone precursors along the shore of Lake Michigan. These 1-min measurements were taken at Spaceport Sheboygan,  
195 which is approximately 9 km north of the Sheboygan, KA monitor highlighted in Figure 2. Here, we use the hourly  
196 averaged EPA NO<sub>2</sub> and HCHO measurements to evaluate the accuracy of prediction of ozone precursors at Sheboygan  
197 for the YNT\_SSNG and AP-XM CMAQ simulations.

198  
199 Figures 3 and 4 show the hourly NO<sub>2</sub> and HCHO comparisons, respectively. There are several periods where observed  
200 NO<sub>2</sub> (black lines, Figure 3) is above 10 ppbv; these periods are generally underestimated by the AP-XM simulation  
201 and overestimated by the YNT\_SSNG simulation (red lines, Figure 3). We find an overall slight positive bias of 0.19  
202 ppbv for the AP-XM and an overall positive bias of 0.68 ppbv for the YNT\_SSNG simulation. We also find that the  
203 correlations are slightly lower and RMS errors are slightly higher in the YNT\_SSNG simulation than in the AP-XM  
204 simulation.

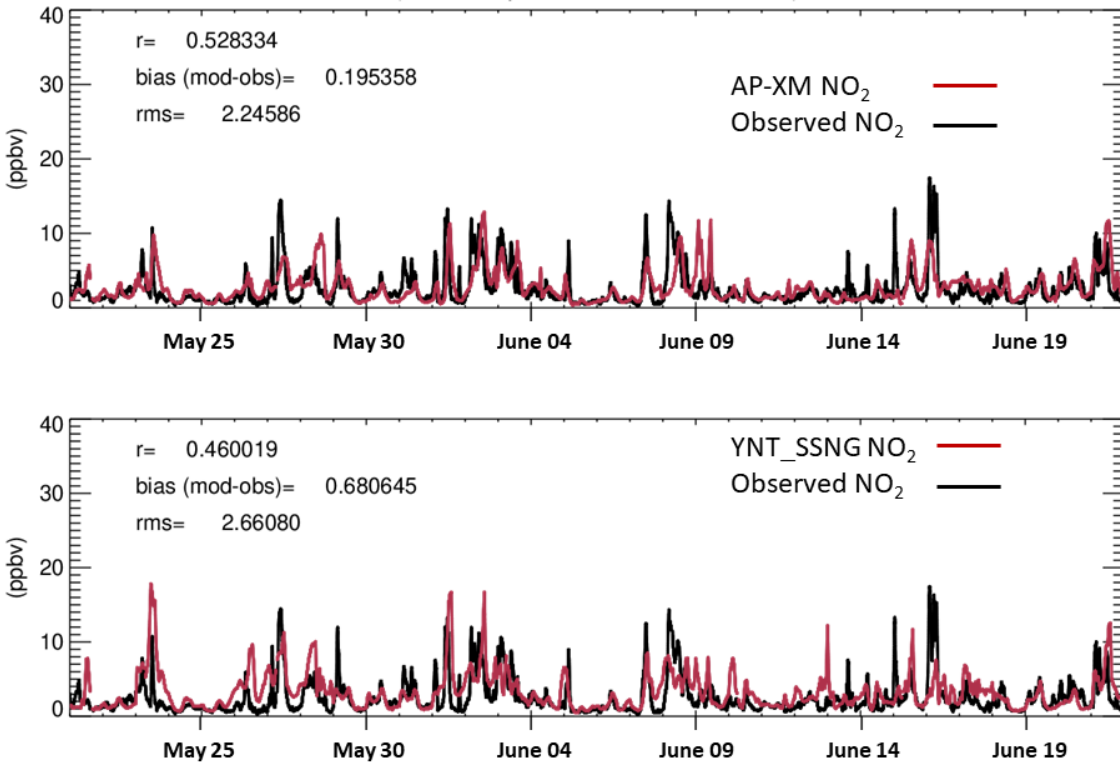
205  
206 Observed HCHO shows peak amounts in excess of 4 ppbv (black lines, Figure 4) which are underestimated in both  
207 simulations (red lines, Figure 4). However, the YNT\_SSNG simulation tends to have overall higher HCHO mixing  
208 ratios than the AP-XM simulation leading to a reduction (-0.26 versus -0.43 ppbv) in the low bias relative to the EPA  
209 measurements. This is in spite of the fact that the YNT\_SSNG uses a more realistic, and lower (relative to climatology)  
210 Green Vegetation Fraction (see Figure 2 in Otkin et al, 2023) which would tend to reduce biogenic VOC emissions.  
211 This suggests that anthropogenic VOC emissions may be playing a role in the reduction of the low biases in the  
212 YNT\_SSNG simulation. Compared to the AP-XM simulation, we also find correlations and RMS errors are slightly  
213 lower in the YNT\_SSNG simulation.

214  
215 The larger high biases in NO<sub>2</sub> and reduced low biases in HCHO in the YNT\_SSNG simulation leads to significant  
216 reductions in high biases in ozone in the YNT\_SSNG compared to the AP-XM simulation (0.07 versus 1.76 ppbv, not  
217 shown) and may be due to more nighttime ozone titration in the YNT\_SSNG simulation.

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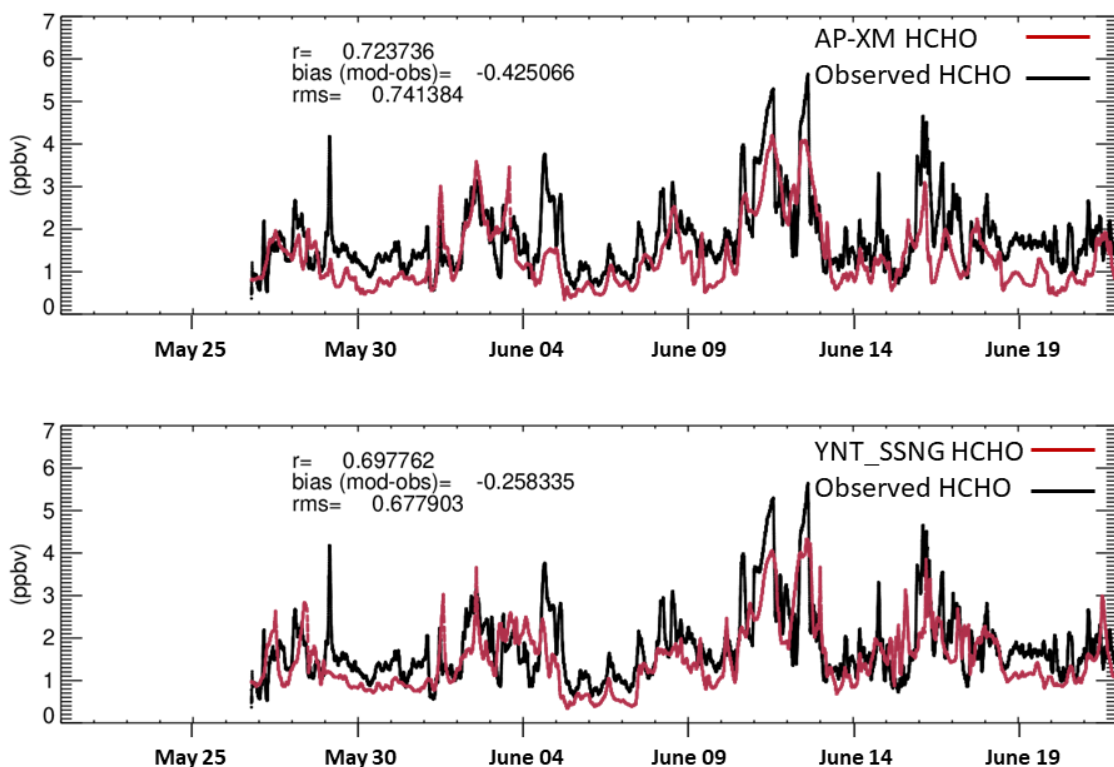
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Figure 3: Timeseries of 1-hour averaged NO<sub>2</sub> at Spaceport Sheboygan for the 1.3km AP-XM (upper) and YNT\_SSNG (lower) CMAQ simulations (red) and EPA observations (black) during the LMOS 2017 time period (May 22-June 21, 2017).



230  
 231 **Figure 4: Timeseries of 1-hour averaged HCHO at Spaceport Sheboygan for the 1.3km AP-XM (upper) and YNT\_SSNG**  
 232 **(lower) CMAQ simulations (red) and EPA observations (black) during the LMOS 2017 time period (May 22-June 21, 2017).**

