Modeling and Data Analysis to Understand the Causes of High Ozone Events in Atlanta, Georgia

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Introduction

The metro Atlanta area is currently violating the 2015 ozone National Ambient Air Quality Standard (70 ppb). Elevated ozone concentrations have large spatial variations among the ground ozone monitors in the metro Atlanta area. To guide future air quality management practices to improve air quality, various types of modeling and data analysis were performed to better understand the causes of ozone exceedances in the metro Atlanta area in 2016 and 2017. Multi-linear regression analysis and Classification and Regression Tree Analysis (CART) analysis were used to understand the relationship between ozone and environmental variables. Low relative humidity, high temperature, and low cloud coverage are three major factors contributing to the ozone exceedances in Atlanta. Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) back trajectory analysis was used to determine the origin of air masses and establish source-receptor relationships on ozone exceedance days. Animations of 5-minute ozone observations and 4-km Weather Research and Forecasting (WRF) model wind vectors were used to better understand ozone formation and transport. The transport of ozone and precursor emissions from the Atlanta urban core has large impacts on the downwind ozone monitors. Finally, 2005-2016 National Aeronautics and Space Administration (NASA) Ozone Monitoring Instrument (OMI) satellite observations for NO_2 and HCHO and 2016-2017 ground observations for NOx and VOC species were analyzed to better understand the impacts of ozone precursors.

Data and Tools

- **Ozone Data**
  Maximum daily 8-hour ozone (MDA8O3) data were analyzed between 1990-2017 at 8 monitors in the Atlanta maintenance area (Figure 1). 1-min data were used for animations.
- **Meteorological Data**
  Meteorological data at Hartsfield-Jackson International Airport was downloaded for 1990-2017 (https://mesonet.agron.iastate.edu). It is further processed into some daily variables for MLR and CART analysis (Table 1).
- **Satellite NO_2 and HCHO columns**
  OMI daily NO_2 columns (NASA) and HCHO columns (http://h2co.aeronomy.be) were downloaded in 2005-2017.
- **Multilinear Regression Model (MLR)**
  Customized IDL (v8.0.1) program is developed for the ozone and meteorological data analysis and MLR model simulations.
- **Classification and Regression Tree Analysis (CART) Model**
  R 3.3.1 program (https://www.r-project.org/).
- **HYSPLIT Model**
  NOAA HYSPLIT model (http://www.arl.noaa.gov/HYSPLIT_info.php).
- **WRF Model**
  WRF ARW version 3.9.1 (https://www.mmm.ucar.edu/weather-research-and-forecasting-model)

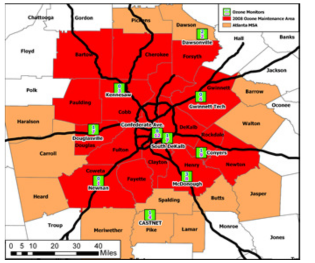


Figure 1. Locations of ozone monitors and the number of ozone exceedance days in 2016 and 2017 in metro Atlanta.

Table 1. Daily meteorological variables used for the MLR analysis and CART analysis

Name	Meaning	Unit
T_{max}	Daily maximum temperature	°F
T_{min}	Daily minimum temperature	°F
TD_{max}	Daily maximum dew point temperature	°F
TD_{min}	Daily minimum dew point temperature	°F
pres1	Mean surface pressure in the morning (6-12 pm)	millibar
pres2	Mean surface pressure in the afternoon (12-6 pm)	millibar
wdir1	Mean wind direction in the morning (6-12 pm)	degree
wdir2	Mean wind direction in the afternoon (12-6 pm)	degree
wsp1	Mean wind speed in the morning (6-12 pm)	m/s
wsp2	Mean wind speed in the afternoon (12-6 pm)	m/s
sky1	Mean cloud coverage in the morning (6-12 pm)	%
sky2	Mean cloud coverage in the afternoon (12-6 pm)	%
O_3-day1	Daily Maximum 8-hr average ozone one day ago (CART)	ppbv
O_3-day2	Daily Maximum 8-hr average ozone two days ago (MLR)	ppbv
wkday	Day of week	n/a
SunAngle	Daily maximum solar elevation angle	degree
relh1	Mean relative humidity in the morning (6-12 pm)	%
relh2	Mean relative humidity in the afternoon (12-6 pm)	%

Ozone Trends in Metro Atlanta

The annual mean MDA8O3 in 1999 is the highest at 71.8 ppb, and decreases to the lowest in 2013 with 47.6 ppb (Figure 2). This generally coincides with Georgia NOx (Figure 3) emission reductions over the same period of time. The annual mean MDA8O3 dropped slightly to 48.7 ppb in 2017, which was the second lowest after 2013.

