# Estimating Surface Level Ozone Under Different Temperature and NOx Regimes at an Urban and Suburban Site in Portland, Oregon

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## Surface Level Ozone (O3) Background

Surface level ozone (SLO) is considered one of the major scientific challenges associated with urban air pollution (Sillman, 1999). This is due to the fact that SLO is both largely influenced by anthropogenic sources and that SLO presents several adverse health effects on humans (American Lung Association, 2022) and the environment (National Research Council, 2004). The Environmental Protection Agency (EPA) identified ozone as a Criteria Pollutant in 1996 and currently regulates ozone with a NAAQS exceedance standard of 70 parts per billion (ppb) over an 8-hour average.

SLO is a secondary pollutant formed through sets of chemical reaction cycles involving volatile organic compounds (VOCs), and oxides of Nitrogen (NOx = NO + NO2). A diurnal cycle is introduced to both the formation and concentration of SLO, as the photolytic cycle, the basis for SLO formation, involves photochemistry. SLO concentrations are also correlated to several meteorological variables, partially dependant on local geography.

Due to the highly complex nature of ozone, we built regression models to predict ozone concentrations at two ozone monitoring stations in Portland, Oregon. These models predict ozone concentrations for changes in both ozone precursors and meteorological variables during the summer months of June, July, and August. These models have both the potential to aid the Oregon Department of Environmental Quality (ODEQ) in forecasting ozone concentrations, and to predict ozone concentrations for changes in climatological variables (such as temperature).

### Ozone Formation - Photolytic Cycle

$$NO2 + h\nu \rightarrow NO + O$$

$$O + O2 \rightarrow O3$$

$$O3 + NO \rightarrow NO2 + O2$$

Note: In this naturally occurring cycle, no net ozone is formed.
Ozone concentrations will not change in the presence of NO.

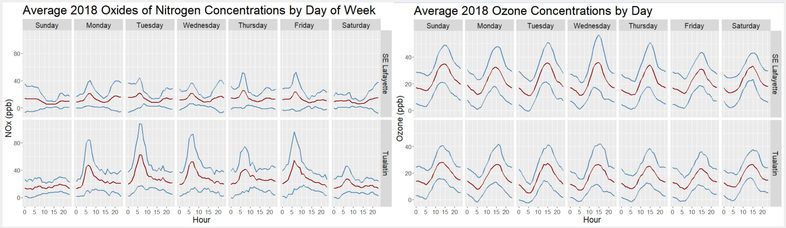
### Ozone Formation - Volatile Organic Compounds (VOCs)

- VOCs are favored to react with NO
- When in the presence of VOCs, daytime ozone builds up
- Organic radicals formed here can lead to additional ozone formation

## Data

Hourly data for the SE Lafayette and Tualatin monitoring stations for the years 2017 through 2021 during the summer months of June, July, and August were obtained through the EPA, ODEQ, and the National Weather Service (NWS). Available O3, NO, NO2, NOx, CO, and PM 2.5 data for all years were obtained through ODEQ. Available meteorological data for both stations were obtained through the EPA and ODEQ. As no temperature observations were available for SE Lafayette in 2021, temperature observations from the National Weather Service station at Portland International Airport (KPDX) were used as a proxy. As no pressure data was available for Tualatin, SE Lafayette was used as a proxy under the assumption that pressure was not significantly affected by the microclimates of each site. Pressure and Humidity are excluded from the regression models due to significant amounts of missing data.

### Example NOx and O3 Signals

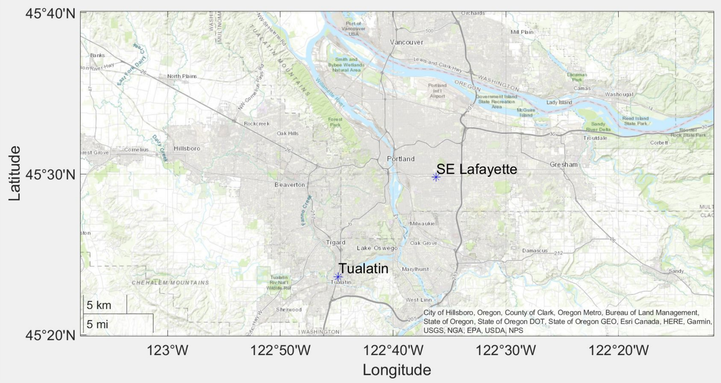



Oxides of Nitrogen (ppb - left) and Ozone (ppb - right) in 2018, hourly by day of week for the Summer months of June, July, and August, as observed at the SE Lafayette and Tualatin stations. Averages in red; one standard deviation in blue.