### 233 3.1.3 Evaluation with Zion IL ground-based NO<sub>2</sub> and isoprene measurements

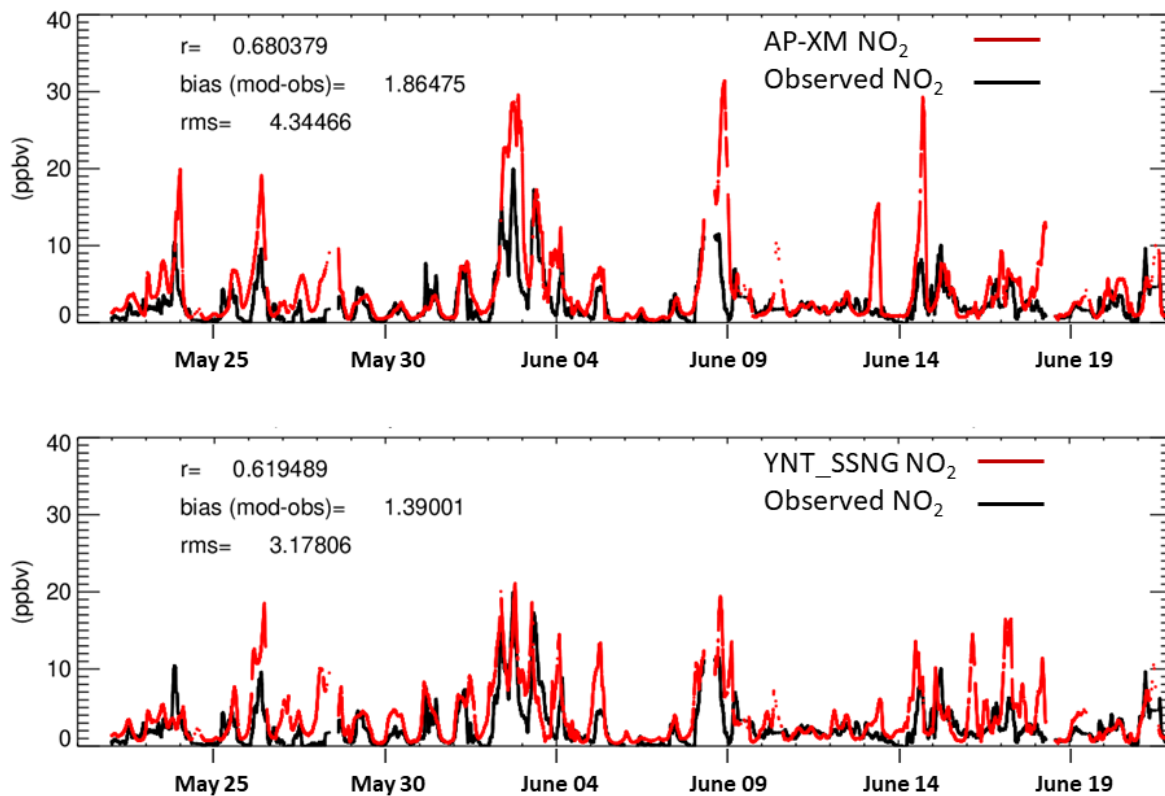
234 During LMOS, the University of Wisconsin deployed a Thermo Scientific NO-NO<sub>2</sub>-NO<sub>2</sub> Analyzer Model 42i  
 235 instrument measuring in-situ NO<sub>2</sub> and the University of Minnesota deployed a Proton-Transfer Quadrupole Interface  
 236 Time-Of-Flight Mass Spectrometer (PTR-QiTOF) measuring isoprene at the LMOS Zion ground site to characterize  
 237 ozone precursors along the shore of Lake Michigan. These 1-min measurements were co-located at the Illinois Air  
 238 Monitoring site (17-097-1007) in Illinois Beach State Park, which is approximately 4 km south of the Chiwaukee  
 239 monitor highlighted in Figure 2. Here, we use the hourly averaged NO<sub>2</sub> and isoprene measurements to evaluate the  
 240 accuracy of prediction of ozone precursors at Zion for the YNT\_SSNG and AP-XM CMAQ simulations.

241  
 242 Figures 5 and 6 show the hourly NO<sub>2</sub> and isoprene comparisons, respectively. There are several periods where  
 243 observed NO<sub>2</sub> (black lines, Figure 5) is above 10 ppbv; these periods are generally overestimated by the AP-XM  
 244 simulation with YNT\_SSNG simulation in much better agreement with observations (red lines, Figure 5). We find an  
 245 overall positive bias of 1.86 ppbv for the AP-XM and an overall positive bias of 1.39 ppbv for the YNT\_SSNG  
 246 simulation. We also find that the correlations are slightly lower and RMS errors are lower in the YNT\_SSNG  
 247 simulation than in the AP-XM simulation.

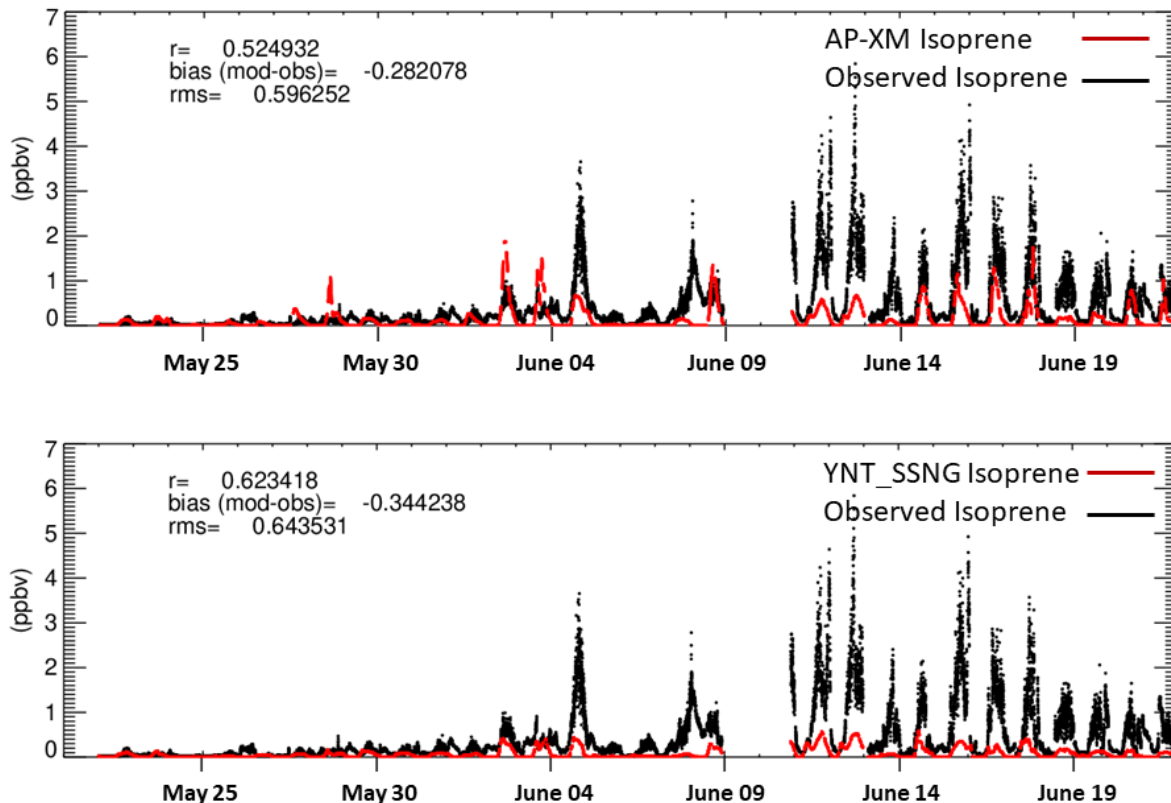
248  
 249 Observed isoprene shows peak amounts in excess of 4 ppbv (black lines, Figure 6) which are significantly  
 250 underestimated in both simulations (red lines, Figure 6). The YNT\_SSNG simulation tends to have overall lower  
 251 isoprene mixing ratios than the AP-XM simulation leading to a larger low bias (-0.34 versus -0.28 ppbv) for the  
 252 YNT\_SSNG simulation relative to the Zion measurements. This is consistent with the use of more realistic, and lower  
 253 (relative to climatology) Green Vegetation Fraction in the YNT\_SSNG simulation (see Figure 2 in Otkin et al, 2023).



254 We also find correlations with observed isoprene are higher and RMS errors are slightly higher in the YNT\_SSNG  
255 simulation.  
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257  
258 **Figure 5: Timeseries of 1-hour averaged NO<sub>2</sub> at Zion for the 1.3km AP-XM (upper) and YNT\_SSNG (lower) CMAQ**  
259 **simulations (red) and observations (black) during the LMOS 2017 time period (May 21-June 22, 2017).**  
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Figure 6: Timeseries of 1-hour averaged isoprene at Zion for the 1.3km AP-XM (upper) and YNT\_SSNG (lower) CMAQ simulations (red) and observations (black) during the LMOS 2017 time period (May 21-June 22, 2017).

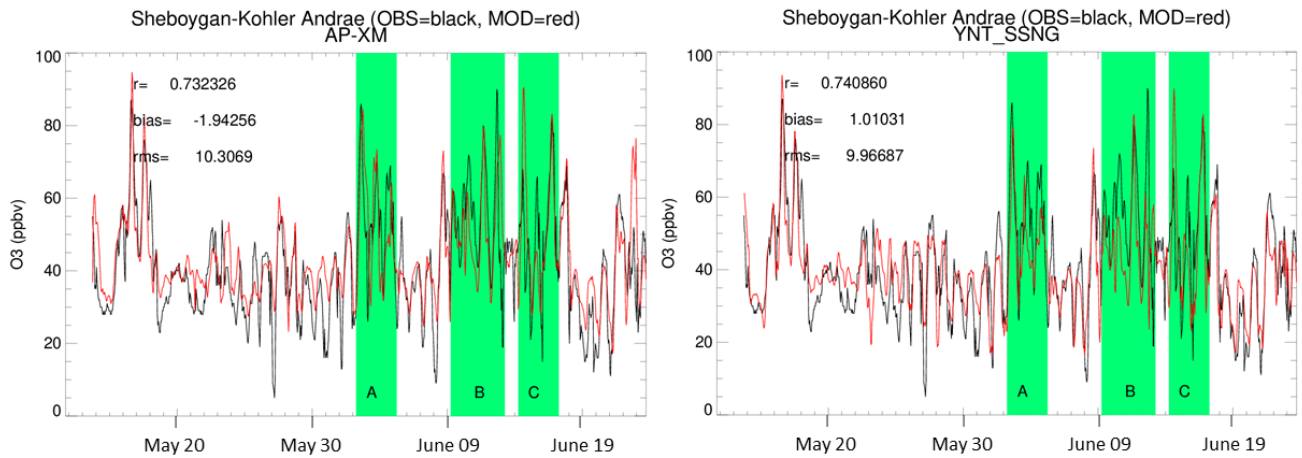
## 266 3.2 Model performance during high-ozone events

### 267 3.2.1 Sheboygan KA and Chiwaukee Prairie 1-hour ozone

268 In this and the following sections, we focus on the two AQS monitors that showed high ozone events during LMOS  
269 most clearly: the Sheboygan Kolher Andrae (KA) monitor (AQS 551170006), located south of Sheboygan, WI, and  
270 the Chiwaukee Prairie monitor (AQS 550590019) is located near the Wisconsin/Illinois border. These two sites are  
271 indicated by red circles in Figure 2.

