

1 Performance of Machine Learning for Ozone Modeling in Southern
2 California during the COVID-19 Shutdown

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12 Abstract

13 We combine machine learning (ML) and geospatial interpolations to create two-dimensional high-
14 resolution ozone concentration fields over the South Coast Air Basin (SoCAB) for the entire year of 2020.
15 Three spatial interpolation methods (bicubic, IDW, and ordinary kriging) were employed. The predicted
16 ozone concentration fields were constructed using 15 building sites predicted by the ML method, and
17 random forest regression was employed to test the predictability of 2020 data based on input data from
18 past years. Spatially interpolated ozone concentrations were evaluated at twelve sites that were
19 independent of the actual spatial interpolations to find the most suitable method for SoCAB. Ordinary
20 kriging interpolation had the best performance overall for 2020: concentrations were overestimated for
21 Anaheim, Compton, LA North Main Street, LAX, Rubidoux, and San Gabriel sites and underestimated for
22 Banning, Glendora, Lake Elsinore, and Mira Loma sites. The model performance improved from the West
23 to the East, exhibiting better predictions for inland sites. The model is best at interpolating ozone
24 concentrations inside the sampling region (bounded by the building sites), with R^2 ranging from 0.56 to
25 0.85 for those sites, as prediction deficiencies occurred at the periphery of the sampling region, with the
26 lowest R^2 of 0.39 for Winchester. All interpolation methods poorly predicted and underestimated ozone
27 concentrations in Crestline during summer (up to 19 ppb). Poor performance for Crestline indicates that
28 the site has a distribution of air pollution level independent from all other sites. Therefore, historical data
29 from coastal and inland sites should not be used to predict ozone in Crestline using data-driven spatial
30 interpolation approaches. The study demonstrates the utility of ML and geospatial techniques for
31 evaluating air pollution levels during anomalous periods. Both ML and CMAQ do not fully capture the
32 irregularities caused by emission reductions during the COVID-19 lockdown period (March – May) in the
33 SoCAB. The results from ML indicate that there has never been a similar pattern in air quality to that of
34 the COVID-19 lockdown in the past. Including 2020 training data in the ML model training improves the
35 model's performance and its ability to predict future abnormalities in air quality.

36 Keywords

37 Ozone, machine learning, COVID-19, modeling, Southern California

38 1. Introduction

39 In the atmosphere, the non-linear relationship between nitrogen oxides (NO_x), volatile organic
40 compounds (VOCs), and ozone is complex. In the United States, the COVID-19 pandemic and the ensuing
41 shutdown presented an unintentionally optimal period to observe, revise, and improve our existing air
42 quality models and observe the sensitivity of the NO_x-VOC-ozone relationship in real time. In California,
43 the pandemic shutdown began on March 16, 2020, where significantly reduced traffic volume was
44 observed. In Los Angeles and Ventura Counties, there was approximately a 30% decrease in vehicle miles
45 traveled (VMT) on weekdays and up to a 40% decrease on weekends in 2020 (Caltrans, 2023). This unusual
46 event temporarily changed the conventional distribution of primary and secondary air pollutants in the
47 South Coast Air Basin (SoCAB). NO_x and VOC emissions declined with the reduction in traffic flow (Jiang
48 et al., 2021). As a result, we expected a drop in ozone concentrations in Southern California. Several
49 studies were published regarding the pandemic that investigated the effects of the COVID-19 shutdown
50 on air pollutants. Jiang et al., used WRF-Chem to simulate the major air pollutants under two scenarios
51 (i.e., before lockdown and during lockdown) and found an increase in ozone in urban areas due to
52 emission reduction during the lockdown (Jiang et al., 2021). The COVID-19 shutdown provided an
53 estimation of the impacts of future large-scale emission reduction strategies on ozone formation in SoCAB
54 (Ivey et al., 2020).

55 Over the past several decades, ozone levels in Southern California significantly decreased as a
56 result of emissions control programs implemented by the South Coast Air Quality Management District
57 (SCAQMD), thereby reducing emissions from mobile sources and shifting to renewable energy sources
58 (Lurmann et al., 2015; South Coast Air Quality Management District, 2017). However, during the past

59 decade, ozone concentrations in the SoCAB have slightly plateaued despite further emissions reductions
60 (Figure 1) (Do et al., 2023).

61 This paper focuses on the performance of deterministic and statistical models under rapid
62 changes in emissions and meteorological conditions. Furthermore, we aim to answer the question of
63 whether there were other periods with emissions changes similar to the COVID-19 lockdown period within
64 the past few decades. Chemical transport models (CTM) are conventionally used for air quality research
65 and regulatory purposes. The Community Multiscale Air Quality (CMAQ) modeling system, developed by
66 the U.S. Environmental Protection Agency (EPA), is well-known for multi-day air quality simulations to
67 estimate air pollutant concentrations with prescribed emissions and meteorology inputs (Ooka et al.,
68 2011; Rao et al., 1996; D. C. Wong et al., 2012). From the model outputs, scientists and regulators can
69 better predict the interactions between future emissions, meteorology, and air pollutants to strengthen
70 recommendations for emissions control programs. Zhu et al. used CMAQ to investigate the sensitivity of
71 ozone and particulate matter less than 2.5 microns ($PM_{2.5}$) to incremental changes in volatile organic
72 compounds (VOC) by updating the VOC emissions from recent literature, and simulated maximum daily
73 8-hour ozone concentrations increased by 17.4 ppb and 15.6 ppb in summer and winter, respectively (Zhu
74 et al., 2019). With a similar approach, Karamchandani et al., found that near-recent regulatory modeling
75 for SoCAB generally underestimated the response of ozone design values to the changes in precursor
76 emissions (Karamchandani et al., 2017).

77 Recently, ML as an alternative modeling approach has attracted more attention from air quality
78 researchers. Although ML and chemical transport models have a similar goal to accurately predict air
79 pollution, ML heavily depends on the quality and quantity of data available. Conversely, CTMs are based
80 on first principles equations and are initiated with interpolated observation data, hence avoiding most
81 obstacles introduced by data missingness in observations. In contrast with CTMs, which produce larger-
82 scale, spatially resolved outputs, ML only provides predictions strictly at trained locations when used for

83 ambient air quality applications. SCAQMD operates 38 air monitoring stations in Southern California over
84 an area of approximately 10,743 square miles, including SoCAB, portions of the Salton Sea Air Basin, and
85 Mojave Desert Air Basin, with an average of 283 square miles per monitoring station (Miyasato et al.,
86 2016; South Coast Air Quality Management District, 2017). Due to the relative sparseness of monitoring
87 stations and locality of air pollutants, using air monitoring stations to represent spatially-varying air quality
88 over a large area may result in incorrect information (Apte et al., 2017). To overcome this limitation when
89 high-resolution measurements are not available, researchers opt to use spatial interpolation methods
90 (e.g., nearest neighbors, linear or polynomial interpolation, continuous natural neighbor interpolation,
91 etc.) (Joseph et al., 2013). Yu et al., evaluated 14 unique spatial modeling methods for eight air pollutants
92 in Atlanta, Georgia for developing spatiotemporal air pollutant concentrations fields (Yu et al., 2018).
93 Wong et al., assessed four spatial interpolation methods (spatial averaging, nearest neighbor, inverse
94 distance weighting (IDW), and kriging) to estimate ozone and PM₁₀ air concentrations (Wong et al., 2004).
95 In this paper, we compare three spatial interpolation techniques to the CMAQ model and evaluate biases
96 related to COVID-19 lockdown anomalies.

97 2. Study Area and Datasets

98 This study targeted the Southern California region, including Los Angeles, Orange County,
99 Riverside, and San Bernardino counties. The region has been historically challenged with poor air quality,
100 with especially higher ozone concentrations than the rest of the United States. The coastal areas tend to
101 have higher relative humidity (RH) and lower temperatures than inland Southern California. Since the turn
102 of the century, SoCAB has been designated as a nonattainment area for the 1997 8-hour ozone standard
103 (80 ppb), with design values for ozone well above the 2015 standard of 70 ppb (Figure 1). In 2019, the
104 maximum daily 8-hour average (MDA8) ozone concentration in SoCAB was 108 ppb at the design value
105 location with a classification of “extreme” (Redlands, California) (California Air Resources Board, 2023).

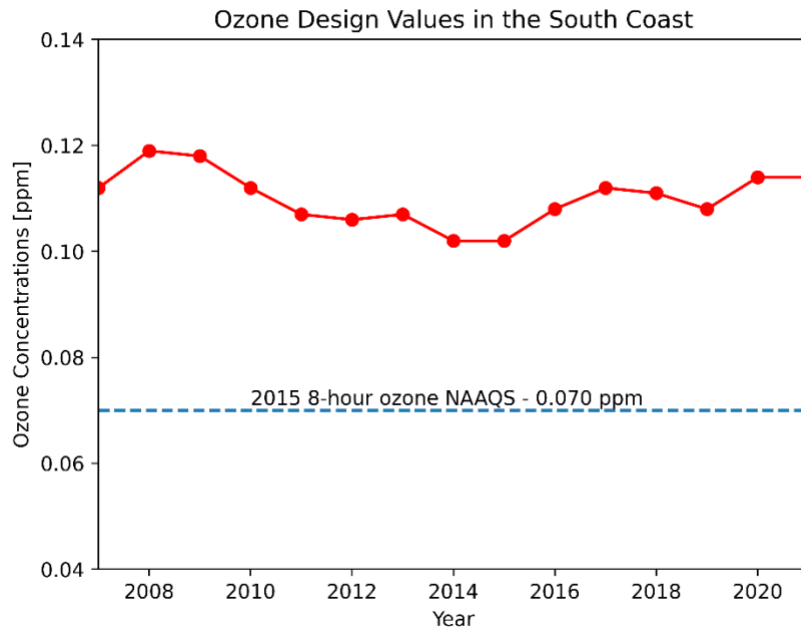


Figure 1. Ozone design values for the South Coast Air Basin from 2006 to 2020 (<https://www.epa.gov/air-trends/air-quality-design-values>).

2.1 Model Input Data

The input meteorological data for the CMAQ simulation were generated using the Weather Research and Forecasting (WRF) model. WRF was initiated using initial and boundary condition meteorology data from the North American Mesoscale (NAM) Forecast System integrated with high-resolution sea surface temperature (SST) from the Group for High Resolution Sea Surface Temperature. We used the WRF Objective Analysis program to improve the meteorological simulation, and this step blends observed surface and upper air observations with background WRF fields. The surface and upper air observations are sourced from NCEP ADP Global Surface Observational Weather Data (ds461) and NCEP ADP Global Upper Air Observational Weather Data (ds351) via the National Center for Atmospheric Research’s Research Data Archive, respectively (Wang et al., 2017).

We re-projected gridded 4 km emissions from 2019 for the year 2020 using a two-step adjustment to account for changes due to the COVID-19 (Zhu et al., 2023). In the first step, a linear projection factor

121 (Eq. 1) was applied to 2019 gridded emissions based on SCAQMD basin-wide, total annual emissions
122 spanning from 2012 to 2034, where the District’s future projections began in the year 2020. The correction
123 factor was calculated for seven air pollutant groups (total organic gases, reactive organic gases, CO, NO_x,
124 SO_x, NH₃, PM).

125
$$\text{Linear projection factor} = \frac{2020 \text{ emis} - 2019 \text{ emis}}{2019 \text{ emis}} \quad (1)$$

126 The second step accounted for traffic reductions due to the COVID-19 lockdown, and reductions
127 were highest from March to May 2020 then slowly but not fully rebounding to pre-lockdown levels toward
128 the end of 2020 (Caltrans, 2023). SCAQMD basin-wide projections understandably did not reflect the
129 decrease in mobile source emissions due to traffic reductions. Moreover, weekly traffic metrics in 2020
130 were acquired for the total flow, flow change, and speed change at 2991 locations in Southern California
131 (Tanvir et al., 2023). Since the traffic data were not evenly distributed over the study domain, we used k-
132 nearest neighbors (k-NN) to obtain the traffic data for grid cells (locations) that had no more than five
133 reported data points (k value ≤ 5). For the grid cells with more than five reported data points, we
134 normalized traffic volume and then averaged the normalized data.

135 2.2 Machine Learning Inputs

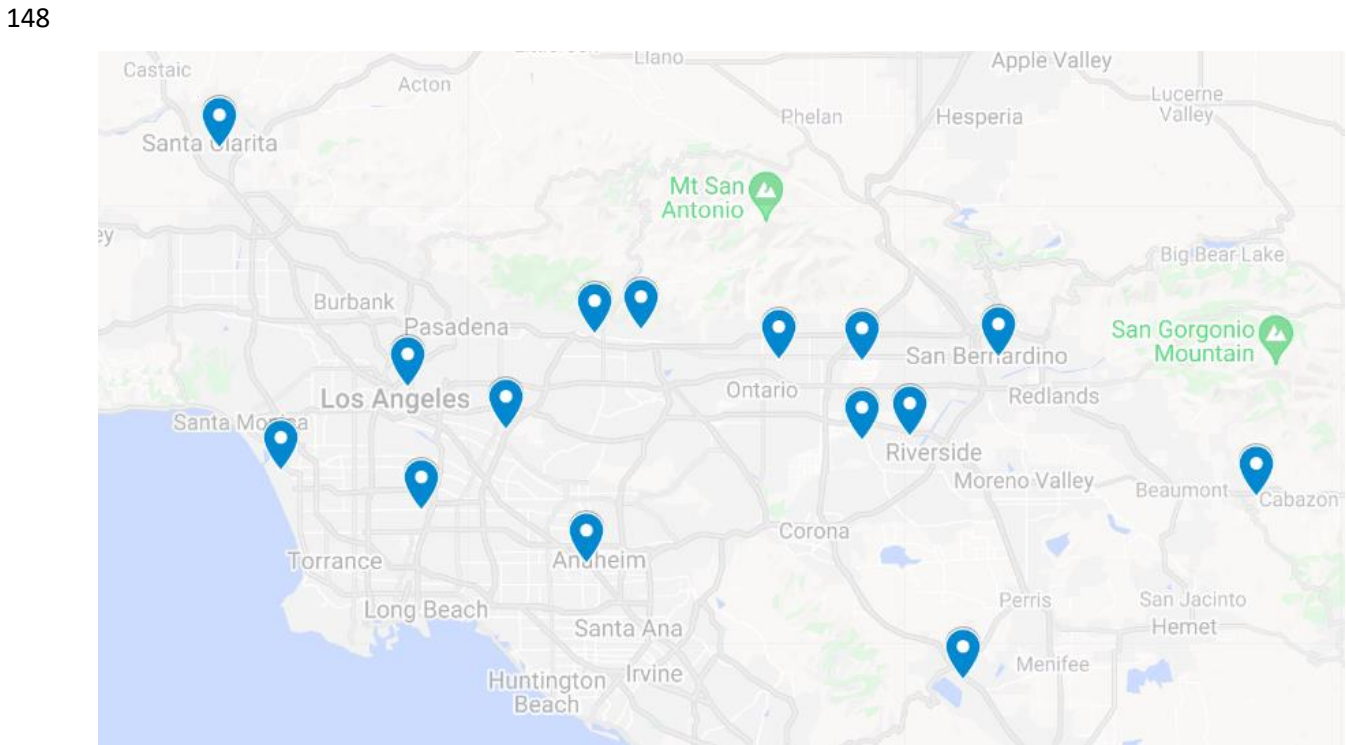
136 We used two air quality features (i.e., NO₂ and NO) and four meteorological features (i.e.,
137 temperature, relative humidity, wind speed, and wind direction) from 15 air monitoring sites in SoCAB
138 (Figure 2). Hourly meteorological and air quality data used for ML training and validation were obtained
139 from the Air Quality System (AQS) data mart
140 (https://aq5.epa.gov/aqsweb/airdata/download_files.html#Raw, last access Jan. 19, 2023). We checked
141 the data to ensure the hourly data was available for all training features. If there was a missing data point
142 for one of the features, we removed the invalid hour and all corresponding features. The date range of