### Monitoring Stations

**SE Lafayette** - Urban, Background **Tualatin** - Urban, Near Road

- No volatile organic compound (VOC) measurements at either site
- Sites present several microclimatic differences that pust be considered separately given the complex ozone chemistry
- Tualatin station is located next to the I-5 highway with a strong influence from local emissions




## Methods

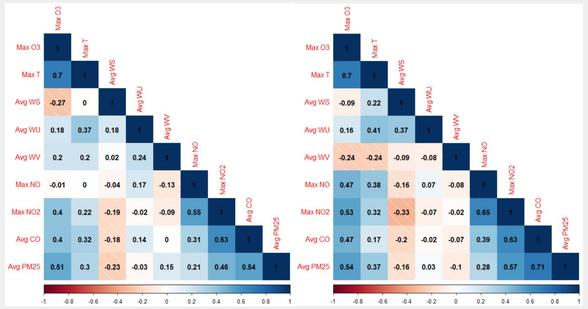
Two separate models are created; one for each site. This distinction is important due to the unique microclimatic features each site displays, directly related to their geographical location. Each model predicts daily maximum surface level ozone concentrations from a linear regression, dependent on the variables of:

Temperature - daily maximum
Wind Speed - daily average
Wind Direction - daily average (unit vector components)
Nitrogen Monoxide - daily maximum
Nitrogen Dioxide - daily maximum
Carbon Monoxide - daily average
Particulate Matter (2.5 μm) - daily average

Temperature is the most highly correlated variable at both sites. Each site presents different correlations to ozone concentrations. The Tualatin station's location relative to the I-5 highway directly influences pollutant measurements, depending on whether or not pollutants are blown towards, away, or remain stagnant relative to the station. The wind's influence on ozone concentrations can be seen in the varying model coefficients at each site. The assumed cause for a near zero correlation of ozone concentrations to NO at Tualatin is a NOx limited regime. This effect would also explain the varying model coefficients for pollutants at each site, though has not been verified as VOC concentrations are not measured at either site.

To make each model we have broken our datasets for both stations into "test" and "train" subsets. The coefficients for each model using the "train" data sets are presented below. The "test" datasets contained a random 20% of the available data, while the "train" datasets contained a random 80% of the available data. From this random sample, the SE Lafayette model slightly underpredicts ozone concentrations at a 0.871 linear relationship to actual concentrations while the Tualatin model closely predicts ozone concentrations at a 0.950 linear relationship to actual concentrations. Nearly a third of the variance within each model is unexplained, and is likely a significant result of the absence of VOCs within our models. The verification of inflation factor for each variable within each model is between 1 and 2.8, meaning there is no concern of multicollinearity within our models.

### Correlation Plots

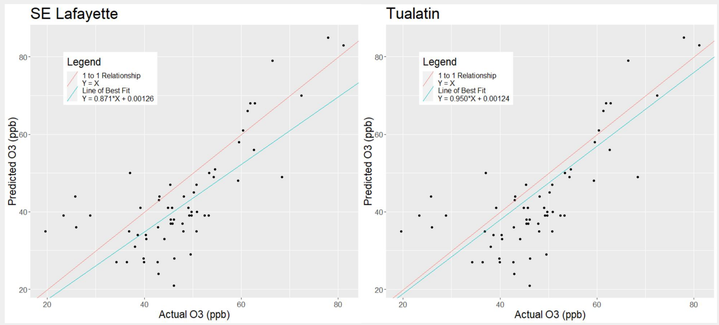



Correlation Plots for years 2017-2021 of average daily values during the months of June, July, and August
Left: SE Lafayette, Right: Tualatin

### Model Coefficients

| SE Lafayette | O3 (ppm) Estimate | Tualatin | O3 (ppm) Estimate |
|---|---|---|---|
| **Intercept** | 5.930e-01 | **Intercept** | 3.656e-01 |
| **Max T (K)** | 2.115e-03 | **Max T (K)** | 1.337e-03 |
| **Avg WS (Knots)** | -1.232e-03 | **Avg WS (Knots)** | -2.537e-03 |
| **Avg WU (X- Component)** | -8.716e-04 | **Avg WU (X- Component)** | 1.329e-03 |
| **Avg WV (Y- Component)** | -5.382e-03 | **Avg WV (Y- Component)** | 1.257e-03 |
| **Max NO (ppb)** | 2.534e-04 | **Max NO (ppb)** | -2.345e-04 |
| **Max NO2 (ppb)** | 1.833e-04 | **Max NO2 (ppb)** | 7.493e-04 |
| **Avg CO (ppm)** | 2.347e-02 | **Avg CO (ppm)** | -8.714e-03 |
| **Avg PM 2.5 (μg/m^3)** | 2.177e-04 | **Avg PM 2.5 (μg/m^3)** | 5.179e-04 |
| | **R^2 = 0.694** | | **R^2 = 0.6885** |