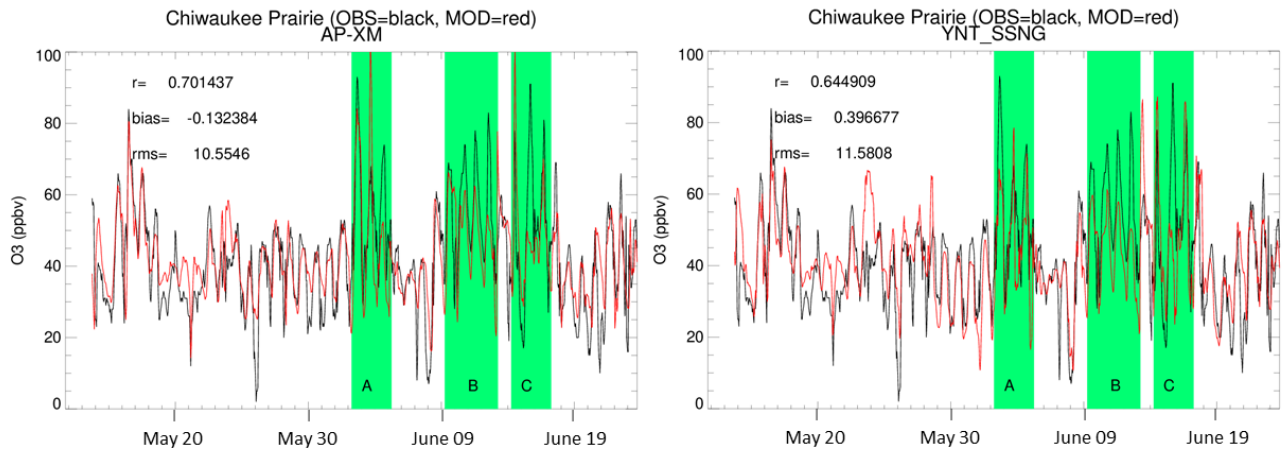
272  
273 Figures 7 and 8 show the hourly AQS observed and CMAQ AP-XM and YNT\_SSNG simulated O<sub>3</sub> for Sheboygan  
274 KA and Chiwaukee Prairie monitors. Comparisons with AQS observations and the two simulations at Sheboygan KA  
275 show similar correlations (0.74 versus 0.73), reduced biases (1.01 versus -1.9 ppbv) and similar RMSE (9.97 versus  
276 10.3 ppbv) for the YNT\_SSNG relative to the AP-XM simulation. Similar comparisons at Chiwaukee Prairie show  
277 decreased correlations (0.64 versus 0.70), higher biases (0.4 versus -0.13 ppbv) and increased RMSE (11.58 versus  
278 11.58 ppbv) for the YNT\_SSNG relative to the AP-XM simulation. Student T-Tests between the AP-XM and  
279 YNT\_SSNG simulations at each site show that the simulations have statistically significant differences (99%  
280 confidence level) in mean ozone concentration at Sheboygan KA but not at Chiwaukee Prairie. While the overall  
281 hourly ozone statistics at Sheboygan KA and Chiwaukee Prairie are relatively similar between the AP-XM and  
282 YNT\_SSNG simulations at these sites, the simulations during high ozone events are quite different. This is illustrated  
283 by looking at composite statistics during events A, B, and C.

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Figure 7: Timeseries of 1-h ozone at Sheboygan-Kohler Andrae AQS monitor (551170006) for the 1.3km AP-XM (left) and YNT\_SSNG (right) CMAQ simulations (red) and AQS observations (black) during the LMOS 2017 time period (May 22- June 21, 2017). The green highlighting shows the periods of high ozone events A, B, and C.



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Figure 8: Same as in Figure 5 but for Chiwaukee Prairie AQS monitor (550590019).

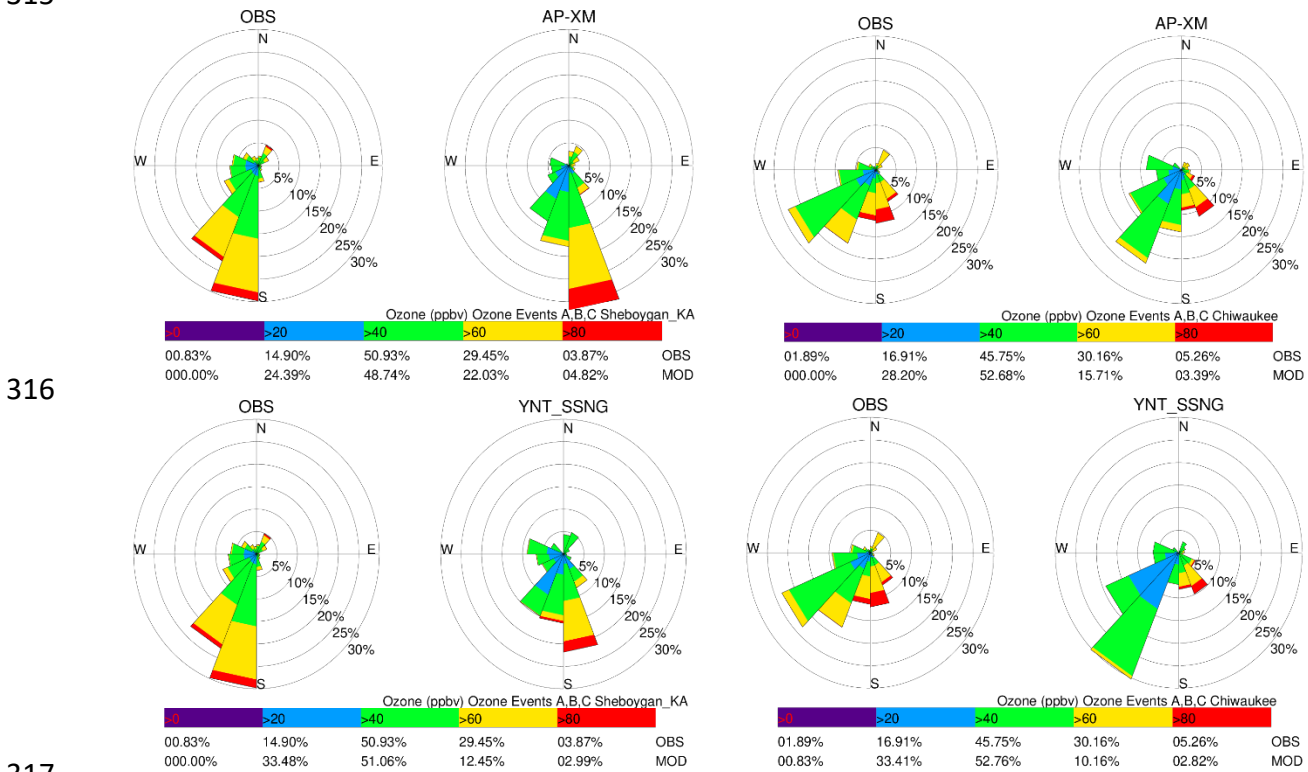
### 294 3.2.2 Composite ozone wind roses during high ozone events A, B, C

295 Figure 9 shows observed and simulated composite ozone wind roses from the 1.3km AP-XM and YNT\_SSNG  
296 simulations at the Sheboygan KA and Chiwaukee Prairie monitors during high ozone events A, B, and C. At  
297 Sheboygan KA, the observed wind direction is most frequently (>50%) from the south-southwest (SSW), which is  
298 also the direction where the majority of the higher (>60ppbv) ozone is observed. The AP-XM simulation predicts  
299 winds which are most frequently (>30%) from the south-southeast (SSE) with the majority of the higher ozone coming  
300 from this direction. The YNT\_SSNG simulation predicts winds which are more variable but also most frequently  
301 (>20%) from the SSE with most of the higher ozone coming from this direction. The overall frequency of higher  
302 ozone in the AP-XM simulation (~27%) is closer to the observed percentage (~33%) than the YNT\_SSNG simulation  
303 (~15%). These comparisons show that the AP-XM meteorology best captures the observed ozone wind rose at  
304 Sheboygan KA during high ozone events.

305

306 At Chiwaukee Prairie the observed winds are more variable and are most frequently (>40%) from the southwest.  
307 While some of the observed higher ozone comes from the southwest, the highest (> 80 ppbv) ozone comes from the  
308 SSE. Both the AP-XM and YNT\_SSNG simulations frequently predict southwest winds (~30% and ~50%,

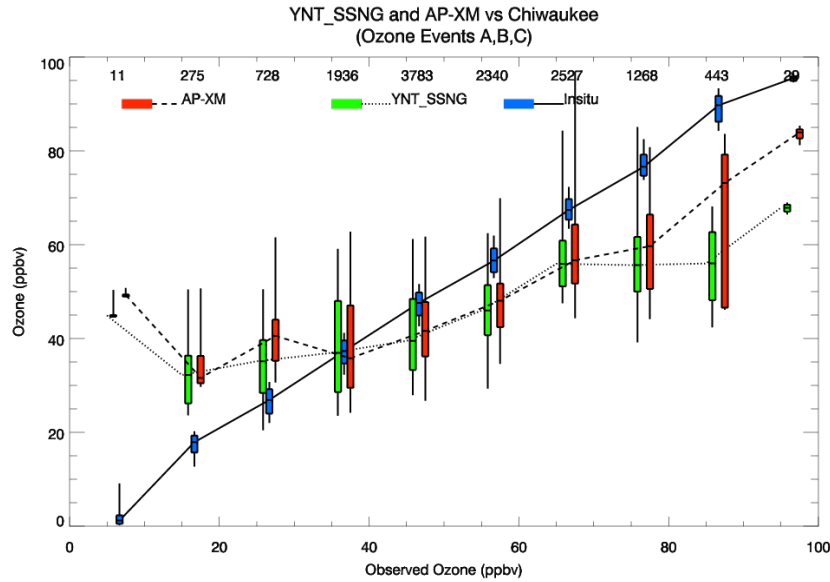
309 respectively) with lower ozone (< 60 ppbv) than observed. Both the AP-XM and YNT\_SSNG simulations show the  
 310 highest ozone coming from the SSE, but the AP-XM simulation more accurately captures the observed percentages  
 311 of high ozone coming from the SSE at Chiwaukee Prairie. The overall frequency of higher ozone in the AP-XM  
 312 (~19%) and YNT\_SSNG (~13%) are both lower than the observed percentage (~35%). These comparisons show that  
 313 the AP-XM simulation best captures the observed ozone wind rose at Chiwaukee Prairie during high ozone events but  
 314 that both simulations have a low bias in ozone when winds are from the southwest.  
 315