143 the model training data was 2009-2010 and 2016-2019 for all 15 sites (Figure 2). The period from 2011-
 144 2015 was not included in our models due to the limited availability of wind direction and wind speed at
 145 the sites. We used 2020 data for model testing and evaluation (

146 Table 1).

147 *Table 1. Data summary for machine learning modeling.*

| | |
|------------------------------------|--|
| Ground Monitoring Locations | Anaheim, Azusa, Banning, Compton, Fontana, Glendora, Lake Elsinore, LAX, LA North Main Street, Mira Loma, Rubidoux, San Gabriel, Santa Clarita, San Bernardino, Upland |
| Features | NO ₂ , NO, temperature, relative humidity, wind speed, wind direction |
| Label | Ozone |
| Data sources | EPA AQS data mart, CARB AQMIS |
| Training years | 2009, 2010, 2016, 2017, 2018, 2019 |
| Evaluation year | 2020 |



149
 150 *Figure 2. Data from 15 air monitoring stations (Anaheim, Azusa, Banning, Compton, Fontana, Glendora, Lake Elsinore, LAX, LA*
 151 *North Main Street, Mira Loma, Rubidoux, San Gabriel, Santa Clarita, San Bernardino, Upland) were used for ML model predictions*
 152 *of ozone concentrations.*

3. Methods

We carried out a parallel approach using both ML and CMAQ to predict 2-D ozone concentrations as shown in Figure 4. The deterministic model (top panel) utilized WRF and CMAQ to simulate ozone concentrations based on a set of emissions and meteorology inputs. In contrast, the ML model (bottom panel) relied on observational meteorology and air quality data to predict ozone concentrations. ML and CMAQ models are

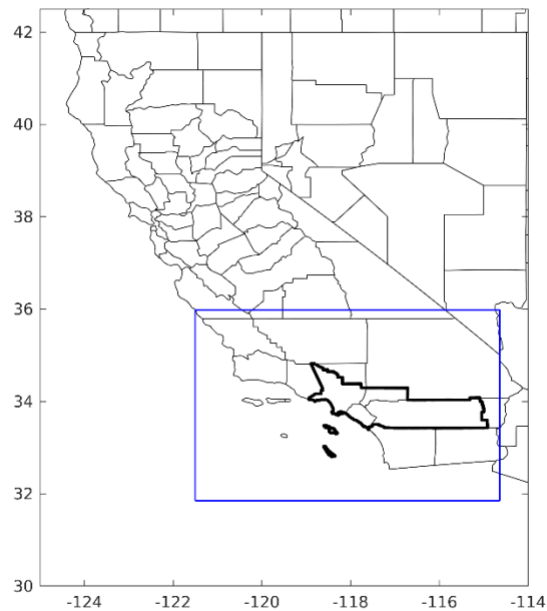


Figure 3. The third and inner-most domain (blue boundary) with 4 km horizontal grid spacing covered the entire SCAQMD region (thick black lines).

evaluated with observational data to assess their performance, especially in response to the irregular emissions patterns of 2020. Additionally, predictions from ML and interpolation were explored to examine the NO_x and VOC limited regimes in Southern California, providing insights into how the models perform in different regions.

3.1 CMAQ Modeling

In this study, we compared the performance of both CMAQ and ML with spatial interpolations of ozone concentrations in SoCAB for the year 2020. The CMAQ simulation covered three distinct periods to study the impact of COVID-19 lockdown on air pollutant concentrations: pre-lockdown (Jan 1st to Mar 18th), lockdown (Mar 16th to May 15th), and post-lockdown (after May 16th) periods. Meteorological modeling was carried out using the Weather Research and Forecasting (WRF) model version 3.9 with 4 km horizontal grid spacing, 11 vertical layers for the finest domain (10 layers near the surface), and 156 x 102 grid cells (Figure 3). There were two parent domains with coarser horizontal grid spacing (36 km and

176 12 km for domain 1 and domain 2, respectively). WRF configurations were optimized for SoCAB, and they
177 included the use of USGS land use, thermal diffusion surface physics, and Yonsei University planetary
178 boundary layer scheme (Hong et al., 2006; Huang et al., 2014). The CMAQ simulation used the modified
179 2020 emissions and previously described WRF simulations as inputs. The choice of chemical mechanism
180 was SAPRC07tc_ae6_aq, i.e., SAPRC07tc photochemical mechanism, aerosol module 6, and aqueous
181 chemistry (Byun & Schere, 2006; Carter, 2010).

182 3.2 Machine Learning

183 In a preceding study, we tested multiple ML algorithms to obtain a better method that resulted
184 in the highest prediction accuracy for ozone concentrations in the SoCAB. Those included neural network,
185 support vector machine, k-nearest neighbors, and random forest (Do et al., 2023). Here, we selected
186 random forest regression (RFR), as RFR is the most suitable ML algorithm for predicting ozone
187 concentrations in SoCAB (Do et al., 2023). For reference, RFR is a supervised learning algorithm with a
188 tree-based ensemble method, i.e., a combination of multiple decision trees trained on an independent
189 collection of input variables. In this application, RFR selected a random collection of features from the six
190 input features for each decision tree to reduce bias, and the output of RFR is the average result from all
191 decision trees (Rodriguez-Galiano et al., 2015; Zhang and Ma, 2012).

192 In this study, we selected six training features to predict ozone concentrations, which included
193 two air quality features (NO and NO₂) and four meteorological features (temperature, relative humidity,
194 wind speed, and wind direction). The two air quality features are directly related to ozone formation in
195 the troposphere. Ozone undergoes the photolytic cycle during the day and is removed by NO_x during
196 nighttime (Brune, 2001; Liu et al., 1980; Trousdell et al., 2019). The four meteorological features were well
197 studied in our previous work and were shown as the most important features to capture the variability in
198 annual ozone, especially in SoCAB (Camalier et al., 2007; Gao et al., 2022; Jaffe, 2020).

199 We used the scikit-learn 0.22 library supported by the Python programming language to train our
 200 RFR model. Again, the input features are NO₂, NO, temperature, relative humidity, wind speed, and wind
 201 direction, and the label is ozone. We tuned the algorithm by varying the number of decision trees, the
 202 depth of the tree, sample split, and the sample leaf to obtain the best prediction accuracy. We used the
 203 same model tuning approached described in Do et al. (2023) (Table 2) (Do et al., 2023).

204 *Table 2. Optimal RFR configurations for the study*

| Hyperparameter | Description |
|----------------------------|--|
| n_estimators = 16 | The number of trees in the forest. |
| max_features = 'auto' | The number of features to consider when looking for the best split. |
| max_depth=None | The maximum depth of the tree. |
| min_samples_split=5 | The minimum number of samples required to split an internal node. |
| min_samples_leaf=30 | The minimum number of samples required to be at a leaf node. |
| min_weight_fraction_leaf=0 | The minimum weighted fraction of the sum total of weights required to be at a leaf node. |
| max_leaf_nodes=None | Best nodes are defined as relative reduction in impurity. |
| n_jobs=8 | The number of jobs to run in parallel. |

205

206 3.3 Spatial Interpolation

207 To generate a two-dimensional ozone concentration map, we first ran the RFR model to obtain
 208 the ozone concentrations at each air monitoring location (15 sites), which served as the model building
 209 sites. In other words, we applied a pointwise ML algorithm to predict ozone concentration at each trained
 210 location. Next, we spatially interpolated the output over the target Southern California region. We applied
 211 three different spatial interpolation methods (ordinary kriging, inverse distance weighting (IDW), and
 212 bicubic interpolation) and comparatively evaluated the performance of each method. Each interpolation
 213 approach is described below.

214 Ordinary kriging was applied to interpolate ozone concentration at the 10 km resolution over the
 215 study area. Ordinary kriging is a well-known spatial interpolation method developed by Danie G. Krige.
 216 Generally, kriging predicts the values for unknown locations by performing a series of linear combinations
 217 of values at known locations. Equation 1 expresses the generic form of the estimator to predict the
 218 optimum value Z^* of an unknown location by combining the known values Z_i with their weights λ_i (Oliver
 219 and Webster, 1990). We can write the variance σ^2 as an optimization problem (Eq. 2) that can be solved
 220 using the Lagrange multiplier μ (Eq. 3).

$$221 \quad Z^*(u) = \sum_{i=1}^n \lambda_i Z(u_i) \quad (1)$$

$$222 \quad \sigma^2(u) = \text{Var}[Z(u) - Z^*(u)] = - \sum_{j=1}^n \sum_{i=1}^n \lambda_j \lambda_i \gamma(u_i - u_j) + 2 \sum_{i=1}^n \lambda_i \gamma(u_i - u) \quad (2)$$

$$223 \quad \sum_{j=1}^n \lambda_j (u_i - u_j) + \mu = \gamma(u_i - u) \quad (3)$$

224 and

$$225 \quad \sum_{j=1}^n \lambda_j = 1 \quad (4)$$

226 μ is the Lagrange multiplier, u_i and u_j are the distance of known locations from unknown locations u , γ
 227 is the variogram, and $i = 1, \dots, n$. Equations 1 and 2 are called the kriging system, and λ is the kriging
 228 weight. The values for λ_i and the optimum value Z^* are obtained by solving the kriging system and
 229 Equation 1 (Yamamoto, 2000).

230 Bicubic interpolation is another method for interpolating data points on a two-dimensional grid.
 231 The interpolated surface can be written in terms of two variables (Eq. 5). The polynomial p consists of
 232 sixteen coefficients a_{ij} that are solved with sixteen boundary conditions (i.e., $(x = 0, y = 0)$, $(x = 1, y =$

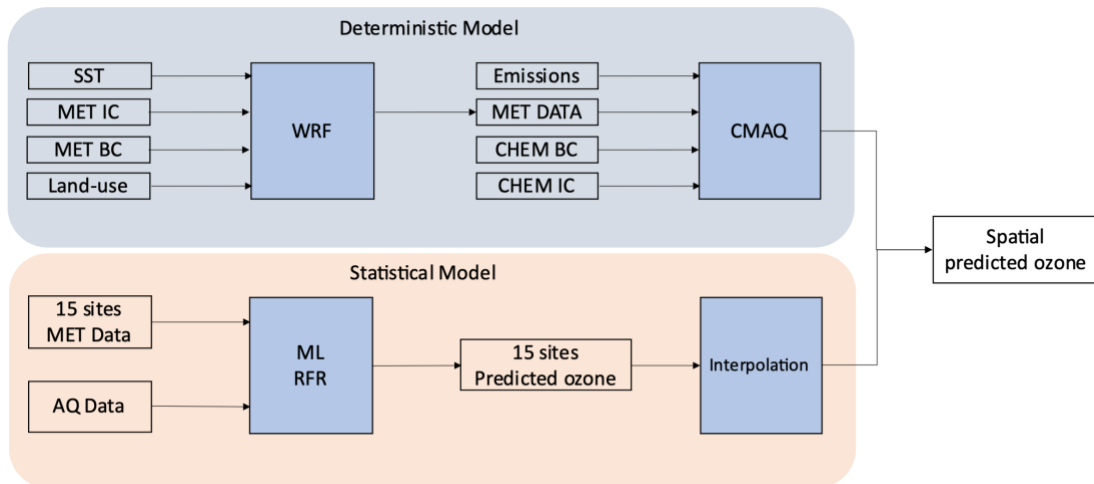
233 0), (x = 0, y = 1), (x = 1, y = 1)) and its derivatives with respect to x, y, and xy (Seiler and Seiler,
 234 1989).

235
$$p(x, y) = \sum_{i=0}^3 \sum_{j=0}^3 a_{ij} x^i y^j \tag{5}$$

236 The IDW interpolation method accounts for the distances between the interpolated points and
 237 the measured locations. The assumption for IDW is that points close to each other are more alike and
 238 have more significant influence than those farther apart. Thus, the nearest measured values have greater
 239 weights assigned. Equation 6 shows that the predicted value Z(x) is inversely proportional to the distance
 240 between the measured and interpolated points d(x, x_i).

241
$$Z(x) = \frac{\sum_{i=1}^n \frac{Z_i}{d(x, x_i)^p}}{\sum_{i=1}^n \frac{1}{d(x, x_i)^p}} \tag{6}$$

242 where Z(x) is the predicted value, d is the distance, x is the unknown point, x_i is the known location, Z_i
 243 is the value of a known location, and p is the power (Bartier and Keller, 1996).