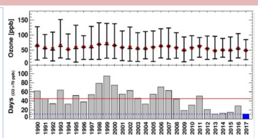


Figure 2. Mean MDA8O3 concentrations (top) and the number of ozone exceedance days (bottom) in April to October in 1990-2017 in the Metro Atlanta area. The red solid line is the average for 1990-2017.

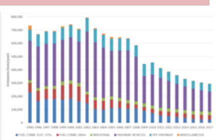
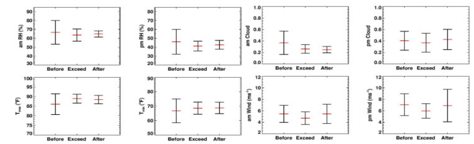


Figure 3. Georgia NOx emission trends by source sectors during 1990-2017.

Meteorological Conditions on Ozone Exceedance Days



High ozone day conditions:
- High T_{max}/T_{min}
- Low am/pm RH
- Low am/pm cloud
- Low am/pm wind

Figure 4. Comparison of meteorological variables in 2017 on the ozone exceedance day, and the day before and after the exceedance. The red bar is the mean, and the upper and lower bars (black) represent the standard deviations.

Multilinear Regression Model Analysis

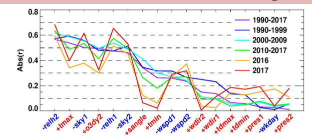


Figure 5. Correlation coefficients of MDA8O3 and environmental variables during ozone season by time periods during 1990-2017. Variables with positive correlation with MDA8O3 are labeled in red, and variables with negative correlation are labeled in blue.

MLR model were developed using daily variables in metro Atlanta (Table 1). High ozone events were strongly associated with high daily T_{max} and low relative humidity. It is also related to low cloudiness and low wind speed. A MLR forecast model based data in 2011-2017 was developed for the daily ozone forecast in metro Atlanta.

Table 2. The coefficients of the MLR ozone model using dataset during 2011-2017

Variable	Coefficient	Variable	Coefficient	Variable	Coefficient
Constant	502.491	TD_{max}	-0.026798	wdir2	-0.0035269
O_3-day2	0.190632	TD_{min}	-0.233327	wspd1	-0.0843647
sky1	-2.66874	SunAngle	0.215487	wspd2	-1.0357
sky2	-2.77572	pres1	-1.06601	relh1	-0.175021
T_{max}	0.575724	pres2	0.615537	relh2	-0.306425
T_{min}	-0.039365	wdir1	-0.010442	wkday	-0.475764

Classification and Regression Tree (CART) Analysis

CART (Breiman et al., 1984) is a non-parametric statistical tool which can estimate the hierarchs of the importance of each variable, especially for the nonlinear relationship between these variables. Regression tree and classification tree CART analysis were done separately in this study. Low PM relative humidity and high daily T_{max} were identified as important conditions on high ozone days.

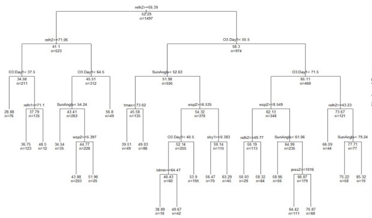


Figure 6. Best split for the regression tree CART analysis for Atlanta ozone during 2011-2017. Tree splits to the left meet the specified criteria and tree splits to the right do not meet the specified criteria.

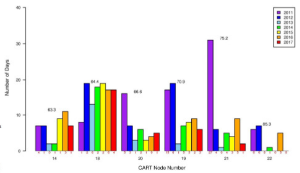


Figure 7. Number of days in 2011-2017 in the 6 high ozone nodes found in the regression tree CART analysis. Average ozone concentrations (black numbers on top) and number of ozone exceedance days (red numbers on bottom) are labeled for each node.