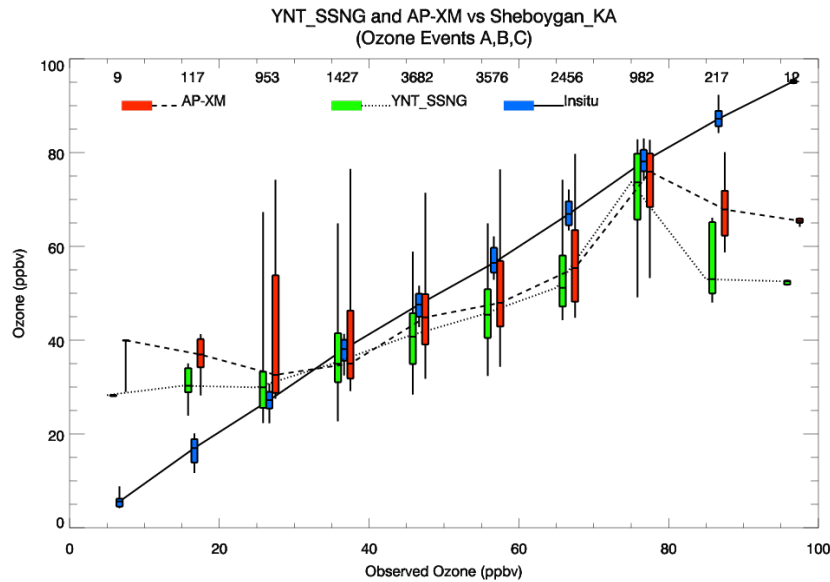
316  
 317  
 318  
 319 **Figure 9: Observed (OBS) and simulated wind roses using 1-h ozone and wind directions at the Sheboygan-Kohler Andrae**  
 320 **AQS monitor (551170006, left columns) and Chiwaukee Prairie AQS monitor (550590019, right columns) for the 1.3km**  
 321 **AP-XM (upper rows) and YNT\_SSNG (lower rows) CMAQ simulations during high ozone events A, B, and C. Wind**  
 322 **directions are divided into 22.5 degree bins and the percentage of winds within each directional bin are indicated by the**  
 323 **percentages on the wind rose plots. The colors within each wind directional bin indicate the distribution of observed and**  
 324 **simulated ozone within 20ppbv bins as indicated by the color bars. The overall percentage of observed (OBS) and simulated**  
 325 **(MOD) ozone within each ozone bin is indicated below the color bar for each site and simulation.**

### 326 3.2.3 1-h ozone concentration and wind direction during high ozone events A, B, C

327 While the ozone wind roses presented above provide a comparison of the joint distribution of simulated and observed  
 328 winds and ozone at these two stations, they do not provide a quantitative estimate of the errors in the simulations. In  
 329 this section we have binned simulated and observed ozone and wind direction to provide a more quantitative  
 330 characterization of the simulated biases. Figure 10 shows bar and whisker plots of 1.3km YNT\_SSNG and AP-XM  
 331 CMAQ ozone simulations and 1-h averaged observed ozone at Chiwaukee Prairie and Sheboygan KA during high  
 332 ozone events A, B, and C. Both simulations show systematic high biases for lower observed ozone concentrations (<  
 333 ~40 ppbv) and low biases for higher ozone concentrations (> 50 ppbv) at both sites. These results are consistent with  
 334 the 8-hour maximum ozone biases for the 1.3km domain wide comparison (Figure 1). The AP-XM simulation shows  
 335 better agreement with observed ozone for the highest ozone (>85 ppbv) at both sites during high ozone events but  
 336 shows a wider spread in the simulated distribution within each of these high observed ozone bins at Chiwaukee Prairie.  
 337 The AP-XM and YNT\_SSNG CMAQ simulations show similar distributions for observed ozone less than 80 ppbv.  
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 339



340  
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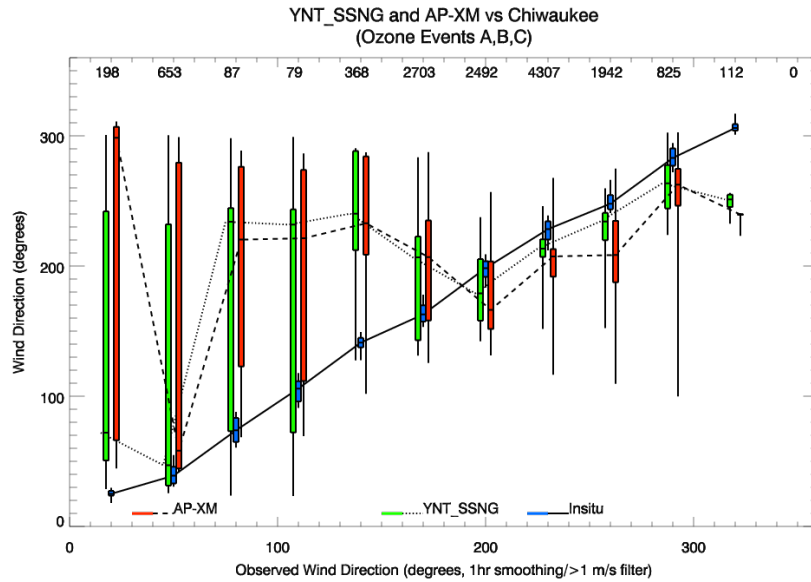


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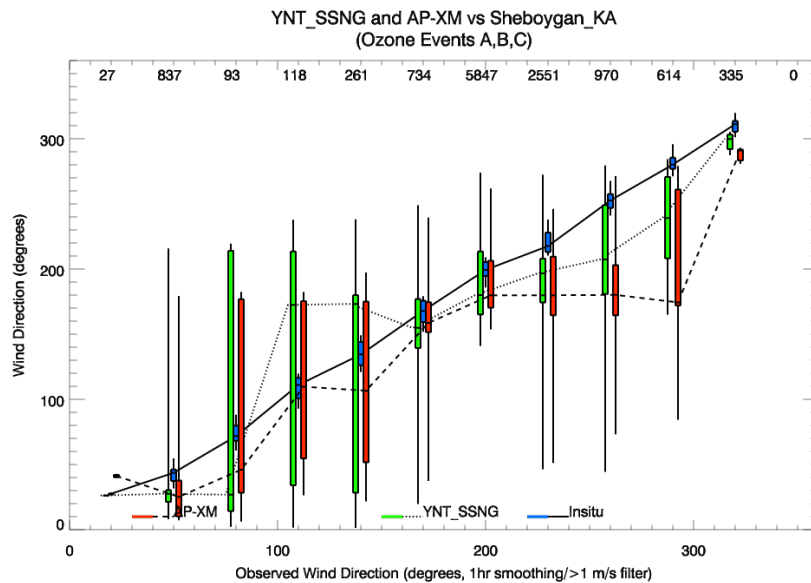
344 **Figure 10. Bar and whisker plots showing the binned median ozone concentrations from the 1.3km AP-XM (dashed) and**  
 345 **YNT\_SSNG (dotted) CMAQ simulations and observed ozone (solid) at Chiwaukee Prairie (upper) and Sheboygan KA**  
 346 **(lower) during high ozone events A, B, and C. The vertical bars show the 50% and the vertical lines show the 95% for the**  
 347 **AP-XM (red) and YNT\_SSNG (green) CMAQ simulations and observed ozone (blue). The total observed count within**  
 348 **each 5 ppbv bin is indicated on the top of each panel.**

349 Figure 11 shows bar and whisker plots of 1.3km YNT\_SSNG and AP-XM CMAQ wind direction simulations and 1-  
 350 h averaged observed wind direction for wind-speeds greater than 1 m/s at Chiwaukee Prairie and Sheboygan KA  
 351 during high ozone events A, B, and C. The 1 m/s threshold was included to reduce the impact of light and variable  
 352 winds at these sites. Both simulations show a large westerly median bias and large variations in wind direction when  
 353 the observed winds have an easterly component (0-180°) at Chiwaukee Prairie. This could be associated with errors  
 354 in the timing of the arrival of the lake breeze, but a more detailed analysis along the lines of Wagner et al, (2022)  
 355 would have to be performed to confirm this. Winds with an easterly component account for 30% of the observed wind  
 356 directions at this site. Both simulations show a smaller easterly bias in median wind direction when the observed  
 357 winds have a westerly component (180-360°) at Chiwaukee Prairie, but the YNT\_SSNG simulation is in better

358 agreement with observations during these periods. The AP-XM simulation shows a small easterly bias when the  
 359 observed winds have an easterly component at Sheboygan KA while the YNT\_SSNG simulation still shows some  
 360 westerly biases in median wind direction for these cases. Both simulations show somewhat larger easterly median  
 361 biases when the observed winds have a westerly component at Sheboygan KA, but the YNT\_SSNG simulation is  
 362 better agreement with observations for these cases.  
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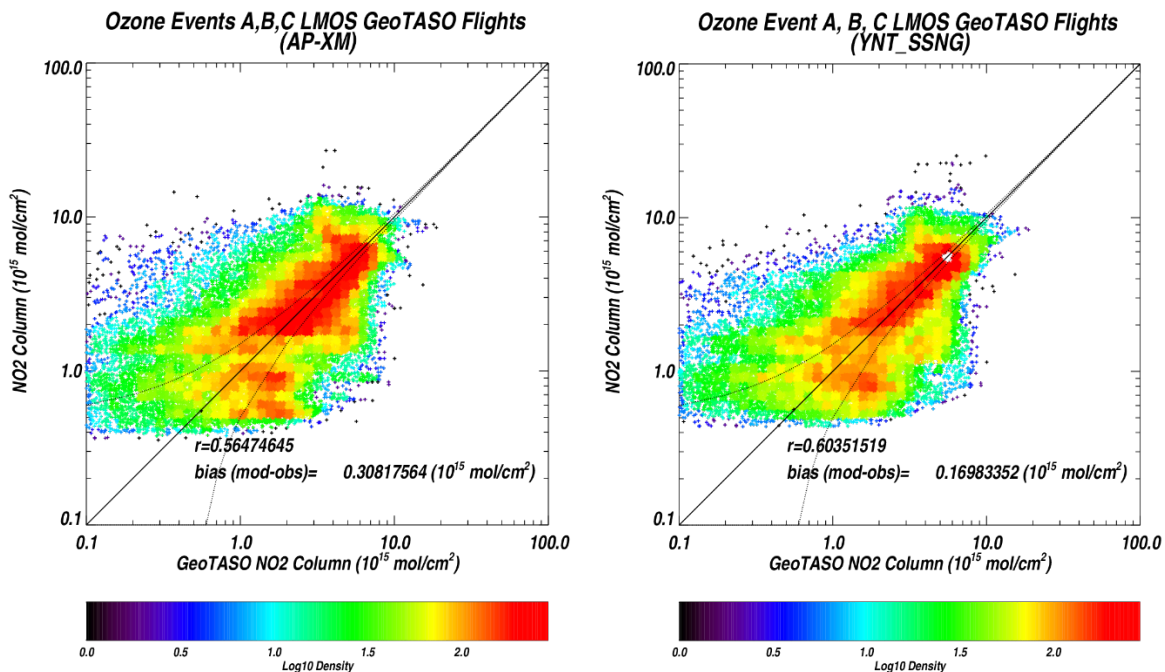