244
 245 *Figure 4. Flow diagram of the deterministic (CMAQ) and ML models for predicting 2D ozone concentrations in Southern California,*
 246 *where SST is sea surface temperature, MET IC and MET BC are meteorology initial and boundary conditions, CHEM IC and CHEM*
 247 *BC are chemistry initial and boundary conditions, AQ Data is air quality data (NO and NO₂), MET Data is meteorology data*
 248 *(temperature, relative humidity, wind speed, and wind direction).*

249 4. Model Evaluation

250 Figure 5 shows a snapshot of the
251 ozone concentrations over the
252 interpolation region at 4:00 PM on June
253 22, 2020 (the highest ozone episode of
254 the day), using ordinary kriging. The
255 colored dots with a white border are the
256 actual values at the evaluation sites, and
257 those without a white border are the RFR

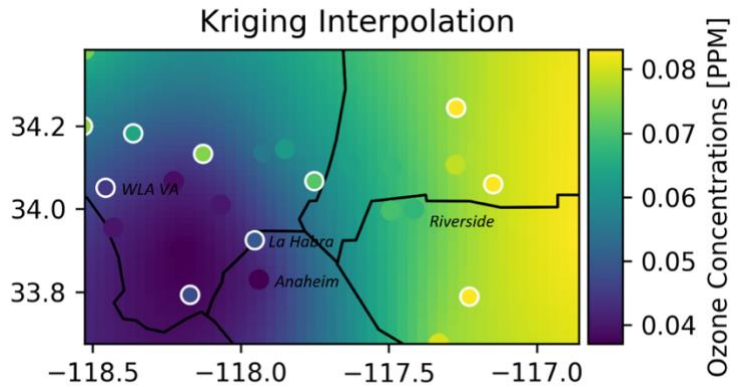


Figure 55. Hourly ozone heatmap (16:00 on June 22, 2020) using ordinary kriging. The dots with white borders are the evaluation sites, and dots without borders are the training sites.

258 predicted values for training sites. The model successfully reconstructed the spatial trends in the region
259 where the lowest ozone levels were in the southwest (coastal) and the highest were in the east (inland),
260 and there was good agreement with the actual ozone concentrations. Figures S2 and S3 show the heatmap
261 for bicubic and IDW interpolation for the same timestamp. Although all interpolation methods predicted
262 the lowest ozone concentrations in the Southwest, the highest ozone concentrations were predicted in
263 the Northeast of the study region for bicubic and in the North for IDW. The concentration gradient
264 increased from south to north for bicubic and IDW, but from west to east for ordinary kriging.

265 The performance of the models was evaluated based on commonly used statistical metrics: mean
266 bias (MB), correlation coefficient, root mean square error, and R^2 (equations listed in SI). The models were
267 evaluated based on data from 27 air monitoring stations in SoCAB, of which 15 sites were used to evaluate
268 the training sites, and the other 12 sites were used to evaluate the performance of the three interpolation
269 methods at non-training sites. Table 3 and Table 4 highlight R^2 for daily average ozone for the bicubic,
270 IDW, and ordinary kriging interpolations, as well as R^2 for the CMAQ comparison. We used the entire year

271 to evaluate the interpolation methods, but we only used the five highest ozone months from May to
 272 September for the CMAQ evaluation.

273
 274 *Table 3. Daily average R² at the 15 building sites for three interpolation methods for the year 2020. R² for CMAQ was computed*
 275 *using the five highest ozone months May - September of 2020.*

| Sites | Bicubic R ² | IDW R ² | Ordinary Kriging R ² | CMAQ R ² |
|------------------|------------------------|--------------------|---------------------------------|---------------------|
| Anaheim | 0.66 | 0.67 | 0.74 | 0.41 |
| Azusa | 0.52 | 0.64 | 0.77 | 0.59 |
| Banning | 0.17 | 0.46 | 0.73 | 0.26 |
| Compton | 0.65 | 0.67 | 0.77 | 0.48 |
| Fontana | 0.88 | 0.89 | 0.87 | 0.59 |
| Glendora | 0.46 | 0.53 | 0.72 | 0.52 |
| Lake Elsinore | 0.52 | 0.70 | 0.79 | 0.56 |
| LA North Main ST | 0.36 | 0.67 | 0.78 | 0.48 |
| LAX | 0.31 | 0.48 | 0.65 | 0.25 |
| Mira Loma | 0.56 | 0.71 | 0.86 | 0.67 |
| Rubidoux | 0.46 | 0.65 | 0.86 | 0.68 |
| San Bernardino | 0.68 | 0.85 | 0.86 | 0.67 |
| San Gabriel | 0.53 | 0.77 | 0.81 | 0.62 |
| Santa Clarita | 0.27 | 0.72 | 0.84 | 0.61 |
| Upland | 0.76 | 0.80 | 0.86 | 0.61 |

276
 277 *Table 4. Daily average R² at 12 evaluation sites, and these were not used spatial interpolation. R² for CMAQ was computed using*
 278 *the five highest ozone months, May - September of 2020.*

| Sites | Bicubic R ² | IDW R ² | Ordinary Kriging R ² | CMAQ R ² |
|-----------------|------------------------|--------------------|---------------------------------|---------------------|
| Crestline | 0.35 | 0.42 | 0.42 | 0.23 |
| La Habra | 0.75 | 0.80 | 0.77 | 0.44 |
| Long Beach | 0.46 | 0.60 | 0.56 | 0.30 |
| Mission Viejo | 0.15 | 0.36 | 0.49 | 0.39 |
| North Hollywood | 0.67 | 0.67 | 0.79 | 0.59 |
| Pasadena | 0.55 | 0.71 | 0.78 | 0.57 |
| Perris | 0.55 | 0.72 | 0.80 | 0.56 |
| Pomona | 0.71 | 0.83 | 0.84 | 0.68 |
| Redlands | 0.60 | 0.74 | 0.71 | 0.57 |
| Reseda | 0.63 | 0.63 | 0.71 | 0.01 |
| West LA | 0.29 | 0.56 | 0.60 | 0.28 |
| Winchester | 0.37 | 0.40 | 0.39 | 0.45 |

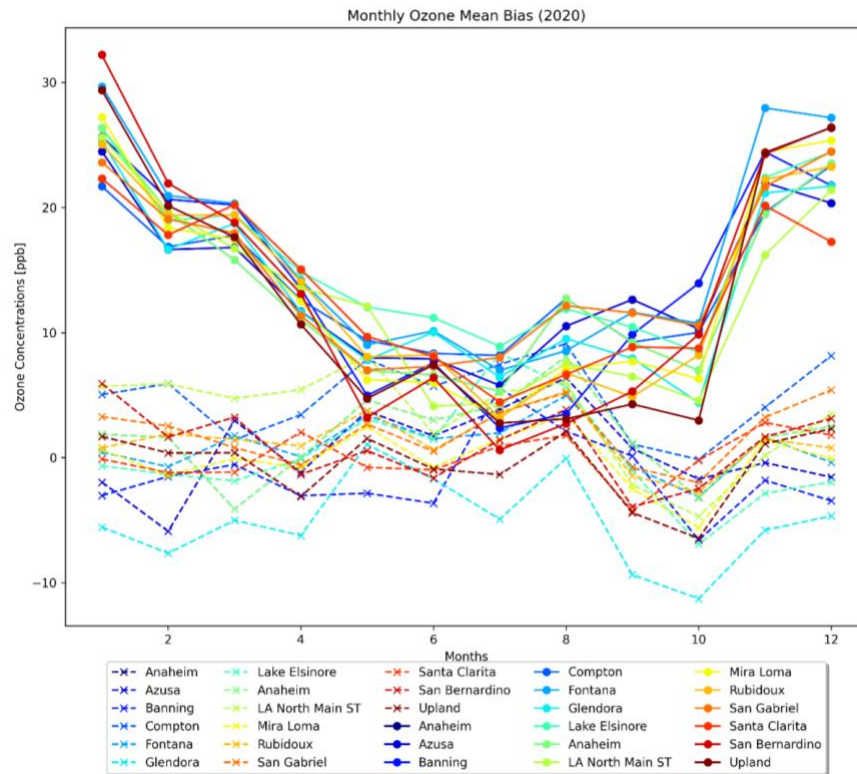
279
 280 The bicubic R² indicates the poorest performance of the three interpolation methods. The lowest
 281 R² values for the 12 evaluation sites were 0.15 and 0.29, Mission Viejo and West LA, respectively (Table

282 4). The poor performance resulted from the method used to calculate the coefficients a_{ij} (Eq. 5), for which
283 the values of coefficients did not depend on the distance between interpolating points but were
284 dependent on the formation of a smooth curve. Bicubic is best for evenly distributed points, such as
285 interpolating image pixels. IDW showed a significant improvement compared to bicubic interpolation. The
286 lowest R^2 was 0.36 for Mission Viejo, and the highest R^2 was 0.83 for Pomona. Since IDW accounts for the
287 distances between the interpolation points and the data points, farther data points have less influence on
288 the interpolation points. Ordinary kriging resulted in the best interpolation method, with the lowest R^2 of
289 0.39 for Winchester and the highest R^2 of 0.84 for Pomona. Kriging not only accounts for the distance
290 between building points and interpolated data by assigning larger weight λ_i to the near neighbors, but it
291 also considers the variability of data by considering the variance of input data, σ^2 . The basis of the
292 variogram function represents the spatial variability of data. The variance depends not on observation
293 values but on the variogram model and geometry (Kebaili Bargaoui and Chebbi, 2009) (Eq. 2).

294 ML with interpolation gave a poor performance for Crestline and Winchester locations. Crestline
295 is located in the mountains and to the northeast of SoCAB, which is elevated terrain associated with upper
296 air and a different air mass at times. Crestline ozone was not well-correlated with coastal or inland sites.
297 Thus, interpolated Crestline ozone based on coastal or inland data points will likely yield poor results. The
298 Winchester air monitoring site is located near the Skinner Reservoir (Figure S1), far away from other data
299 points (Lake Elsinore and Banning). Low R^2 for Winchester can be explained by the influence of the lake
300 and local meteorology and air quality. The ordinary kriging model performed well for locations bounded
301 by data points with R^2 above 0.56. However, poor interpolation results occurred for peripheral locations
302 in SoCAB (Crestline, Mission Viejo, and Winchester). LAX ozone levels were not well correlated with
303 meteorology, and training the ML model with fewer meteorological features did not affect the
304 performance of the LAX location. Overall, model performance increased from the West to the East, with
305 better prediction for inland sites.

306 The distribution of the monthly mean bias (MB) for ordinary kriging interpolation centered around
307 zero with the range between +9 ppb for Compton (August) and -11 ppb for Glendora (October). Eleven
308 building sites have a net positive monthly MB, and four have a net negative monthly MB (Figure 6). The
309 results from the CMAQ simulation overestimated the ozone levels. CMAQ's best performance was from
310 May to October when the MBs were the smallest. In general, ozone concentrations in the SoCAB are
311 highest during the summer and lowest in the winter, corresponding with the temperature. Even though
312 the CMAQ simulation captures diurnal variation, the seasonal variation is not as well-represented (Figure
313 S4, S5, S7, and S11). Lower performing CMAQ results could come from uncertainties in emissions
314 estimates. CMAQ generally overestimated ozone concentrations because the simulated nighttime ozone
315 concentrations were higher than those observed, potentially due to underestimated nighttime NO_x
316 emissions (Zhu et al., 2023). In other words, that there was not enough NO_x emitted in the model during
317 the daytime for ozone formation and at night for ozone removal (Awang and Ramli, 2017; Brown et al.,
318 2004).

319 Training features can be varied to study the sensitivity to modeled ozone response. For example,
320 we can perturb the temperature, RH, or emissions values and examine the ozone levels corresponding to
321 the change in the features. However, because the formation of ozone results from a complex combination
322 of chemical reactions, resulting impacts are nonlinear and interdependent. Therefore, when using ML to
323 test for sensitivity to a feature, one should consider feature dependencies. For example, in testing
324 temperature impacts on ozone concentration, we must consider both how temperature impacts
325 photolysis rates (NO₂ degradation) as well as simultaneous correlations/anticorrelation with other
326 meteorological variables, such as RH or wind speed.



327

328 *Figure 6. Monthly mean bias computed for 2020 for 15 sites using the kriging interpolation method (dash lines), and CMAQ*
 329 *simulation (solid lines). The colors of the lines correspond to the evaluation locations.*

330 5. Discussion

331 The reduction in traffic volumes during the lockdown from March to May led to a decrease in
 332 observed CO and NO_x (Ivey et al., 2020; Tanvir et al., 2023). As a result, we expected an overall reduction
 333 in ozone levels over the SoCAB region. The average diurnal ozone concentrations before the lockdown
 334 (Jan - Feb) in 2020 were noticeably greater than the average from 2016 – 2019 for all 15 building sites.
 335 Figure 7 shows the averaged diurnal profiles of three 2020 periods for inland sites, Lake Elsinore and
 336 Fontana: pre-lockdown (a, d), lockdown (b, e), and post-lockdown (c, f) periods. Before the lockdown, the
 337 2020 ozone concentrations (red line) in Lake Elsinore and Fontana exceeded the four-year average (blue
 338 line), indicating a recent worsening of ozone trends in Southern California. The ML model with the
 339 interpolation method (black line) successfully predicted this ozone trend before the lockdown. During the
 340 lockdown, observed ozone levels in 2020 significantly decreased in Lake Elsinore, dropping below the four-

341 year average. After the lockdown, ozone levels in 2020 rebounded but remained lower than the pre-
342 lockdown period. The ML model effectively captured these ozone trends throughout the three periods of
343 2020 for the Lake Elsinore site. In contrast, ozone levels in Fontana did not decrease significantly below
344 the four-year average during the lockdown and remained high afterward. It is important to note that Lake
345 Elsinore is located in a remote area surrounded by trees. During the lockdown, Lake Elsinore showed a
346 drop in ozone concentrations, indicating that the location is in a NO_x limited atmosphere, where
347 fluctuations in NO_x have a significant impact on ozone levels. On the other hand, Fontana is an urban site,
348 and the ozone levels did not exhibit significant improvement during the lockdown, suggesting that
349 Fontana is located in a VOC limited regime.

350 Post-lockdown differences compared to the four-year average were not significant across the 15
351 sites. The RFR model captured ozone trends throughout 2020, although slightly lower during and despite
352 the observed reduction in NO_x, suggesting that meteorological features would play an important role in
353 predicting ozone levels during anomalous episodes in addition to air quality features. Actual and modeled
354 discrepancies also indicate anomalous ozone behavior during lockdown. For instance, several sites in the
355 SoCAB showed an increase in ozone levels based on the diurnal profile implying that the urban locations
356 in the SoCAB were VOCs-limited regimes, where reduction in NO_x reduction-initiated ozone enhancement
357 (Parker et al., 2020).