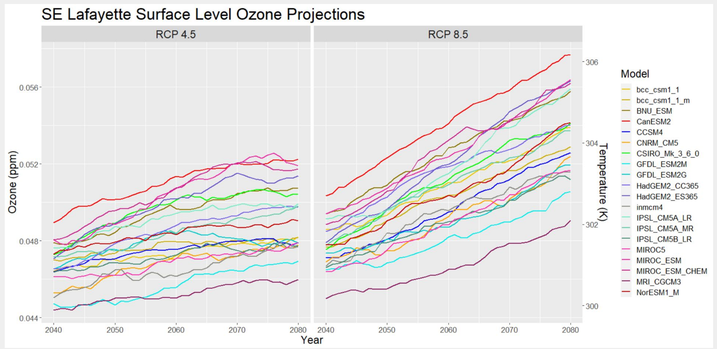
### Model Verification



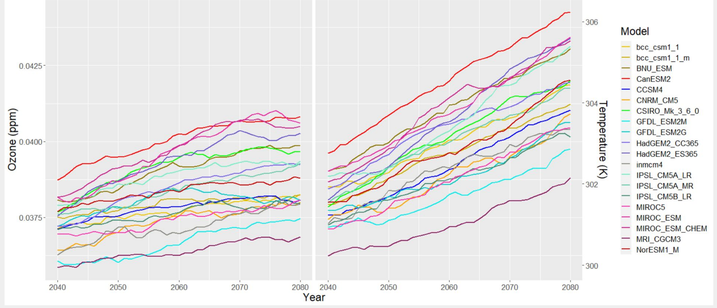

Actual versus predicted ozone concentrations using the "test" data sets (blue) for the SE Lafayette (left) and Tualatin (right) linear regression models.

## Ozone Predictions for Climatological Changes in Temperature

The following surface level ozone projections are for changes in daily maximum temperature under IPCC scenarios RCP4.5 and RCP8.5. Climate data were obtained from the Multivariate Adaptive Constructed Analogs (MACA), providing statistically downscaled climate model projections from 20 different models. From the outputs by MACA, a centered 31 year average by day of year was performed for each model to eliminate variance due to random scenarios. A resulting data set of projections for maximum temperature by day was obtained for the years 2040 through 2080 for each model, for each scenario, at each ozone monitoring station. Maximum temperature values during the summer months of June, July, and August were then averaged by year for each model, to show average maximum surface level ozone projections during the summer months for years 2040 through 2080, for each model, for each scenario, at each ozone monitoring station.




SE Lafayette surface level ozone projections by year, for changes in average daily maximum temperature during the Summer months of June, July, and August. Temperature projections for IPCC scenarios RCP 4.5 and 8.5, are obtained from statistically downscaled climate models.




Tualatin surface level ozone projections by year, for changes in average daily maximum temperature during the Summer months of June, July, and August. Temperature projections for IPCC scenarios RCP 4.5 and 8.5, are obtained from statistically downscaled climate models.

## Discussion

The projections presented show a general increase in average maximum daily ozone concentrations for both scenarios RCP4.5 and RCP8.5 for the summer months of June, July, and August during the time period of years 2040 through 2080. These projections do not show a proportion of how many days during a given summer will reach the EPA regulatory value of 70 ppb. It is expected that the proportion of days in a year reaching the EPA regulatory value of 70 ppb will increase, however it cannot be concluded upon in the context of these presented projections. It is important to note that the the EPA regulatory value is also expected to decrease as time passes. Should a decrease in the EPA regulatory value occur, the likelihood that a day will reach the EPA regulatory value will likely also increase, assuming all other variables remain constant!

These predictions, from a climatological viewpoint, make the assumption that all other variables influencing ozone concentrations will remain constant. This assumption is unlikely, and a new model should be created with a representative base of any changing precursor emission concentrations and ratios.

It is important to remember the context of the presented surface level ozone projections. For both scenarios, projections are presented from year 2040, however both scenarios begin at the same base starting point. The base starting point for each scenario is the average observed values during the Summer months of years 2017 through 2021 at each respective station. We do not currently know which climate models used in this research are "good" or "bad," and they should all be considered as our "best" available models.

## References

American Lung Association. (2022). State of the Air 2022.

National Research Council. (2004). Research priorities for airborne particulate matter: IV. Continuing research progress.

Sillman, Sanford. (1999). The relation between ozone, NOx and hydrocarbons in urban and polluted rural environments. Atmospheric Environment, 33(12), 1821–1845. https://doi.org/10.1016/S1352-2310(98)00345-8

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