370  
 371 **Figure 11.** Bar and whisker plots showing the binned median wind direction from the 1.3km AP-XM (dashed) and  
 372 YNT\_SSNG (dotted) CMAQ simulations and observed wind direction (solid) at Chiwaukee Prairie (upper) and Sheboygan  
 373 KA (lower) during high ozone events A, B, and C. The vertical bars show the 50% and the vertical lines show the 95% for  
 374 the AP-XM (red) and YNT\_SSNG (green) CMAQ simulations and 1-hour averaged observed wind direction (blue). The  
 375 total observed count within each 20° bin is indicated on the top of the figures.

376 **3.2.4 GEOTASO comparisons during high ozone events A, B, C**

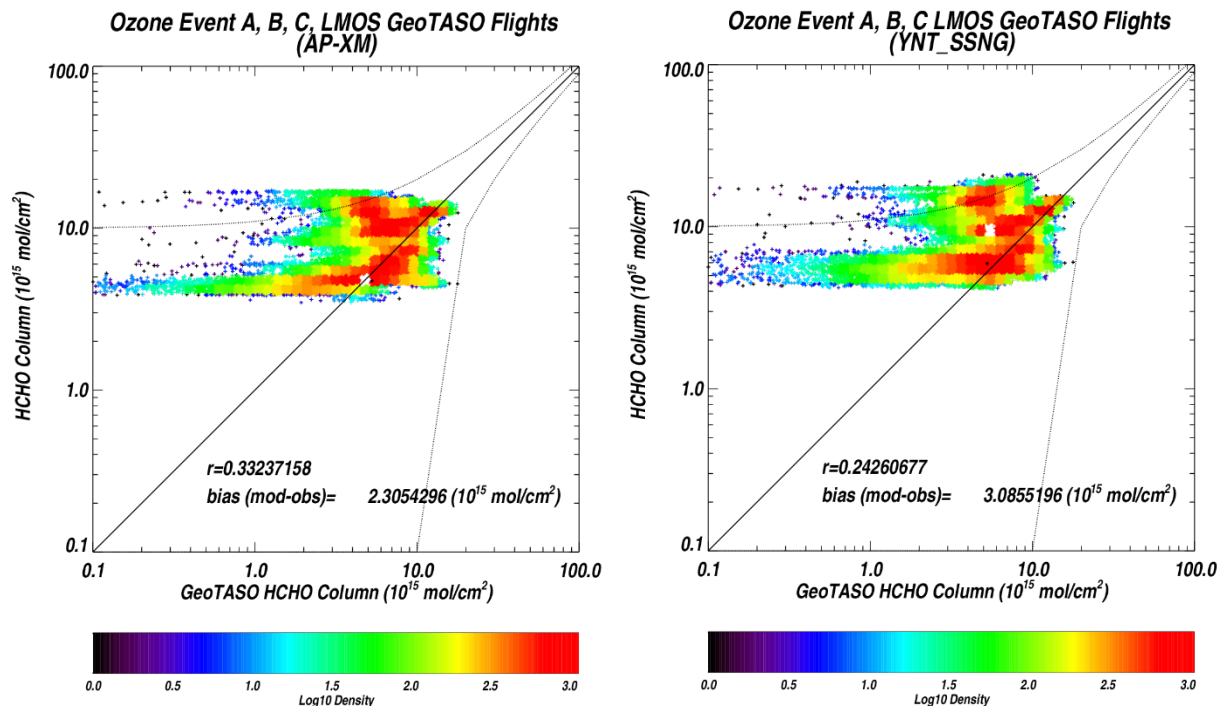
377 Here, we use GeoTASO (Nowlan et al., 2016) NO<sub>2</sub> and HCHO column measurements to verify ozone precursors  
 378 within the YNT\_SSNG and AP-XM simulations during high ozone events A, B, and C. Figure 12 shows the results  
 379 of the NO<sub>2</sub> column analysis. Compared to observed NO<sub>2</sub> column measurements, the YNT\_SSNG and AP-XM  
 380 simulations have similar correlation (0.60 vs. 0.57) and the YNT\_SSNG has a substantially reduced bias (0.17 x 10<sup>15</sup>  
 381 vs. 0.31 x 10<sup>15</sup> mol/cm<sup>2</sup>). Figure 13 shows the results of the HCHO column analysis. Compared to observed HCHO  
 382 column measurements, the YNT\_SSNG has a lower correlation than the AP-XM simulation (0.24 vs. 0.33) and a  
 383 larger bias (3.1 x 10<sup>15</sup> vs. 2.3 x 10<sup>15</sup> mol/cm<sup>2</sup>).  
 384

385 Nowlan et al. (2018) used comparisons between the GEOstationary Coastal and Air Pollution Events (GEO-CAPE)  
 386 Airborne Simulator (GCAS, which is similar to the GeoTASO instrument) NO<sub>2</sub> and HCHO retrievals and columns  
 387 estimated from airborne in-situ NO<sub>2</sub> and HCHO profiles to estimate mean precisions of 1 x 10<sup>15</sup> mol/cm<sup>2</sup> and 19 x  
 388 10<sup>15</sup> mol/cm<sup>2</sup> for the native (250m) resolution NO<sub>2</sub> and HCHO retrievals, respectively. The LMOS 2017 GeoTASO  
 389 radiances were co-added onto a 1km grid during the 2017 LMOS campaign so we anticipate that the precision of the  
 390 1km retrievals are better by a factor of 2. Given the relatively high precision of GeoTASO NO<sub>2</sub> compared to the  
 391 column amounts observed during high ozone events A, B and C, we conclude that the high bias in NO<sub>2</sub> columns in  
 392 the AP-XM simulation is significant, with more AP-XM NO<sub>2</sub> columns found outside the estimated +/- 0.5 x 10<sup>15</sup>  
 393 mol/cm<sup>2</sup> precision range then found in the YNT\_SSNG simulation. We have less confidence in the significance of the  
 394 differences between the YNT\_SSNG and AP-XM HCHO columns relative to the GeoTASO retrievals since the  
 395 observed HCHO columns are on the order of the precision of the instrument (10 x 10<sup>15</sup> mol/cm<sup>2</sup>) and the biases in the  
 396 column HCHO simulations are both mostly less than the GeoTASO precision during high ozone events A, B, and C.  
 397 Overall, our results show the YNT\_SSNG simulation has an improved representation NO<sub>2</sub>, which is a primary ozone  
 398 precursor, during these high ozone events.  
 399  
 400



401  
 402 **Figure 12. Scatter plots of 1.3km AP-XM (left) and YNT\_SSNG (right) NO<sub>2</sub> columns versus GEOTASO NO<sub>2</sub> columns (x**  
 403 **10<sup>15</sup> mol/cm<sup>2</sup>) during LMOS 2017 high ozone events A, B, and C. The dashed lines show the precision (+/-) of the GEOTASO**  
 404 **NO<sub>2</sub> columns**

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 406  
 407



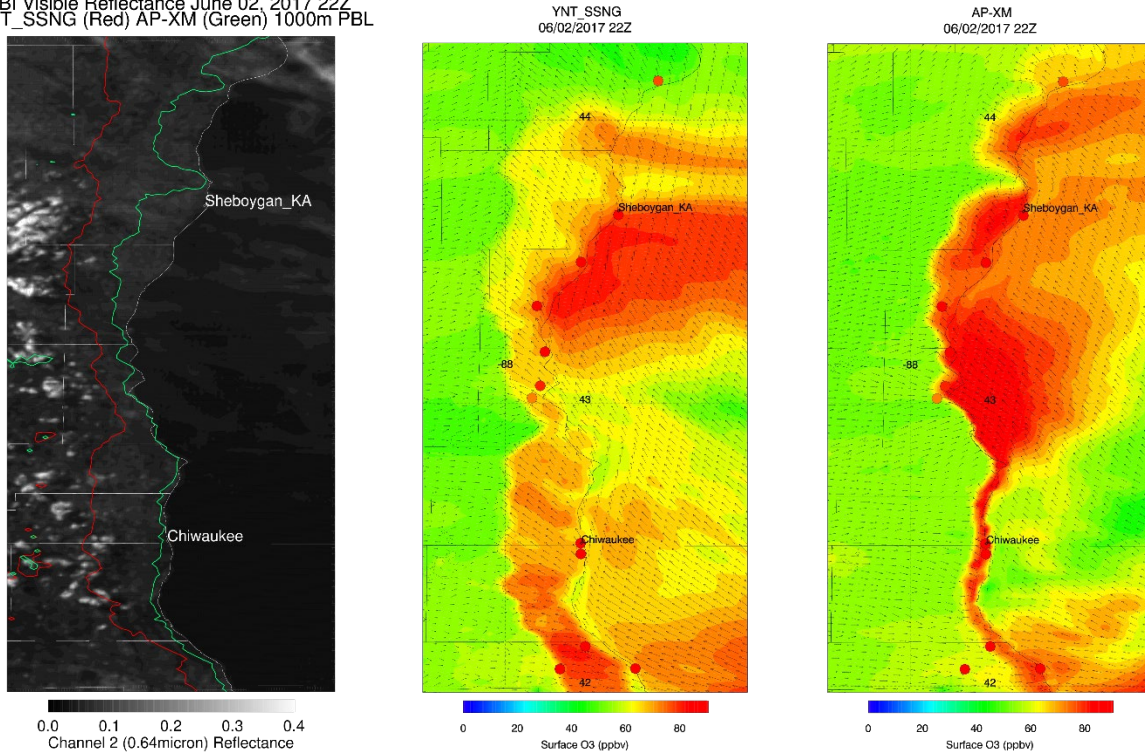
408  
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Figure 13. Same as in Figure 10 but for HCHO columns.