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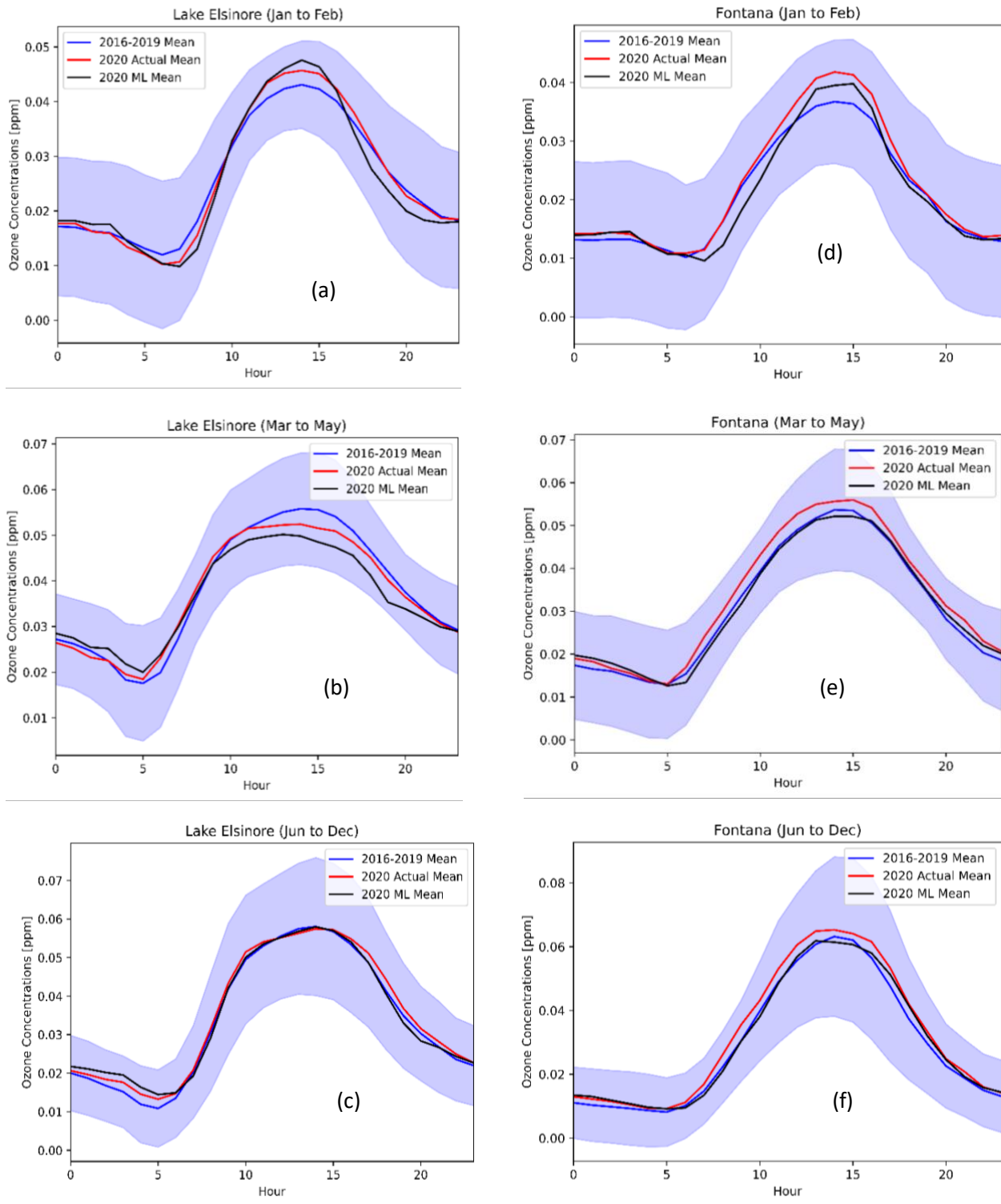


Figure 77. Averaged diurnal profiles of 2016 - 2019 (blue), actual 2020 (red), and ML predicted 2020 (black) ozone concentrations (ppm) at Lake Elsinore (a, b, c) and Fontana (d, e, f) for three different periods: (a,d) pre-lockdown (Jan to Feb), (b,e) lockdown (Mar to May), and (c,f) post-lockdown (after May). The shaded area is the standard deviation of the 2016 - 2019 measurements. Additional sites are provided in the SI.

360 6. Conclusion

361 This study highlights the advantages of spatial interpolation methods for ozone predictions during
362 anomalous environmental events. With modern processor architectures (e.g., AMD Zen 3 or Intel Alder
363 Lake), training the RFR model and performing high-resolution interpolation over the SoCAB region for one
364 prediction year took less than five minutes of walltime with a 16-core processor. In contrast, CMAQ
365 walltime was 16 days for a year-long simulation for the SoCAB region. Further, ozone modeling for 2020
366 was challenging because of expected emissions conditions from March to September, during which traffic
367 volume significantly decreased (up to 40% reduction in some locations). We hypothesized that mid-2020
368 ozone levels would decrease semi-proportionally due to the decline in traffic volume. However, the
369 changes in ozone levels in the SoCAB were small in magnitude, but directionally the changes were
370 informative for future emissions reductions planning (increased ozone indicates VOC limitations).
371 Ordinary kriging interpolation using ML building provided daily data, addressed data missingness, and
372 captured 2020 ozone trends with fairly low bias despite the sudden change in emissions. The ML model
373 with the interpolation method successfully captured ozone trends throughout three periods in 2020,
374 particularly in locations operating under a NO_x limited regime, such as Lake Elsinore. However, it faced
375 challenges in predicting ozone levels during the lockdown period in areas characterized by a VOC limited
376 regime, like Fontana. ML inherently relies on patterns learned from historical data to make predictions,
377 especially for inputs that resemble past occurrences. In this study, the ML model struggled to make
378 accurate predictions for VOC limited regime, suggesting that events akin to the COVID-19 lockdown had
379 not been encountered in the past. Unfortunately, due to the unavailability of speciated VOC data, we
380 didn't incorporate them as a training feature in the model. Since ozone formation exhibits a non-linear
381 correlation with both NO_x and VOC, the inclusion of speciated VOC data would likely enhance the model's
382 accuracy, especially for regions with both NO_x and VOC limited regimes. Our ML model provides regulators
383 with valuable insights into NO_x and VOC limited regimes across the Southern California domain, enabling

384 policymakers to devise more effective emission reduction strategies and improve air quality at hyperlocal
385 scales.

386 Data and Source Codes

387 All training and evaluating air quality and meteorology data are available at
388 https://aq5.epa.gov/aq5web/airdata/download_files.html#Raw. Weekly traffic observations in Southern
389 California and emissions are available upon request. Source codes for ML and interpolation were uploaded
390 to GitHub: <https://github.com/kdo037/Machine-Learning-with-Spatial-Interpolation>.

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500

Supplemental Information for:

Performance of Machine Learning for Ozone Modeling in Southern
California during the COVID-19 Shutdown

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Evaluation Metrics

Correlation coefficient

$$CC = \frac{\sum_{i=1}^N (M_i - \bar{M})(O_i - \bar{O})}{[\sum_{i=1}^N (M_i - \bar{M})^2 \sum_{i=1}^N (O_i - \bar{O})^2]^{\frac{1}{2}}} \quad (1)$$

Mean bias:

$$MB = \frac{1}{N} \sum_{i=1}^N (M_i - O_i) \quad (2)$$

Mean absolute error:

$$MAE = \frac{1}{N} \sum_{i=1}^N |M_i - O_i| \quad (3)$$

Root mean square error:

$$RMSE = \left[\frac{1}{N} \sum_{i=1}^N (M_i - O_i)^2 \right]^{\frac{1}{2}} \quad (4)$$

Relative root mean square error:

$$rRMSE = \frac{\left[\frac{1}{N} \sum_{i=1}^N (M_i - O_i)^2 \right]^{\frac{1}{2}}}{\frac{1}{N} \sum_{i=1}^N O_i} \quad (5)$$

Mean normalized bias:

$$MNB = \frac{1}{N} \sum_{i=1}^N \frac{M_i - O_i}{O_i} \quad (6)$$

Mean normalized absolute error:

$$MNAE = \frac{1}{N} \sum_{i=1}^N \frac{|M_i - O_i|}{O_i} \quad (7)$$

Normalized mean bias:

$$NMB = \frac{\sum_{i=1}^N (M_i - O_i)}{\sum_{i=1}^N O_i} \quad (8)$$

Normalized mean absolute error:

$$NMAE = \frac{\sum_{i=1}^N |M_i - O_i|}{\sum_{i=1}^N O_i} \quad (9)$$

Fractional bias:

$$FB = \frac{1}{N} \sum_{i=1}^N \frac{M_i - O_i}{(M_i + O_i)/2} \quad (10)$$

Fractional absolute error:

$$FAE = \frac{1}{N} \sum_{i=1}^N \frac{|M_i - O_i|}{(M_i + O_i)/2} \quad (11)$$

Model mean:

$$\bar{M} = \frac{1}{N} \sum_{i=1}^N M_i \quad (12)$$

Observational mean:

$$\bar{O} = \frac{1}{N} \sum_{i=1}^N O_i \quad (13)$$

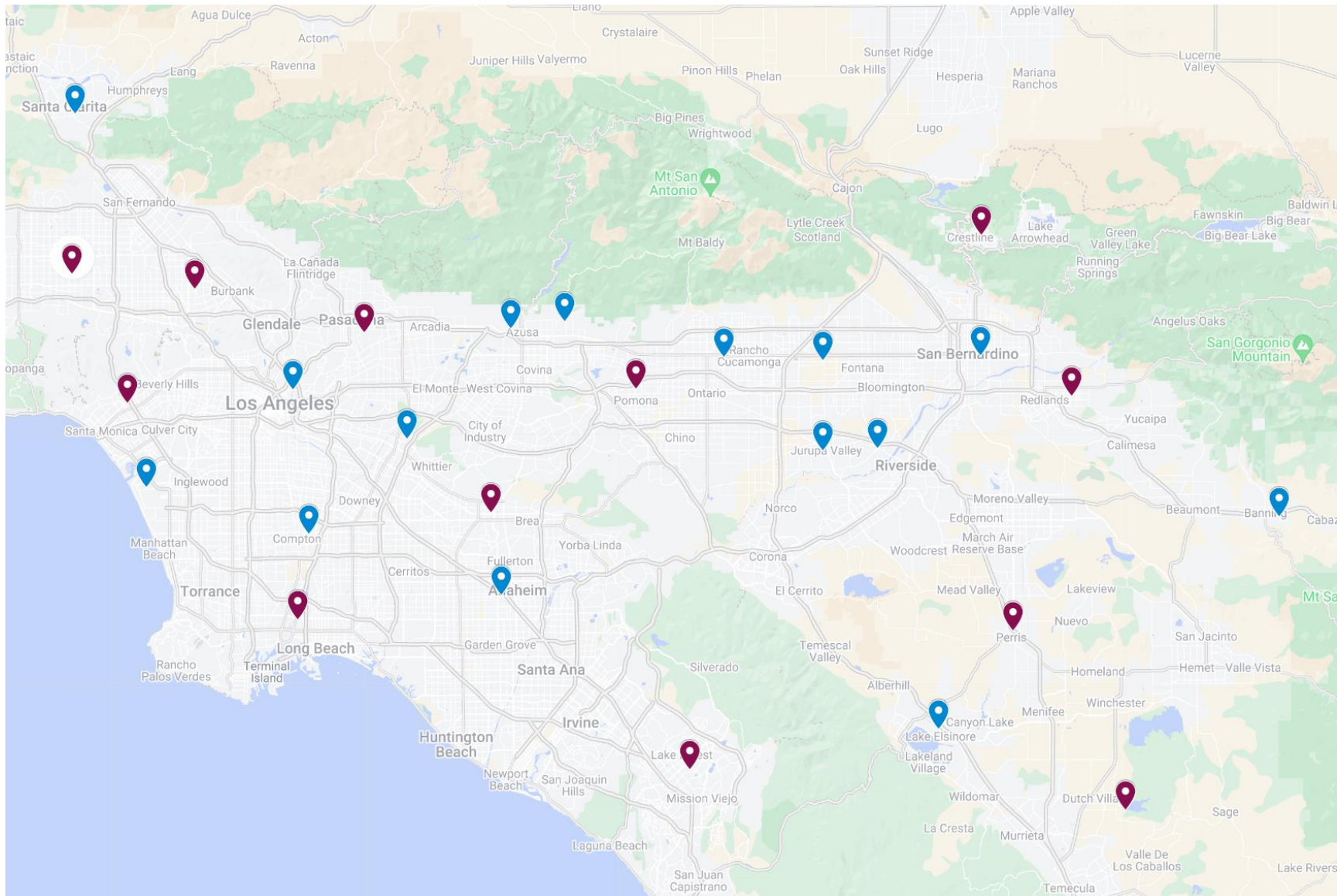


Figure S1. The map shows 27 air monitoring sites in the SoCAB. Blue labels were used for interpolation points, and red labels were used for interpolation performance evaluation.

