

The Study of Oxidant Formation Mechanism in an Urban Environment

Abstract

The goal of this study was to investigate the possibility of finding a simple statistical model to predict ozone (O₃) excess days based on measurements of meteorological variables. Data used in this experiment was collected from the Georgia Department of Natural Resource's ambient monitoring site and Clark Atlanta University's meteorological database. Variables such as wind speed, wind direction, relative humidity, temperature and solar intensity were used in the analysis. By correlating ozone data with the meteorological variables mentioned above, it can be concluded which variables contribute to ozone formation in Douglasville.

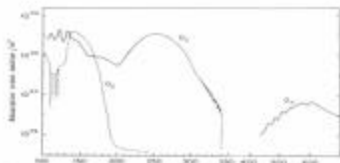


Figure 4. The absorption cross-section of the absorption cross-section of ozone at 25°C and 1013 mb. The vertical dashed line indicates the wavelength of the maximum absorption cross-section of ozone at 25°C. The horizontal dashed line indicates the wavelength of the maximum absorption cross-section of ozone at 25°C. The vertical dashed line indicates the wavelength of the maximum absorption cross-section of ozone at 25°C. The horizontal dashed line indicates the wavelength of the maximum absorption cross-section of ozone at 25°C.

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TABLE 3-8 Wavelengths (Å) below Which It Is Energetically Possible to Produce the Indicated Species from O₃ Photolysis*

Species	O ₃ (¹ Σ _g ⁺) ^b	O ₃ (¹ Δ _g ⁺)	O ₃ (¹ Σ _g ⁺)	O ₃ (¹ Σ _g ⁺)	O ₃ (¹ Σ _g ⁺)
O(¹ P) ^c	11,400	5900 ^d	4600 ^e	2300	1700
O(¹ D)	4,100 ^f	3100	2600	1670 ^g	1500 ^g
O(³ S)	2,340 ^h	1940	1750	1290 ^g	1080 ^g

* From McNesby and O'Kabe.²¹
^b Ground state.
^c Forbidden transition.

Source: The Urban Smog

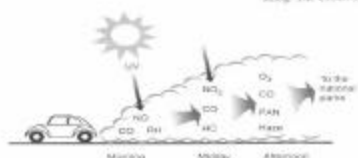


Figure 8.2. Smog formation is the primary cause of urban air pollution. The key steps are: (1) NO is oxidized to NO₂ by sunlight; (2) NO₂ and CO react to form peroxy radicals; (3) peroxy radicals react to form O₃ and other pollutants.

Source: The Urban Smog



Figure 8.3. The absorption cross-section of NO₂ at 25°C. The vertical dashed line indicates the wavelength of the maximum absorption cross-section of NO₂ at 25°C. The horizontal dashed line indicates the wavelength of the maximum absorption cross-section of NO₂ at 25°C.

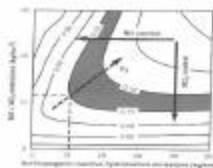


Figure 8.4. The absorption cross-section of NO at 25°C. The vertical dashed line indicates the wavelength of the maximum absorption cross-section of NO at 25°C. The horizontal dashed line indicates the wavelength of the maximum absorption cross-section of NO at 25°C.

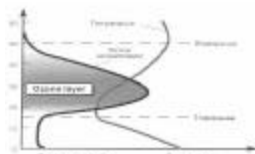


Figure 8.5. The vertical profile of ozone concentration and temperature. The vertical dashed line indicates the altitude of the maximum ozone concentration. The horizontal dashed line indicates the altitude of the maximum temperature.

Background

The ozone molecule consists of three atoms of oxygen joined together by a single bond and a double bond in a bent formation at an angle of 116.8 degrees. Oxygen and ozone absorbs light in the portion of solar spectrum that is harmful to plant and animal life. Ozone itself, absorbs in a region (290-360 nm) in which DNA is particularly sensitive. Hence, the ozone layer in the stratosphere is important to the survival of life at the surface of the planet. In recent years it has been discovered that there is an excessive amount of ozone in the troposphere. This problem was discovered in the 1940's when scientist observed a yellow haze in the boundary layer above Los Angeles on daily bases. From this observation scientist began to run test on this yellow later to be known as smog. Ozone is the main constituent of smog and it is formed from the following reactions:

Due to the increase in tropospheric ozone, studies have been done on the effects of the increased amount of ozone. These studies yielded the result that human health was effected by excessive amounts of ozone. It starts by inhaling air in which your body uses the molecular oxygen, removes unwanted chemicals inhaled, and retain 90% of the ozone inhaled. As result, the inhaled ozone irritates the mucous membrane of the nose throat and other airways, which leads to respiratory infections. Overexposure leads to permanent scarring of lung tissue, loss of lung function and reduced lung elasticity. Symptoms of overexposure are chest pain, coughing, asthma attacks and throat irritation. When the statement "overexposure" is used it is referring to exposure to ozone amounts over 0.08 ppm (parts per million), which is the newer public health standard. The other degrees of hazardous ozone concentration are : 0.12 ppm means a public alert, 0.40 ppm means a public warning and 0.50 ppm means a public emergency. In the Atlanta metro area, Douglasville seems to have a major problem with ozone. It has many days in the summer, which is ozone season, where it was over 0.08 ppm. As result it was used as a case study to determine which variables were useful for predicting ozone.

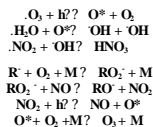
EPA's Ozone Related Emissions Study For Atlanta

VOCs from Auto & Light Trucks/SUVs
 NO_x from Auto & Light Trucks/SUVs

	1970	1980	1999	2005
VOCs	68%	38%	38%	29%
NO _x	68%	62%	33%	24%

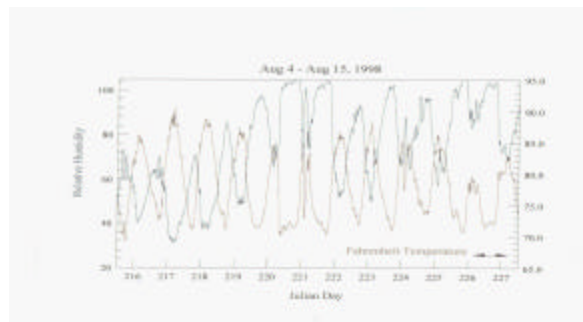
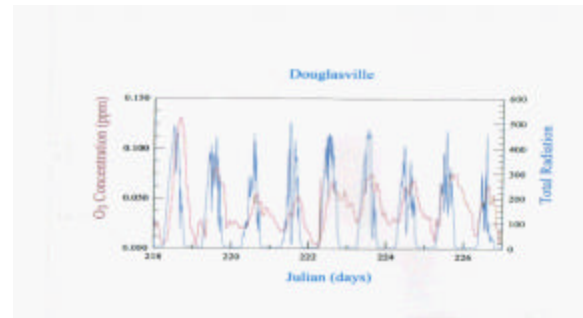
Analysis

The time period used to analyze this data is 216-227 (Aug 4-15, 1998) Julian days at the Douglasville, GA ozone ambient monitoring site. These days were chosen for one, because the ozone concentration remained mostly above 0.08 ppm and day 216 was similar to a typical non-ozone season day (ozone season is may-august). Since **Relative humidity** = (P_{act}/P_{sat}), then P_{act} is proportional to relative humidity. When P_{act} is plotted with the O₃ concentration, they had an inverse relationship. This may be due to increased removal of NO₂ in reaction 3 created by larger amounts of OH produced by reactions 1 and 2, below:



Also, as the total radiation increases so does the O₃ concentration because an increase in radiation will create more free-radical species that convert NO to NO₂ as shown in the last 4 reactions.

In the time frame studied, the temperature and relative humidity had an inverse relationship, as is to be expected when air containing a relatively fixed amount of water vapor is heated during the day. Also the average Interstate highway traffic in Douglasville is 169,478 vehicles per day, which helps contribute to NO_x in the boundary layer. Below are statistical values of a few of the precursors to O₃.



	Maximum	Minimum	Absolute mean	median
Douglasville O ₃ concentration	0.131	0.002	0.3997	.036
Temperature	88.6	70.1	77.7	77.1
Total radiation	1008	8.90	215.18	45.26
Pact.	30.425	14.878	25.57	26.7

Conclusion

From my preliminary examination of the data from one of many Metro Atlanta's ambient ozone monitoring sites, no clear, simple pattern emerged. When the next step is taken, determining a functional relationship between the variables, some that were thought to contribute to ozone were proven to be unconventional variables such as wind direction and traffic data should be used. Next, the level of NO_x should be included in the data used since it is a major ozone precursor. All in all this project needs to be looked at more in depth in order for an accurate conclusion to be drawn.

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