### 411 3.3 June 2, 2017 ozone exceedance event

412 The only ozone exceedance event that had significant inland penetration of the lake breeze at both Chiwaukee and  
 413 Sheboygan KA during LMOS 2017 occurred on June 2<sup>nd</sup>, 2017 (Stanier et al, 2021; Wagner et al, 2022). The  
 414 simulations on this day most clearly illustrate the differences between the AP-XM and YNT\_SSNG results. Figure 14  
 415 shows the observed visible (0.64 micron) reflectance from the Advanced Baseline Imager (ABI) on the NOAA GOES-  
 416 16 satellite and surface ozone concentrations from the YNT\_SSNG and AP-XM simulations, respectively, at 22 GMT  
 417 (5pm CDT) on June 2, 2017. To delineate the simulated continental convective and stable maritime boundary layers  
 418 we also show where the YNT\_SSNG and AP-XM simulated PBL heights are >1 km (Figure 14, Red or Green lines  
 419 in the ABI panel). These contours roughly correspond to the western most edge of the simulated marine boundary  
 420 layer and indicate the extent of the penetration of the lake breeze circulation. The ABI visible reflectances clearly  
 421 show where the stable marine boundary layer suppresses the formation of fair-weather cumulus clouds, which form  
 422 within the turbulent continental boundary layer and are evident to the west of the YNT\_SSNG 1-km PBL height  
 423 contour. The YNT\_SSNG simulation shows a more extensive penetration of high ozone concentrations inland, in  
 424 agreement with the extent of the penetration of the marine boundary layer. In contrast, the AP-XM simulation shows  
 425 very little penetration of the stable marine boundary layer. This lake breeze penetration has a significant impact on the  
 426 simulated surface ozone distributions. While the YNT\_SSNG simulation shows deeper penetration of the lake breeze  
 427 circulation, it also leads to somewhat lower surface ozone concentrations near the shoreline leading to underestimates  
 428 in the observed ozone concentrations at this time.



ABI Visible Reflectance June 02, 2017 22Z  
 YNT\_SSNG (Red) AP-XM (Green) 1000m PBL

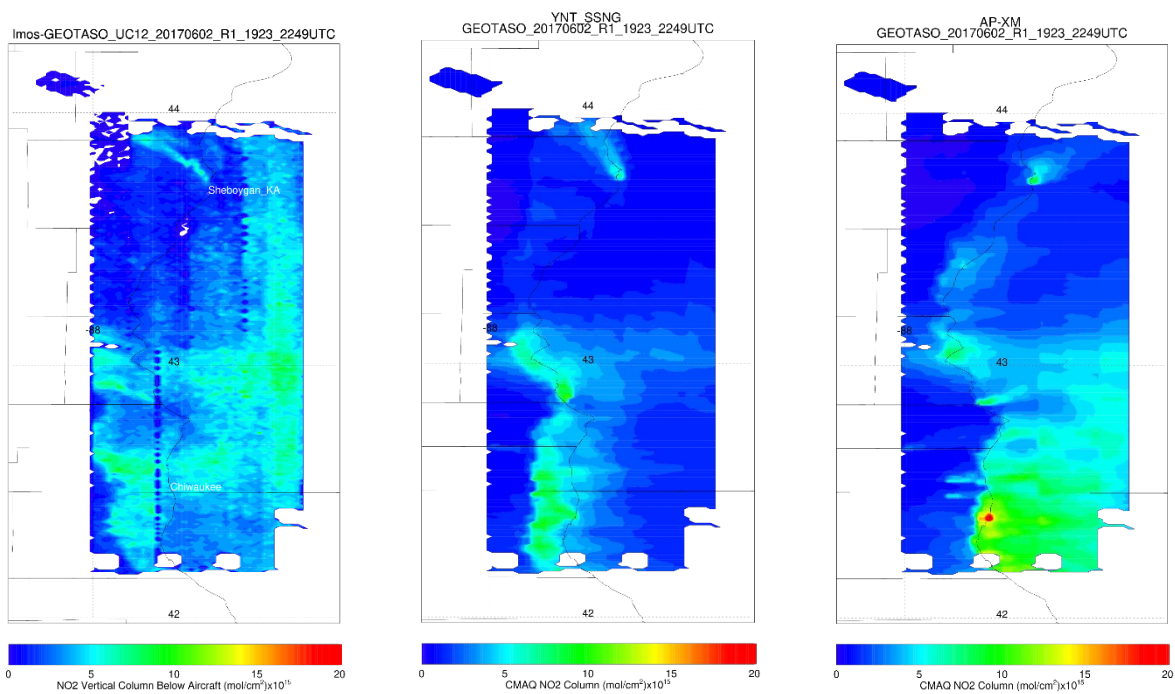


429  
 430 **Figure 14: ABI visible (0.64micron) reflectance (left), YNT\_SSNG surface ozone (ppbv, middle), and AP-XM surface ozone**  
 431 **(ppbv, right) at 22 GMT on June 2, 2017. Observed AQS ozone concentrations at 22 GMT are shown as colored circles.**  
 432 **Location of 1km YNT\_SSNG (Red) and AP-XM (Green) PBL heights are also shown in the ABI (left) panel. The locations**  
 433 **of the Shebogan, KA and Chiwaukee Prairie AQS monitors are labeled in each of the panels.**  
 434

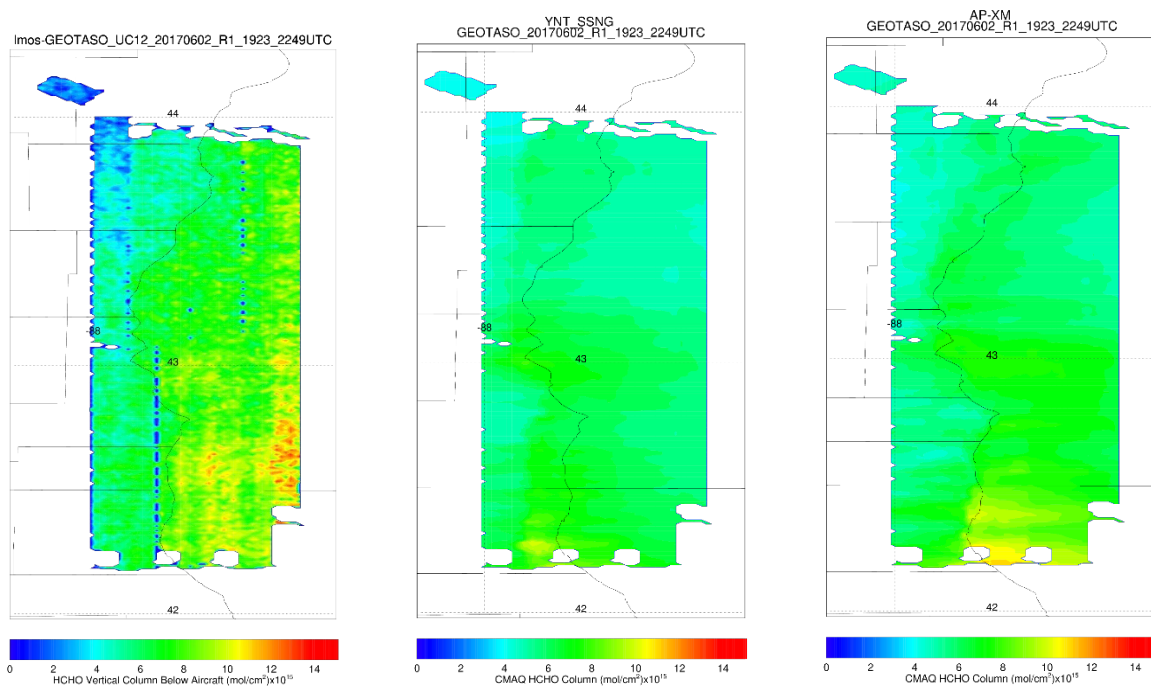
435 Figure 15 shows comparisons between airborne GeoTASO, YNT\_SSNG, and AP-XM column NO<sub>2</sub> along the western  
 436 shore of Lake Michigan on June 2, 2017. Comparisons with column NO<sub>2</sub> distributions provide a means of comparing  
 437 the fidelity of the lake breeze transport of ozone precursors during this high ozone event. Observed NO<sub>2</sub> columns peak  
 438 near 10 x 10<sup>15</sup> mol/cm<sup>2</sup> and show penetration of the high NO<sub>2</sub> column amounts inland by the lake breeze circulation,  
 439 consistent with the ABI visible reflectances. The observed NO<sub>2</sub> columns also show enhancements over the lake on the  
 440 eastern part of the GeoTASO raster pattern that are best captured by the AP-XM simulation. The GeoTASO NO<sub>2</sub>  
 441 columns show peak amounts of 10 x 10<sup>15</sup> mol/cm<sup>2</sup> and significant inland penetration of higher NO<sub>2</sub> columns over the  
 442 southern portion of the flight track. The YNT\_SSNG NO<sub>2</sub> column shows similar peak amounts and shows similar, but  
 443 not as far inland, penetration of the high NO<sub>2</sub> columns. The AP-XM NO<sub>2</sub> column shows localized NO<sub>2</sub> columns over  
 444 15 x 10<sup>15</sup> mol/cm<sup>2</sup> along the Lake Michigan shoreline and does not predict as much onshore penetration. The narrow  
 445 plume of higher GeoTASO NO<sub>2</sub> column extending to the northwest from the coast north of the Sheboygan KA AQS  
 446 monitor is a signature of the Edgewater coal-fired power plant. The YNT\_SSNG and AP-XM simulations also show  
 447 this plume, but the YNT\_SSNG simulation does a better job of capturing the northwestward transport of the plume  
 448 while the AP-XM simulation shows transport of this narrow plume to the north-northeast.  
 449