Table S1. The R2 for CMAQ was computed for the entire year of 2020.

| Sites | 2020 CMAQ R ² |
|------------------|--------------------------|
| Anaheim | 0.24 |
| Azusa | 0.39 |
| Banning | 0.17 |
| Compton | 0.38 |
| Fontana | 0.36 |
| Glendora | 0.37 |
| Lake Elsinore | 0.43 |
| LA North Main ST | 0.26 |
| LAX | 0.17 |
| Mira Loma | 0.48 |
| Rubidoux | 0.52 |
| San Bernardino | 0.50 |
| San Gabriel | 0.48 |
| Santa Clarita | 0.43 |
| Upland | 0.36 |
| Crestline | 0.22 |
| La Habra | 0.27 |
| Long Beach | 0.15 |
| Mission Viejo | 0.19 |
| North Hollywood | 0.36 |
| Pasadena | 0.32 |
| Perris | 0.47 |
| Pomona | 0.55 |
| Redlands | 0.43 |
| Reseda | 0.36 |
| West LA | 0.18 |
| Winchester | 0.30 |

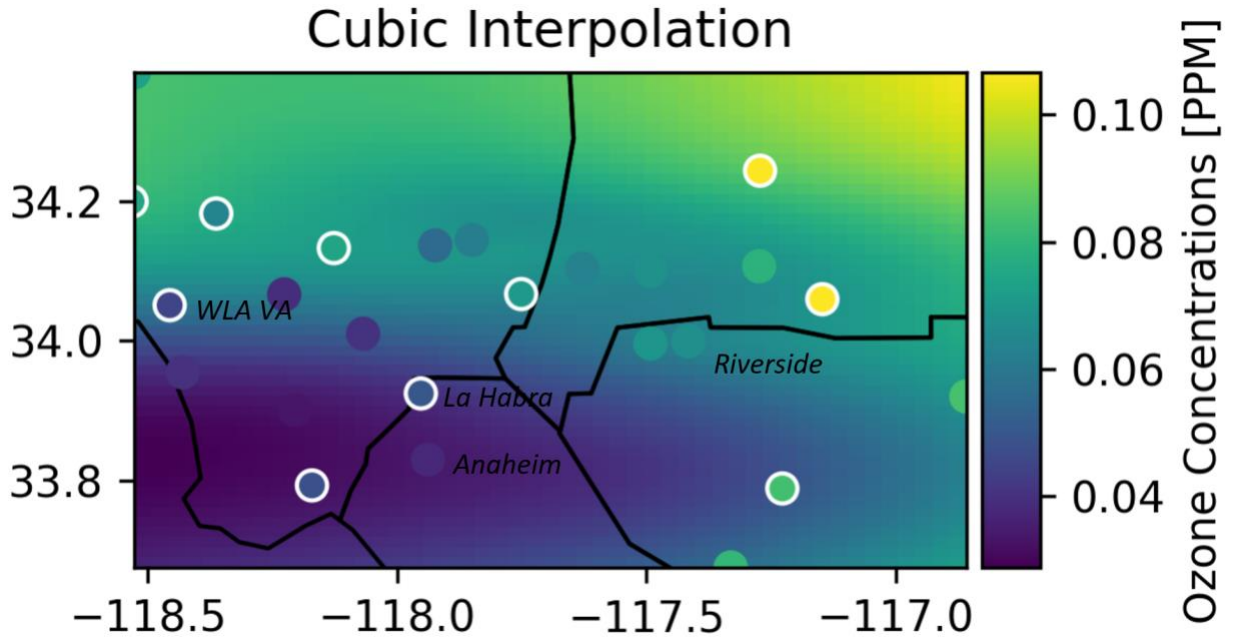


Figure S2. Hourly ozone heatmap (@16pm June 22, 2020) using cubic interpolation.

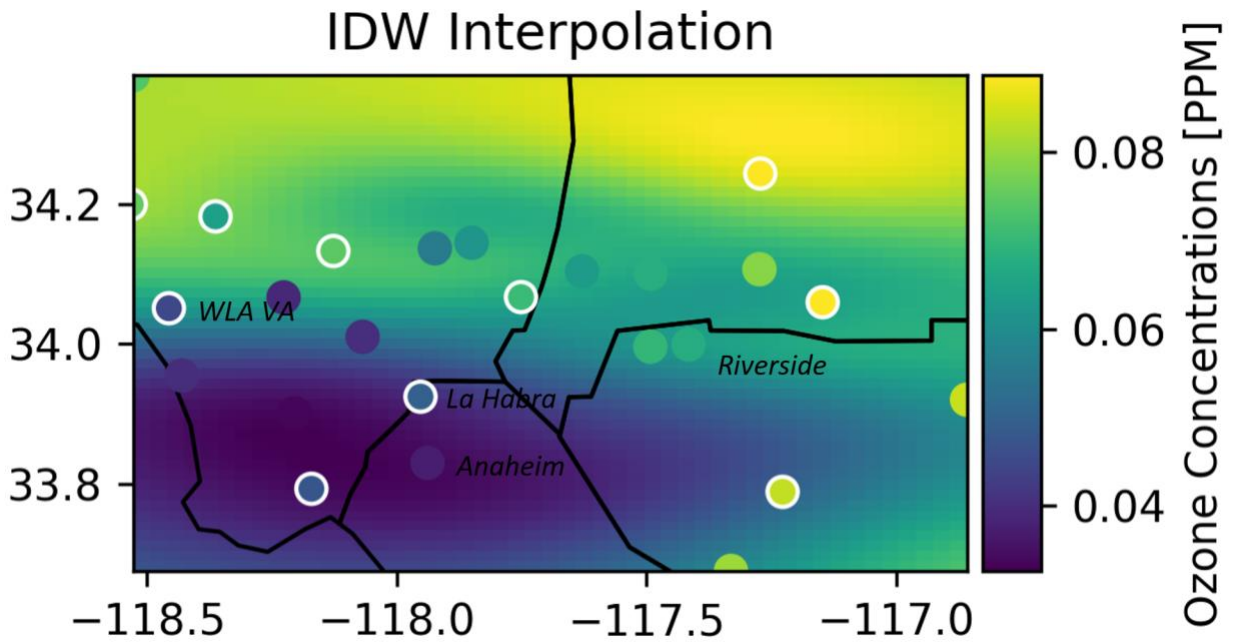


Figure S3. Hourly ozone heatmap (@16pm June 22, 2020) using IDW interpolation.

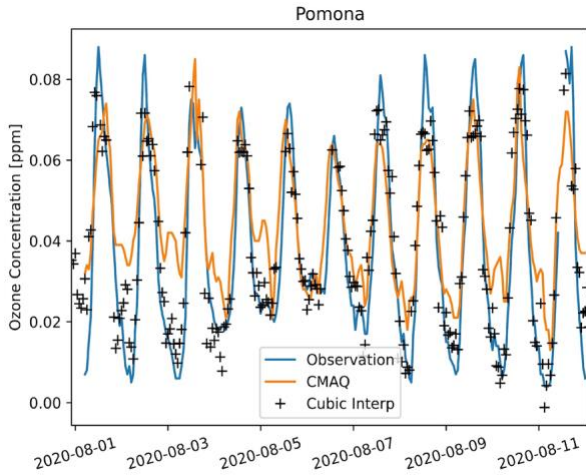


Figure S4. Time series plotting ozone concentrations for CMAQ model, cubic interpolation, and observation

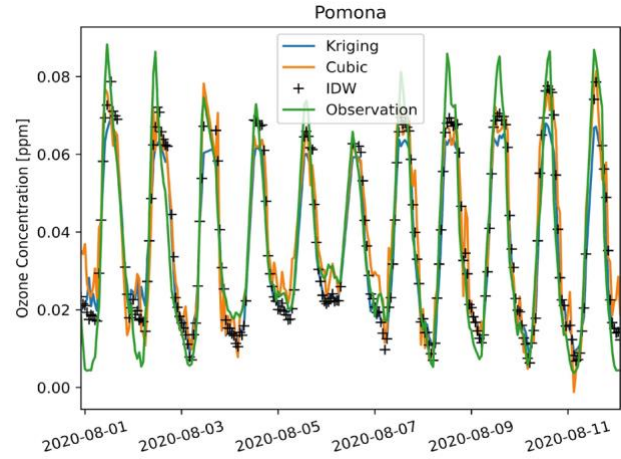


Figure S5. Time series plotting ozone concentrations for three different interpolation methods (kriging, cubic, and IDW) with observation

Table S2. Evaluation was computed using the average of 12 evaluation sites.

| Month | CC | MB | MAGE | RMSE | MNB | MNAE | NMB | NMAE | FB | FAE | MM | OM |
|-------|------|------|------|------|------|------|-------|------|-------|------|------|------|
| 1 | 0.40 | 0.01 | 0.01 | 0.02 | 7.26 | 7.42 | 0.58 | 0.88 | 0.71 | 0.93 | 0.03 | 0.02 |
| 2 | 0.26 | 0.00 | 0.01 | 0.02 | 4.56 | 4.77 | 0.16 | 0.44 | 0.33 | 0.59 | 0.03 | 0.03 |
| 3 | 0.75 | 0.01 | 0.01 | 0.02 | 6.71 | 6.79 | 0.78 | 0.97 | 0.94 | 1.04 | 0.03 | 0.01 |
| 4 | 0.62 | 0.00 | 0.01 | 0.01 | 1.73 | 1.98 | 0.00 | 0.30 | 0.10 | 0.40 | 0.03 | 0.03 |
| 5 | 0.85 | 0.00 | 0.01 | 0.01 | 0.44 | 0.61 | 0.05 | 0.25 | 0.13 | 0.34 | 0.03 | 0.03 |
| 6 | 0.83 | 0.00 | 0.01 | 0.01 | 0.47 | 0.73 | -0.03 | 0.23 | -0.01 | 0.31 | 0.04 | 0.04 |
| 7 | 0.80 | 0.01 | 0.01 | 0.02 | 1.08 | 1.24 | 0.13 | 0.34 | 0.28 | 0.48 | 0.04 | 0.04 |
| 8 | 0.81 | 0.00 | 0.01 | 0.02 | 1.96 | 2.21 | 0.14 | 0.36 | 0.20 | 0.50 | 0.04 | 0.03 |
| 9 | 0.62 | 0.01 | 0.02 | 0.02 | 5.88 | 6.16 | 0.19 | 0.59 | 0.40 | 0.76 | 0.04 | 0.03 |
| 10 | 0.35 | 0.01 | 0.02 | 0.02 | 5.94 | 6.19 | 0.35 | 0.71 | 0.45 | 0.76 | 0.03 | 0.02 |
| 11 | 0.49 | 0.01 | 0.01 | 0.02 | 5.61 | 5.76 | 0.43 | 0.71 | 0.63 | 0.82 | 0.03 | 0.02 |
| 12 | 0.39 | 0.00 | 0.01 | 0.01 | 3.15 | 3.37 | 0.22 | 0.55 | 0.40 | 0.67 | 0.03 | 0.02 |

Monthly Ozone Root Mean Square Error Using Kriging (2020)

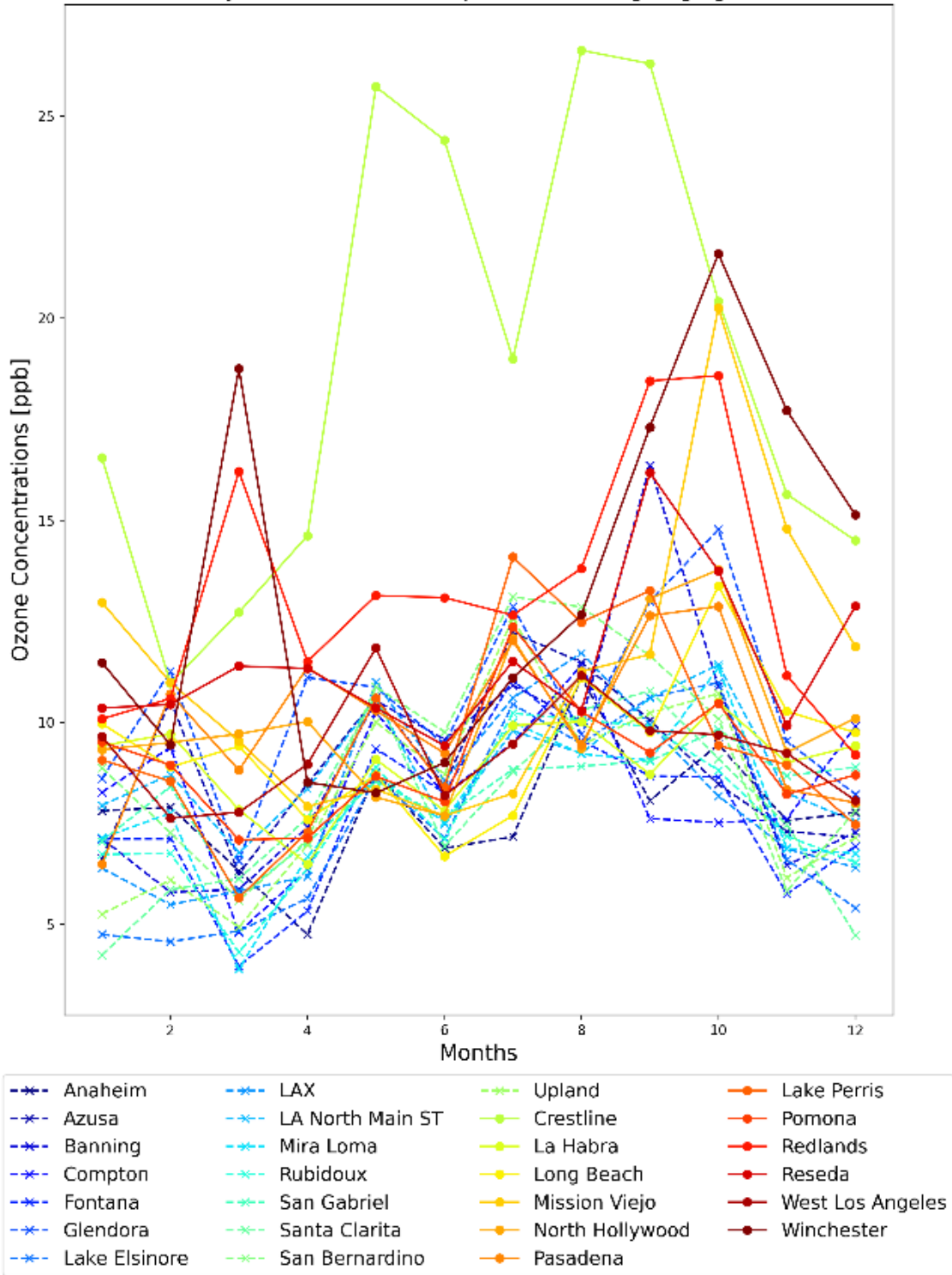


Figure S6. Monthly ozone mean bias from spatial interpolation for 2020 using the Kriging method. The dash lines with x-markers are fifteen building sites, and solid lines with filled dots are the evaluation sites.