Ground Ozone and Wind Animation

- Created animations with wind vectors and ozone concentrations.
- 1-minute ozone observations are summed to 5-minute averages and interpolated across the domain.
- WRF simulations (4-km grid resolution) containing surface wind vectors (wind speed and wind direction).
- The synchronized movements of high ozone and dynamic changes of winds are illustrated.

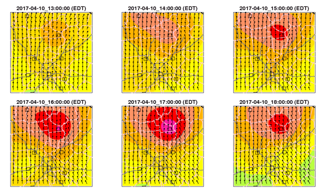


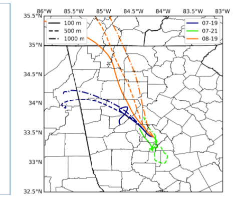
Figure 8. Ozone exceedance at Dawsonville, GA on April 10, 2017.

HYSPLIT Trajectory Analysis

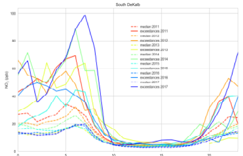
The origin of air masses and establish source-receptor relationships on ozone exceedance days

1. 24-hour back trajectory analysis for each violating ozone monitor in Atlanta
2. 12-km North American Mesoscale (NAM) meteorological fields
3. Three release heights: 100, 500, and 1,000 meters

Findings: High ozone events were generally associated with air masses passing through the Atlanta urban core.



Ground NO_x and VOC Measurements



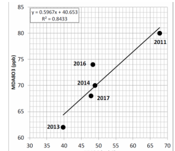


Figure 10. (**Right**) Univariate regression for the 4th highest MDA8O3 and summertime (June-August) average aNMOC concentrations at the South DeKalb monitor in 2011-2017.

Figure 9. (**Left**) Diurnal profile of median NOx for each ozone season (dashes) and exceedance days (solid lines) during 2011-2017.

OMI Satellite NO_2 and HCHO Tropospheric Columns

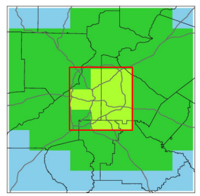
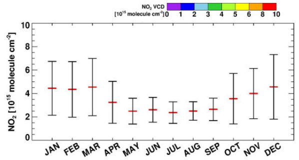
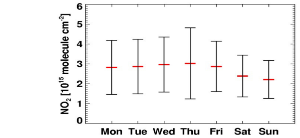
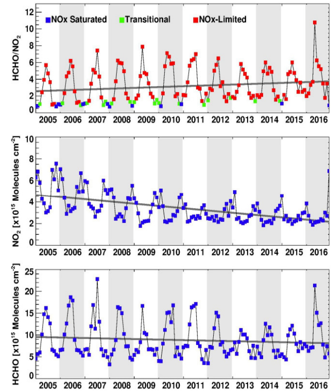


Figure 11. (**Top left**) OMI NO_2 tropospheric columns over metro Atlanta in 2005-2017. (**Middle left**) Monthly mean of OMI NO_2 over metro Atlanta. (**Bottom left**) Mean OMI NO_2 on 7 days of week. (**Right**) Monthly OMI HCHO/NO_2, NO_2, and HCHO columns over metro Atlanta in 2005-2016.







The hot spot of OMI NO_2 columns over the Atlanta urban core clearly shows strong local NOx emissions in the Metro Atlanta area. The decrease of NO_2 columns in ozone season is consistent with the decrease of NOx emissions since 2005 (Figure 3). NO_2 columns are lower in warm months and weekend. OMI HCHO are relatively stable in 2005-2016. The OMI HCHO/NO_2 ratios shows that ozone formation in Metro Atlanta was mostly in the NOx-limited regime during ozone season.

Conclusion

The conditions for high ozone days in metro Atlanta are

- Meteorological conditions
  - Low relative humidity in the afternoon
  - High daily maximum air temperature
  - Low cloud coverage
  - Low wind speed
- High ozone on previous days
- NOx emissions, mainly from local on-road mobile sources
- VOC emissions, mainly from biogenic sources in the summer months with additional contributions from local on-road mobile sources in the evening and morning hours
- Local transport of emissions from the Atlanta urban core to monitors outside the urban core