450 Figure 16 shows comparisons between airborne GeoTASO, YNT\_SSNG, and AP-XM column HCHO along the  
 451 western shore of Lake Michigan on June 2, 2017. HCHO columns vary much less spatially than NO<sub>2</sub> columns, despite  
 452 both anthropogenic and biogenic VOC emissions influencing the former, while the latter is primarily associated with  
 453 anthropogenic emissions. Both simulations capture the observed north-to-south positive gradient providing some  
 454 confidence in the larger scale gradients. However, the GeoTASO HCHO measurements show values in excess of 10  
 455 x 10<sup>15</sup> mol/cm<sup>2</sup> over Lake Michigan that are not captured in either the YNT\_SSNG or AP-XM HCHO column  
 456 simulations. Given the lower precision GeoTASO HCHO columns, the differences between the YNT\_SSNG and AP-  
 457 XM HCHO columns are difficult to quantify with these measurements. We note large differences between simulated  
 458 and observed GeoTASO NO<sub>2</sub> and HCHO over the eastern portion of observations. These observations were collected

459 later during the flight and therefore subject to larger uncertainties related to the impact of stratospheric NO<sub>2</sub> and ozone  
460 absorption interferences.  
461

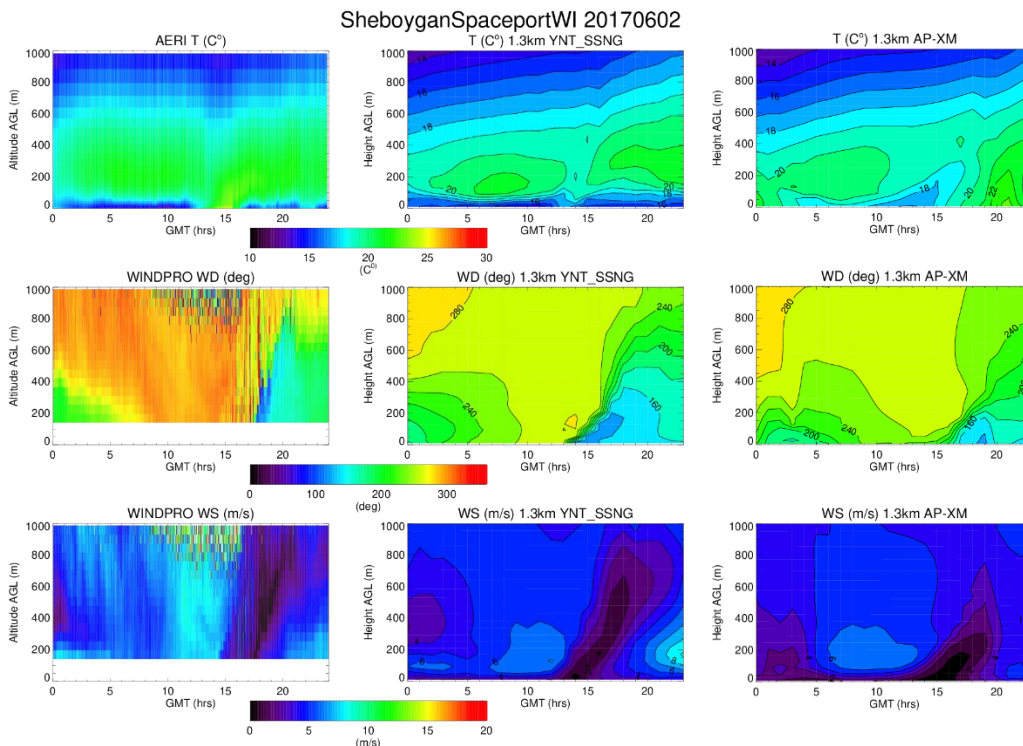


462  
463 **Figure 15: GEOTASO (left), YNT\_SSNG (middle), and AP-XM (right) Column NO<sub>2</sub> (x 10<sup>15</sup> mol/cm<sup>2</sup>) on June 2, 2017. The**  
464 **location of the Sheboygan, KA AQS station is labeled in the GEOTASO column NO<sub>2</sub> panel.**



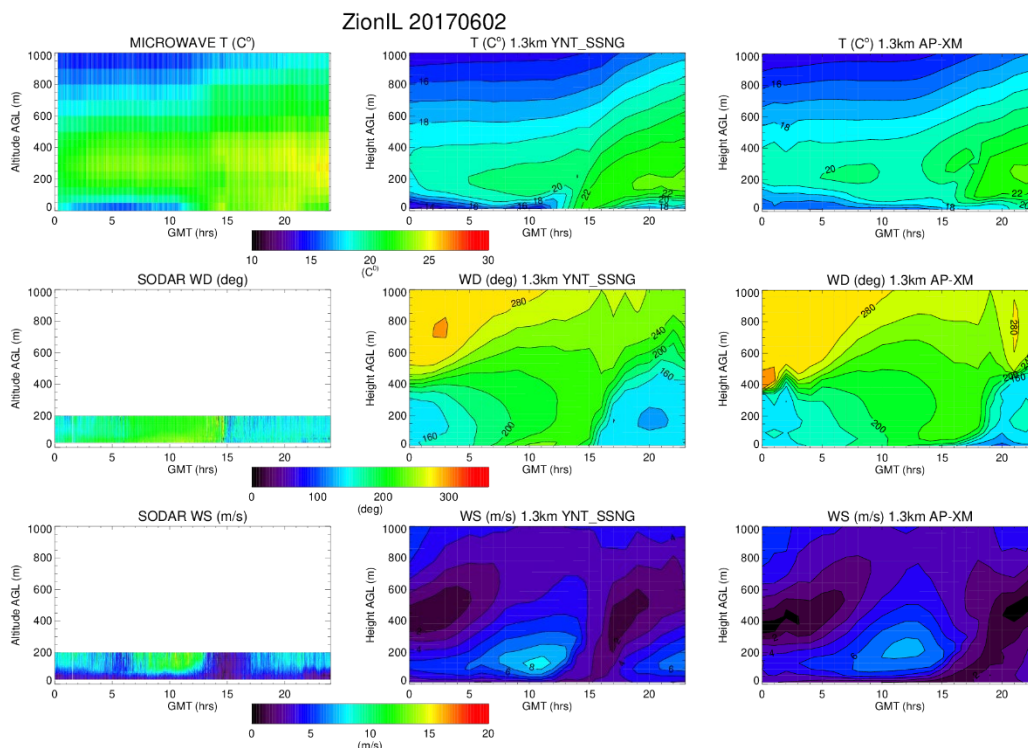
465  
466 **Figure 16: GEOTASO (left), YNT\_SSNG (middle), and AP-XM (right) Column HCHO ( $\times 10^{15} \text{mol/cm}^2$ ) on June 2, 2017.**  
467

468 Figure 17 shows comparisons between observed time height cross-sections of thermodynamic (temperature) and  
469 kinematic (wind) distributions at Sheboygan WI during the June 02, 2017 ozone exceedance event. Observed  
470 temperatures are obtained from the UW-Madison Atmospheric Emitted Radiance Interferometer (AERI) instrument  
471 (Knutson et al, 2004a,b) while wind direction and speed are obtained from a Halo Photonics doppler wind lidar  
472 instrument. Both of these instruments were deployed at the Sheboygan, WI ground site during LMOS 2017 (Stanier  
473 et al, 2021; Wagner et al, 2022). AERI temperatures show a well-defined nocturnal boundary layer with a thin layer  
474 of cold temperatures below 100-m AGL and a warmer layer extending up to approximately 600 m. The continental  
475 convective boundary layer begins to form as the sun rises ( $\sim 12$  GMT [7am CDT]). This is evident in the warmer  
476 surface temperatures near 15 GMT (10am CDT). The AERI measurements show a new shallow layer of cooler air  
477 below 50m arriving at 17 GMT (12pm CDT) associated with the stable marine boundary layer. Observed wind  
478 directions are out of the NW prior to 15 GMT at 7m/s, rapidly diminish around 15 GMT, and switch to the SE around  
479 18 GMT (1pm CDT) when the lake breeze reaches Sheboygan, WI. Both simulations show an easterly bias during the  
480 observed NW winds, which is consistent with the overall statistics during ozone events A, B, and C shown in Figure  
481 11. The YNT\_SSNG simulation captures the thermal structure of the nocturnal boundary layer (temperature  
482 differences are less than  $2^\circ\text{C}$  below 100 m) and timing of the arrival of the maritime boundary layer but underestimates  
483 the near surface (below 200 m) convective boundary layer temperatures by up to  $10^\circ\text{C}$  at 15 GMT. The AP-XM  
484 simulation shows significant (temperature differences are greater than  $5^\circ\text{C}$  below 100 m) overestimates of the  
485 nocturnal boundary layer temperatures and shows a gradual warming of temperatures below 200 m after 15 GMT,  
486 resulting in large (greater than  $7^\circ\text{C}$ ) overestimates in temperatures and no evidence of the cooler lake breeze. Both  
487 simulations underestimate the observed increase in wind speed prior to the arrival of the lake breeze by  $\sim 2$  m/s. The  
488 YNT\_SSNG simulation shows a more rapid shift in wind direction associated with the arrival of the lake breeze than  
489 the AP-XM simulation, but the timing of the switch in wind direction is about 3 hours too early in the YNT\_SSNG  
490 simulation. This results in errors in wind speeds of up to 5 m/s near 200 m in the YNT\_SSNG simulation prior to the  
491 observed reduction in wind speed at 15 GMT. The observed depth of the wind shift is underestimated in both  
492 simulations, but the YNT\_SSN simulation does a better job of capturing the vertical extent of the wind shift and  
493 reduction in wind speed above 200 m. This is most evident above 400 m where the AP-XM wind speeds are  
494 underestimated by up to 5 m/s.