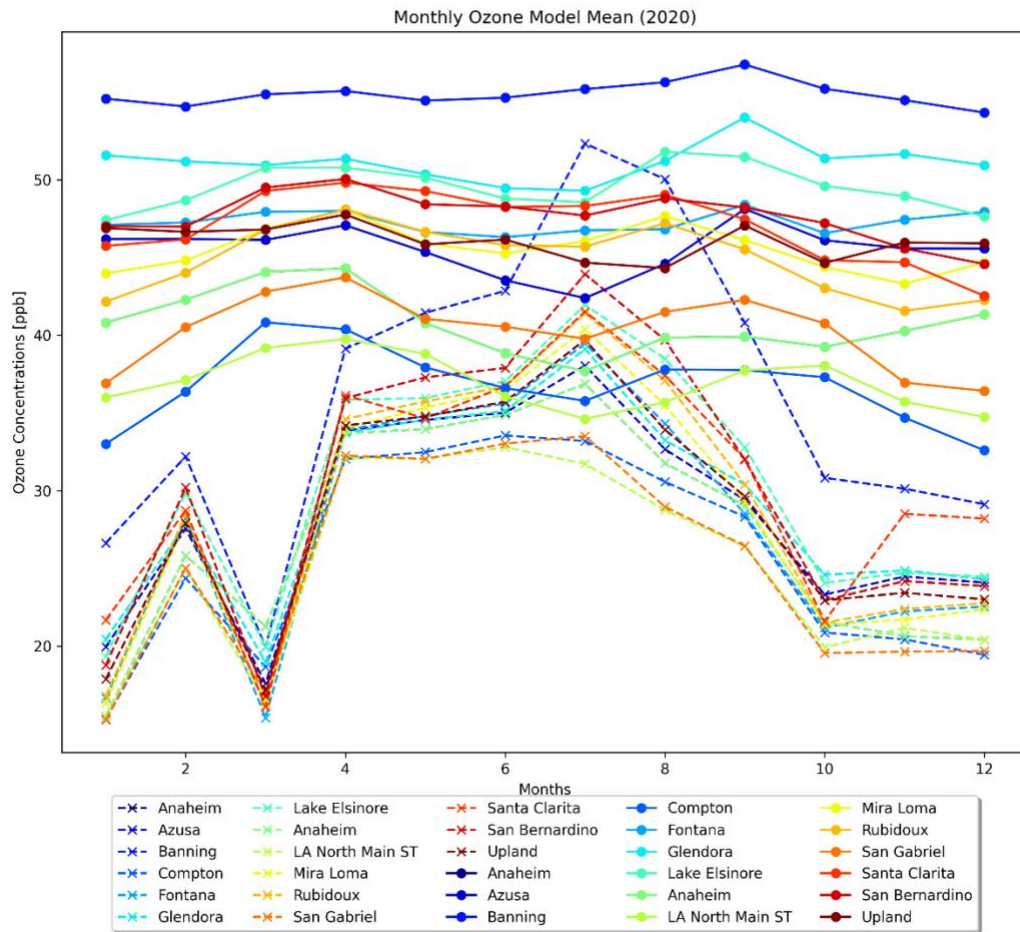


Figure S7. CMAQ (solid lines) vs. ML building sites (dash lines) model mean.

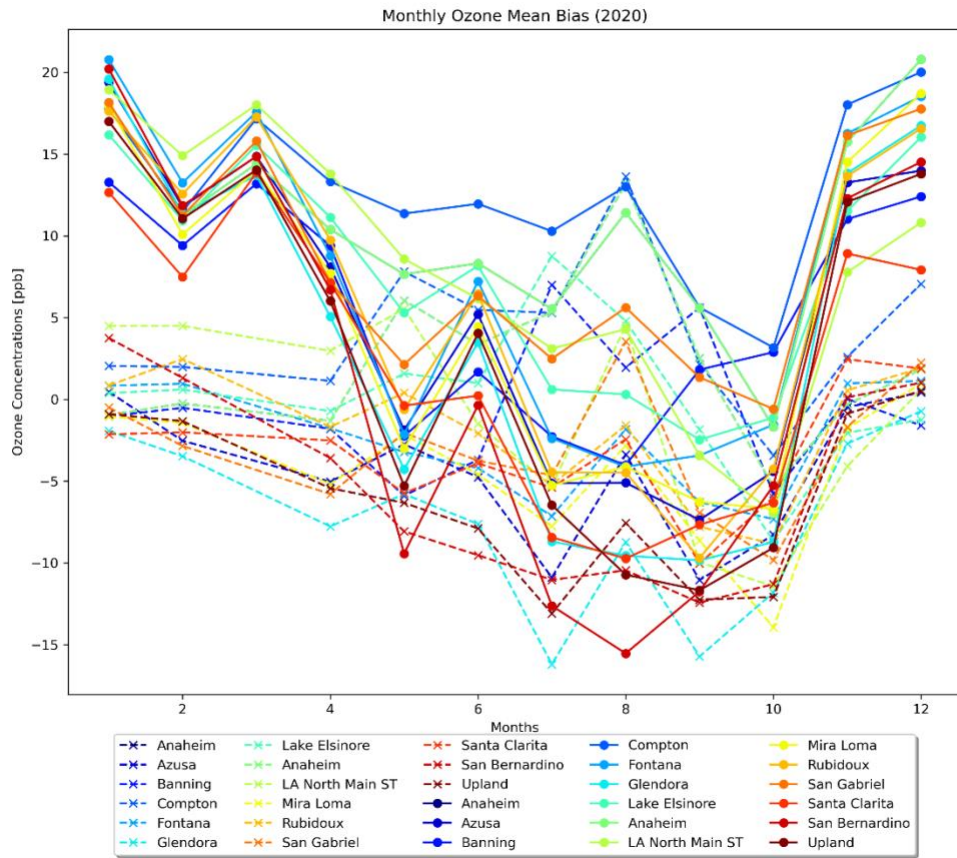


Figure S8. Monthly mean bias computed for 2020 from 9AM to 4PM. Monthly mean bias for 15 sites using kriging interpolation method (dash lines), and CMAQ simulation (solid lines). The colors of the lines corresponded to the evaluation locations.

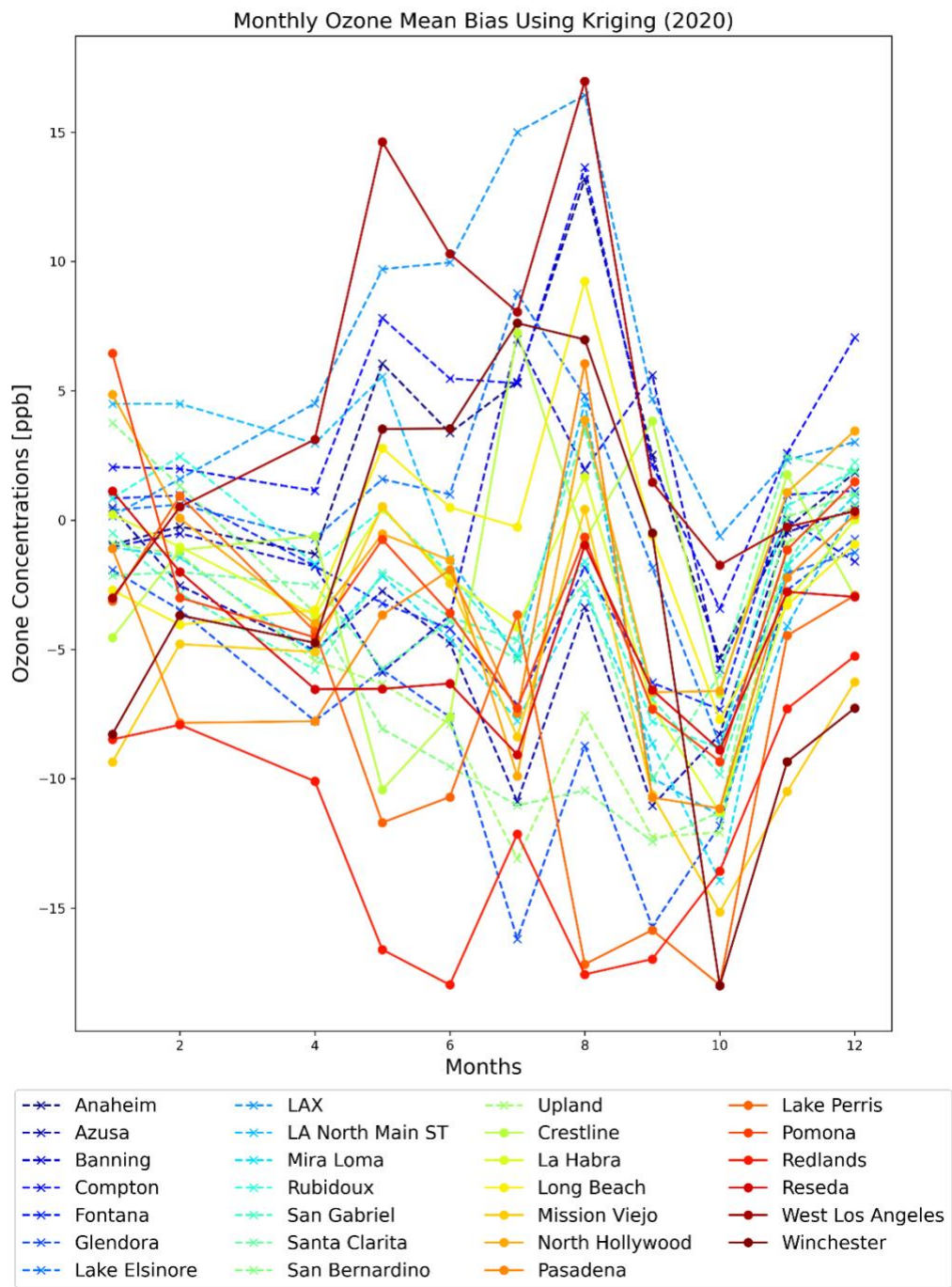


Figure S9. Monthly ozone mean bias from spatial interpolation for 2020 using the Kriging method calculated from 9AM to 4PM. The dash lines with x-markers are fifteen building sites, and solid lines with filled dots are the evaluation sites.