495  
 496 **Figure 17: Time height curtains of observed (left column), YNT\_SSNG (middle column), and AP-XM (right column)**  
 497 **temperature (T, C°, upper row), wind direction (WD, degrees, middle row), and wind speed (WS, m/s, lower row) at**  
 498 **Sheboygan WI on June 2, 2017. Observed temperature is from UW-Madison AERI and observed winds are from the Halo**  
 499 **Photonics doppler wind lidar instrument.**  
 500

501 Figure 18 shows comparisons between observed time-height cross-sections of thermodynamic (temperature) and  
 502 kinematic (wind) distributions at Zion IL during the June 02, 2017 ozone exceedance event. Observed temperatures  
 503 are obtained from the Microwave Radiometer while wind direction and speed were observed using a Sound Detection  
 504 and Ranging (SODAR) instrument, both of which were provided by the University of Northern Iowa. Both of these  
 505 instruments were deployed at the Zion, IL ground site during LMOS 2017 (Stanier et al, 2021; Wagner et al, 2022).  
 506 Microwave temperatures show a well-defined nocturnal boundary layer with a thin layer of cooler temperatures below  
 507 100 m, similar to Sheboygan, WI (Figure 17) but not as cold. The continental convective boundary layer begins to  
 508 form as the sun rises (~12 GMT; 7am CDT). This is evident in the warmer surface temperatures near 15 GMT (10am  
 509 CDT). In contrast to Sheboygan, the Microwave temperatures do not show a signature of the cooler air associated with  
 510 the stable marine boundary layer. This may be due to the fact that the Zion site is further inland than the Sheboygan  
 511 site and turbulent heat fluxes from the warmer land surface warm the marine layer. The SODAR wind direction shows  
 512 a sharp transition from southwesterly to southeasterly winds and a rapid reduction in wind speed (from over 10 m/s to  
 513 less than 5 m/s) at 15 GMT associated with the arrival of the lake breeze at the Zion site. Both the YNT\_SSNG and  
 514 AP-XM simulations overestimate the temperature within the nocturnal boundary layer with the AP-XM showing  
 515 somewhat larger warm biases (>5°C) below 100 m compared to the YNT\_SSNG (<5°C). The YNT\_SSNG simulation  
 516 captures the development of the continental convective boundary layer better than the AP-XM simulation, which  
 517 underestimates the observed temperatures by 5-7°C below 100 m between sunrise (12 GMT) and 15 GMT (10am  
 518 CDT). This cold bias persists until 20 GMT (3pm CDT) in the AP-XM simulation. The YNT\_SSNG simulation shows  
 519 some evidence of a cooler lake breeze moving over the Zion site that leads to a cold bias of 5-7°C at 20 GMT. The  
 520 YNT\_SSNG simulation more accurately captures the timing of the wind shift at 15 GMT, which is delayed by nearly  
 521 3 hours in the AP-XM simulation. Wind speeds are similar in both simulations, although the YNT\_SSNG simulation  
 522 shows slightly higher (8 m/s versus 7 m/s) wind speeds prior to the arrival of the lake breeze and stronger (6 m/s  
 523 versus 3 m/s) low level winds after 20 GMT, which are in better agreement with the SODAR measurements.



524  
 525 **Figure 18: Time height curtains of observed (left column), YNT\_SSNG (middle column), and AP-XM (right column)**  
 526 **temperature (T, C°, upper row), wind direction (WD, degrees, middle row), and wind speed (WS, m/s, lower row) at Zion**  
 527 **III on June 2, 2017. Observed temperatures were obtained using a Microwave Radiometer and observed winds are from a**  
 528 **SODAR instrument provided by Alan Czarnetski at the University of Northern Iowa.**  
 529

#### 530 4. Discussion and Conclusions

531 We have conducted an evaluation of two model simulations employing differing meteorological inputs, with the goal  
 532 of identifying a model configuration best suited for characterizing the spatial and temporal variability of ozone and its  
 533 precursors where lake breezes commonly affect local air quality along the Lake Michigan shoreline. We focus on the  
 534 period of the LMOS campaign, 22 May – 22 June 2017, using the innermost grid of a triple-nested simulation around  
 535 Lake Michigan, with a horizontal resolution of 1.3 km. The AP-XM simulation used the same boundary layer and  
 536 surface physics that are used within CMAQ for WRF inputs; our YNT\_SSNG simulation used different WRF  
 537 parameterizations, as well as constraints to satellite observations of green vegetation fraction and soil temperature and  
 538 moisture, as detailed by Otkin et al. (2023).  
 539

540 Both model simulations reasonably capture observed daily maximum 8-h average ozone amounts over the study  
 541 period, however both simulations underestimated ozone amounts at times with high ozone and overestimated ozone  
 542 when observed amounts were low. These ozone biases are consistent with those simulated by Baker et al. (2023). Both  
 543 model simulations also perform similarly on an hourly basis on high ozone days. We find the AP-XM simulation  
 544 better represents hourly ozone when observed amounts are high (80-90 ppbv), and the YNT\_SSNG simulation overall  
 545 biases are generally smaller (less negative) than those of the AP-XM simulation. Both simulations also tend to  
 546 underestimate amounts of the ozone precursor HCHO, with smaller (less negative) biases in the YNT\_SSNG  
 547 simulation. This is despite that the YNT\_SSNG uses a more realistic, and lower (relative to climatology) Green  
 548 Vegetation Fraction (which would tend to reduce biogenic VOC emissions) suggesting that anthropogenic HCHO  
 549 emissions may be playing a more important role in HCHO concentrations in the YNT\_SSNG simulation. Both  
 550 simulations significantly underestimate isoprene, with larger (more negative) biases in the YNT\_SSNG simulation.  
 551 This is also consistent with the use of more realistic, and lower (relative to climatology) Green Vegetation Fraction in

552 the YNT\_SSNG simulation. We find the simulations are less similar in their representation of NO<sub>2</sub> amounts; while  
553 the AP-XM simulation tends to underestimate NO<sub>2</sub> at monitor sites, the YNT\_SSNG simulation has an overall high  
554 (positive) bias.

555  
556 Since the simulations use identical anthropogenic emissions and chemistry, the differences in modeled ozone and  
557 precursors are linked to any differences in biogenic emissions resulting from the input meteorology and from  
558 differences in boundary layer mixing, horizontal and vertical transport. In Part 1 of this study, Otkin et al. (2022) noted  
559 the AP-XM simulation had an overall low bias in wind speed, the YNT\_SSNG simulation had a positive bias, and the  
560 simulations had similar RMSE. Here, we find many similarities between simulations on high ozone days. At  
561 Chiwaukee Prairie, we find both simulations capture the highest ozone amounts transported from the SSE. On high  
562 ozone days at Sheboygan KA, observed winds tend to be SSW, while both models show highest ozone amounts  
563 transported from the SSE. At Chiwaukee Prairie, both simulations tend to have a westerly bias when observed winds  
564 have an easterly (onshore) component.

565  
566 We find greater differences in column amounts of ozone precursors. The AP-XM simulation has a negative bias in  
567 near-surface NO<sub>2</sub> at Sheboygan, a high bias in near-surface NO<sub>2</sub> at Zion, a positive bias in column NO<sub>2</sub> amounts, and  
568 elevated column amounts concentrated along the Lake Michigan shoreline during the ozone exceedance event on June  
569 2<sup>nd</sup>. The YNT\_SSNG simulation has a small positive bias in NO<sub>2</sub> column amounts, with elevated column amounts  
570 extending further inland on the lake-breeze enhanced ozone event on June 2<sup>nd</sup>. While these differences reflect the  
571 parameterizations used to generate input meteorology, differences in vertical mixing, and ensuing column amounts of  
572 NO<sub>2</sub> and HCHO discussed here, they are further complicated by CMAQ using the ACM2 parameterization for vertical  
573 diffusion—a mismatch for the YNT\_SSNG simulation that influences our evaluation since it leads to differences in  
574 boundary layer mixing. Still, the NO<sub>2</sub> column comparisons provide support for the improved representation of lake  
575 breeze transport of ozone precursors in the YNT\_SSNG simulation. Future model comparisons with upcoming  
576 geostationary observations will allow for maturing analysis for assessing model performance with respect to the  
577 diurnal evolution of precursors during ozone events.

578  
579 Our thermodynamic and kinematic comparison of the AP-XM and YNT\_SSNG simulations show improved  
580 representation of not only the extent, but of the timing of the lake breeze in the YNT\_SSNG simulation at Sheboygan,  
581 WI and Zion, IL for the June 2, 2017 ozone episode. This is consistent with the meteorological analysis presented in  
582 Part 1 of this study, where the YNT\_SSNG had a better representation of diurnal patterns (Otkin et al., 2023).  
583 However, we note that the meteorological inputs to our CMAQ simulations are hourly, as is typically used in air  
584 quality modeling studies. Both simulations would likely benefit from sub-hourly winds given the rapid changes that  
585 can occur in the presence of lake and land breeze circulations. For this, a more tightly coupled model such as WRF-  
586 CMAQ (Wang et al., 2021) would be better suited for a goal of better simulating the fine temporal and spatial scales  
587 of lake breeze transport and chemistry.

588  
589 This analysis complements other studies in evaluating the impact of changing meteorological inputs and  
590 parameterizations on air quality in a complex environment. Appel et al. (2014) also found improved representation of  
591 ozone in environments with bay and sea breezes with the addition of high-resolution SST into the WRF and CMAQ  
592 modeling framework. Cheng et al. (2012) underscored the importance of PBL parameterization in simulating land-sea  
593 breezes and their impacts on near-surface ozone. Similar to our work, Banks and Baldasano (2016) evaluated the  
594 impacts of PBL parameterizations on air quality and also found ambiguous results, with the simulation using the YSU  
595 PBL better capturing observed NO<sub>2</sub>, and the simulation using the ACM2 PBL better capturing observed ozone. Future  
596 work will be able to take advantage of ongoing improvements to both WRF and CMAQ, such as an update to the  
597 calculation of vegetative fraction and PX-LSM soil parameters in WRF (Appel et al., 2021), and should explore the  
598 relationships among spatial and temporal resolution of meteorological parameterizations themselves along with those  
599 of the modeling framework.

600  
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606  
607 **References**

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