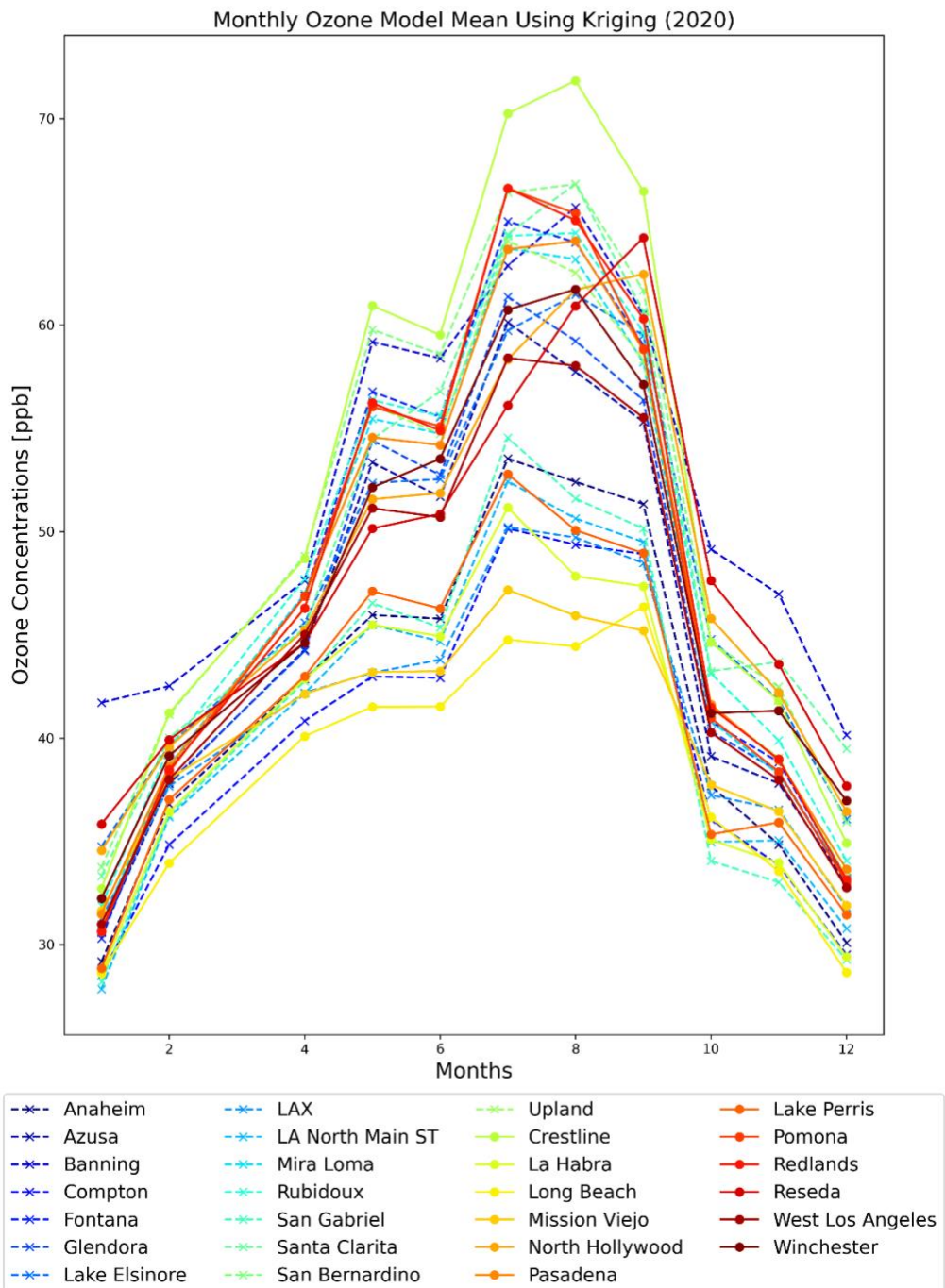


Figure S10. Building sites vs interpolated sites from 9AM to 4PM

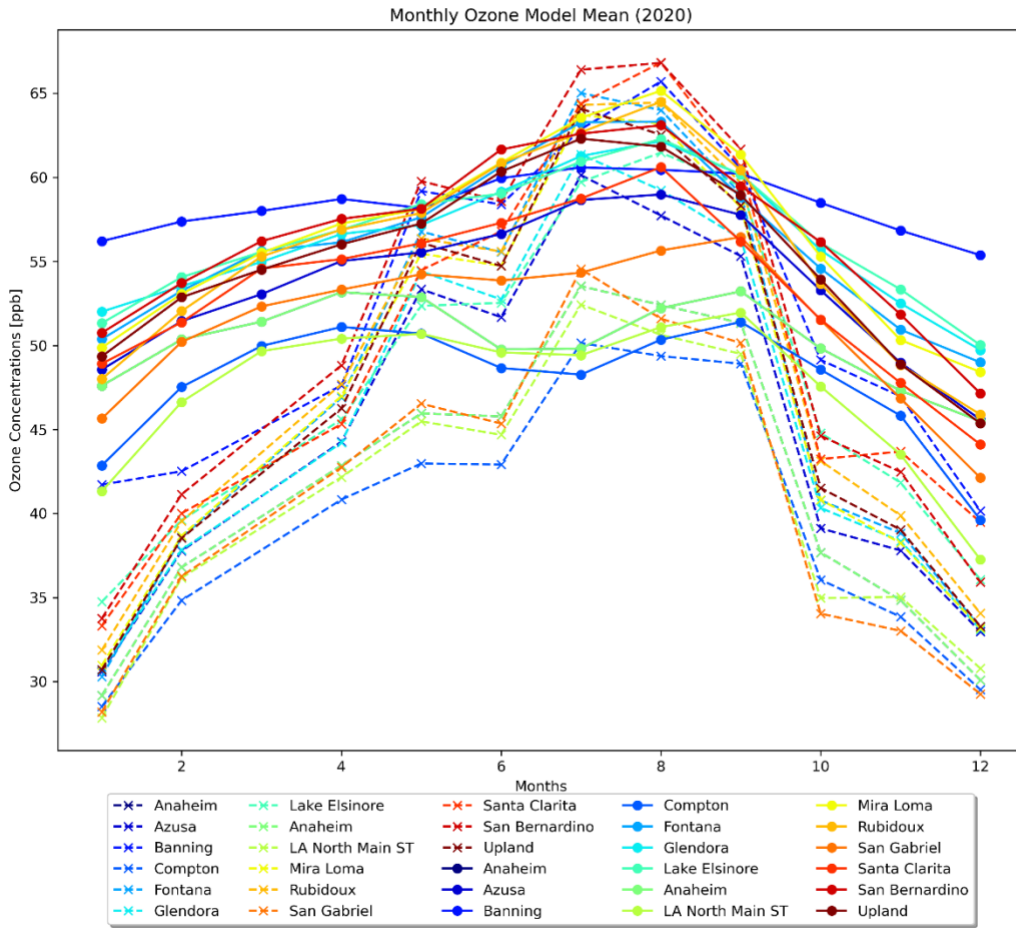


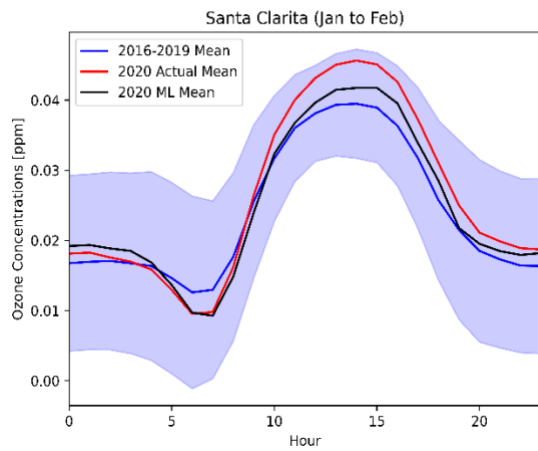
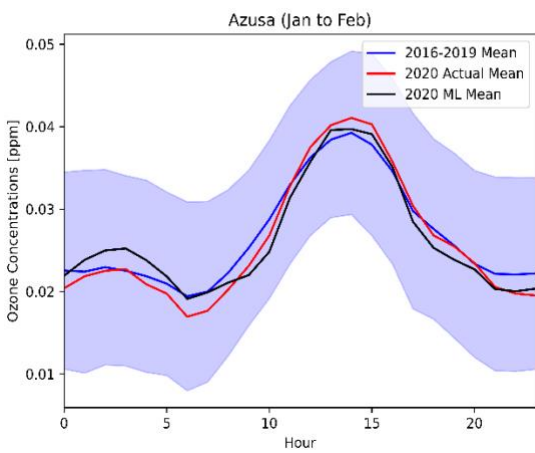
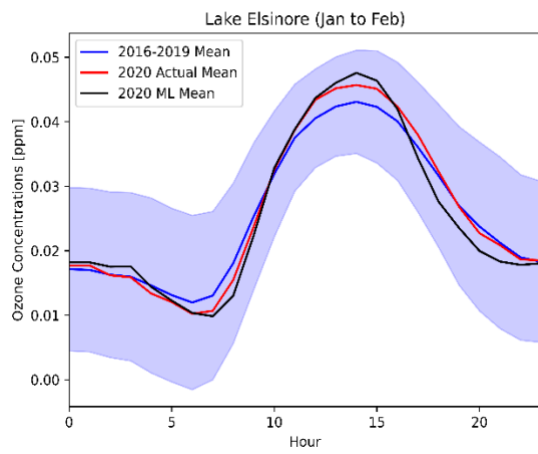
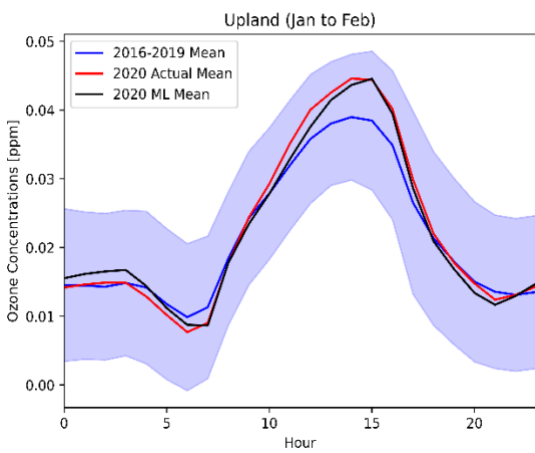
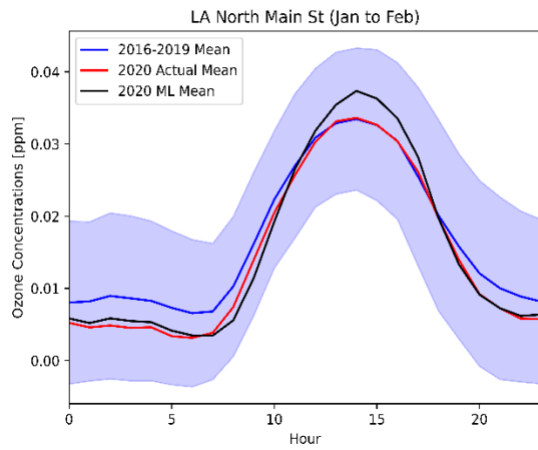
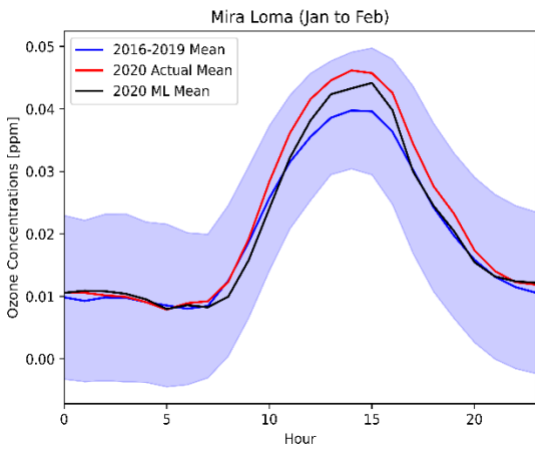
Figure S11. CMAQ (solid lines) vs. ML building sites (dash lines) from 9AM to 4Pm.

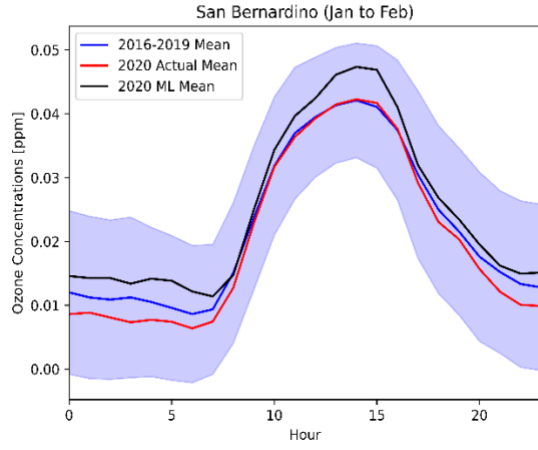
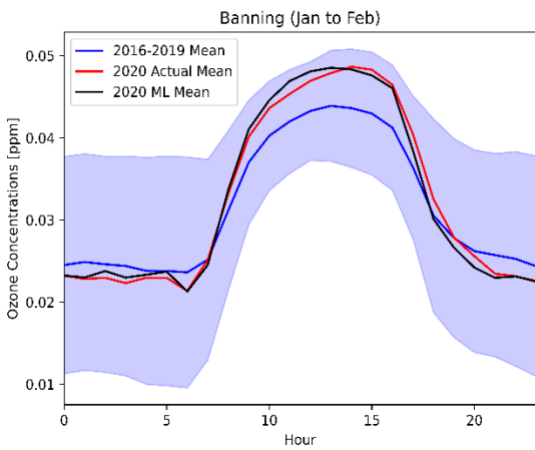
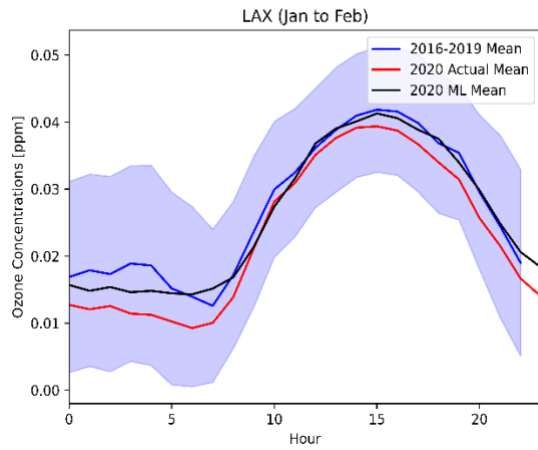
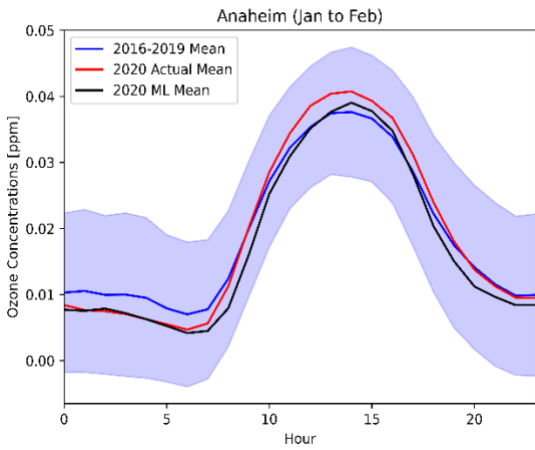
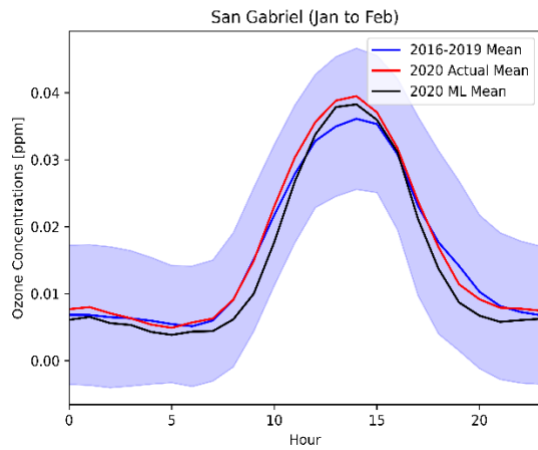
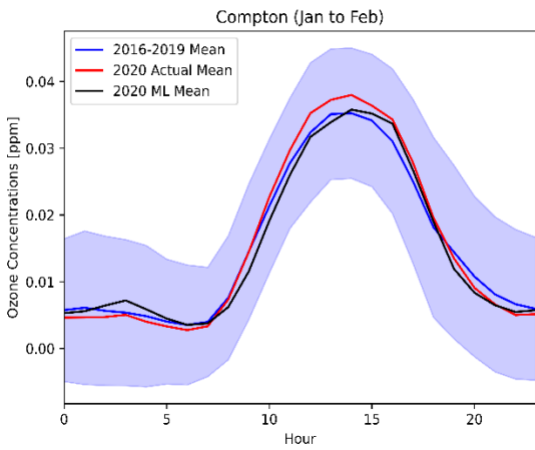
Table S3. The monthly correlation coefficient for fifteen building sites using the Kriging method.

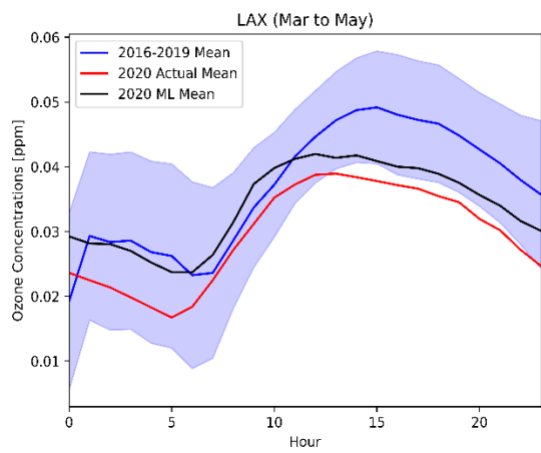
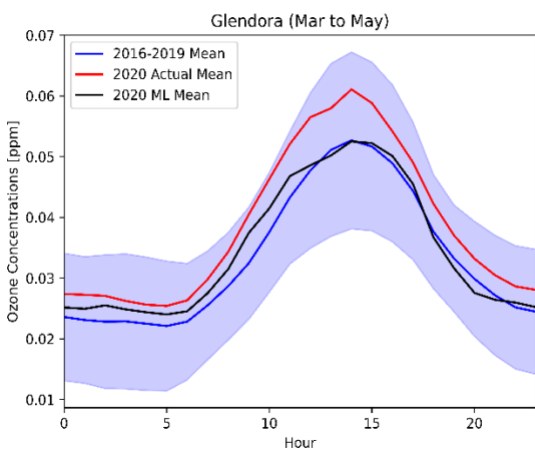
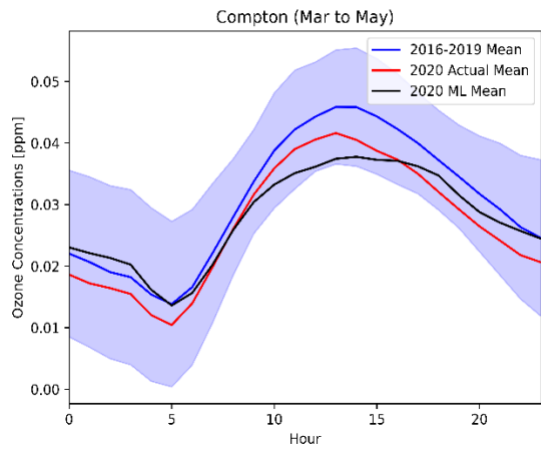
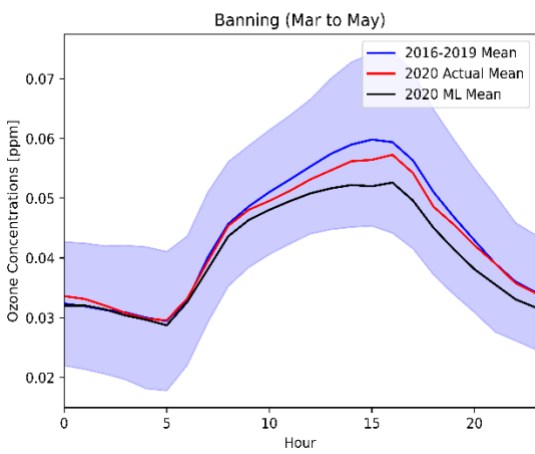
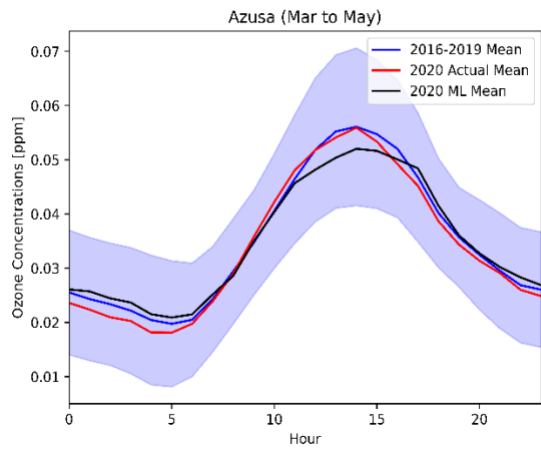
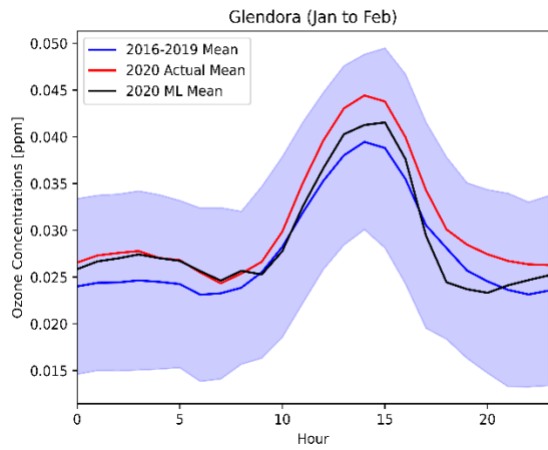
| | Jan | Feb | Mar | Apr | May | Jun | Jul | Aug | Sep | Oct | Nov | Dec |
|-----------------------|------|------|------|------|------|------|------|------|------|------|------|------|
| Anaheim | 0.85 | 0.91 | 0.90 | 0.91 | 0.71 | 0.81 | 0.89 | 0.86 | 0.88 | 0.87 | 0.89 | 0.86 |
| Azusa | 0.80 | 0.66 | 0.96 | 0.89 | 0.85 | 0.91 | 0.93 | 0.91 | 0.95 | 0.90 | 0.86 | 0.75 |
| Banning | 0.89 | 0.87 | 0.94 | 0.81 | 0.86 | 0.88 | 0.80 | 0.84 | 0.66 | 0.86 | 0.92 | 0.87 |
| Compton | 0.87 | 0.91 | 0.92 | 0.90 | 0.77 | 0.80 | 0.91 | 0.86 | 0.88 | 0.89 | 0.90 | 0.88 |
| Fontana | 0.86 | 0.88 | 0.98 | 0.95 | 0.93 | 0.94 | 0.92 | 0.95 | 0.96 | 0.91 | 0.94 | 0.88 |
| Glendora | 0.75 | 0.63 | 0.95 | 0.81 | 0.85 | 0.89 | 0.87 | 0.91 | 0.92 | 0.76 | 0.81 | 0.70 |
| Elsinore | 0.93 | 0.94 | 0.96 | 0.89 | 0.83 | 0.90 | 0.91 | 0.91 | 0.87 | 0.89 | 0.93 | 0.92 |
| LA | 0.87 | 0.90 | 0.93 | 0.89 | 0.84 | 0.87 | 0.96 | 0.92 | 0.92 | 0.87 | 0.90 | 0.89 |
| LAX | 0.90 | 0.92 | 0.89 | 0.86 | 0.58 | 0.70 | 0.86 | 0.79 | 0.75 | 0.83 | 0.89 | 0.87 |
| Mira Loma | 0.90 | 0.90 | 0.98 | 0.95 | 0.91 | 0.93 | 0.92 | 0.93 | 0.95 | 0.91 | 0.93 | 0.90 |
| Rubidoux | 0.90 | 0.92 | 0.98 | 0.94 | 0.91 | 0.93 | 0.93 | 0.94 | 0.95 | 0.94 | 0.92 | 0.90 |
| San Bernardino | 0.90 | 0.92 | 0.96 | 0.93 | 0.91 | 0.94 | 0.89 | 0.92 | 0.94 | 0.93 | 0.95 | 0.87 |
| San Gabriel | 0.86 | 0.92 | 0.94 | 0.92 | 0.85 | 0.86 | 0.93 | 0.91 | 0.92 | 0.87 | 0.88 | 0.87 |
| Santa Clarita | 0.95 | 0.91 | 0.95 | 0.88 | 0.89 | 0.95 | 0.94 | 0.91 | 0.92 | 0.89 | 0.89 | 0.95 |
| Upland | 0.93 | 0.88 | 0.97 | 0.93 | 0.91 | 0.93 | 0.90 | 0.94 | 0.96 | 0.91 | 0.93 | 0.87 |

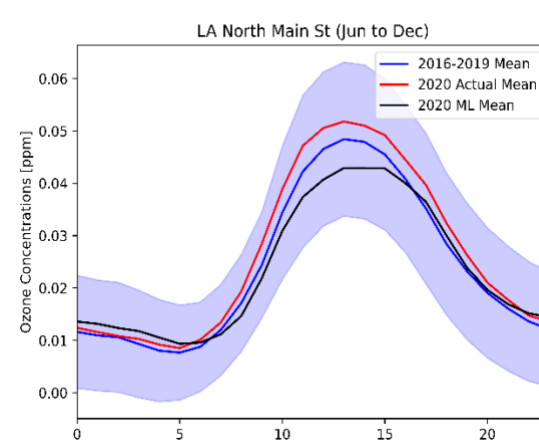
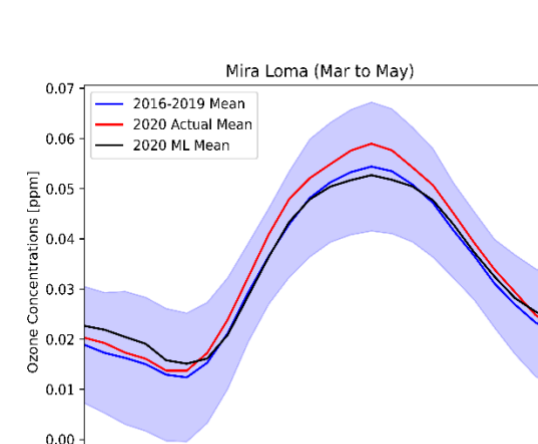
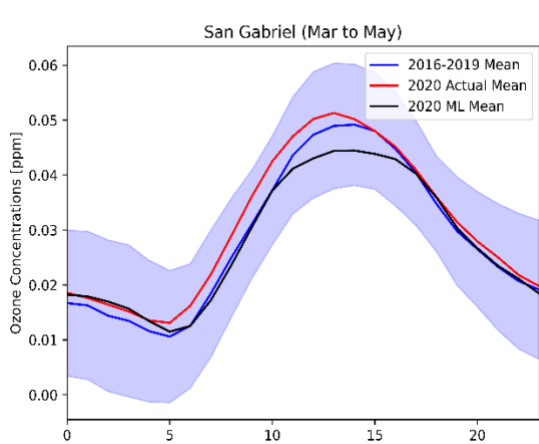
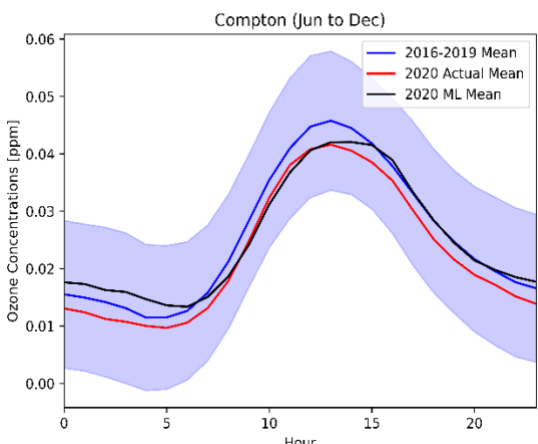
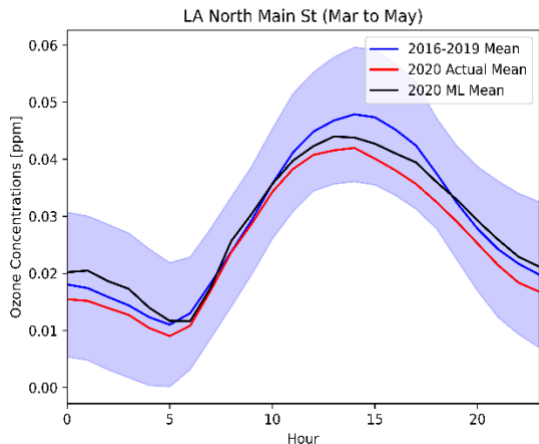
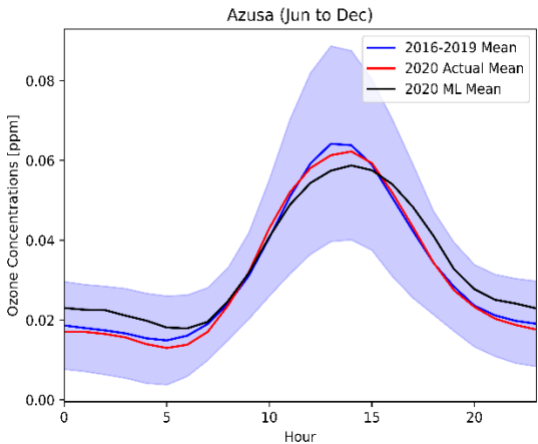
Table S4. The monthly correlation coefficient for twelve evaluation sites using the Kriging method.

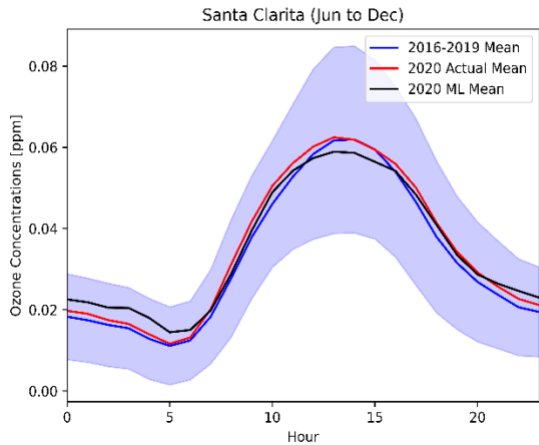
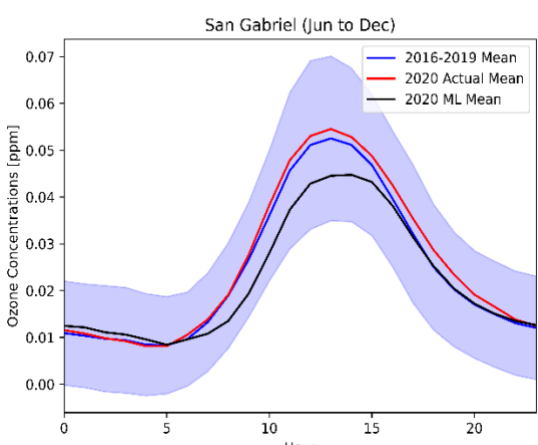
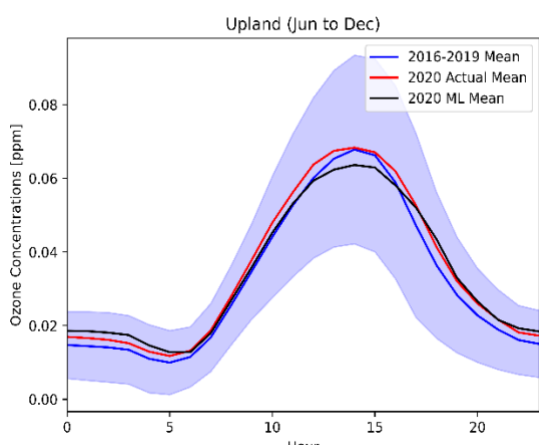
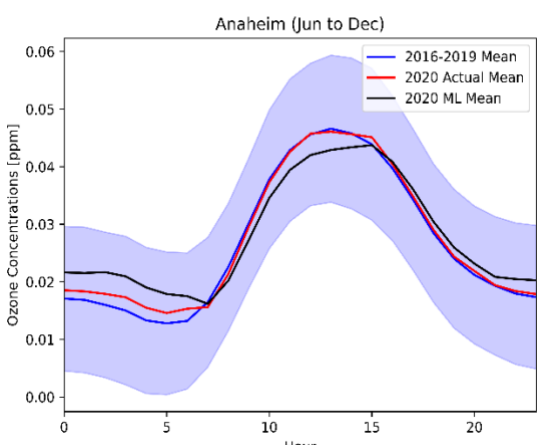
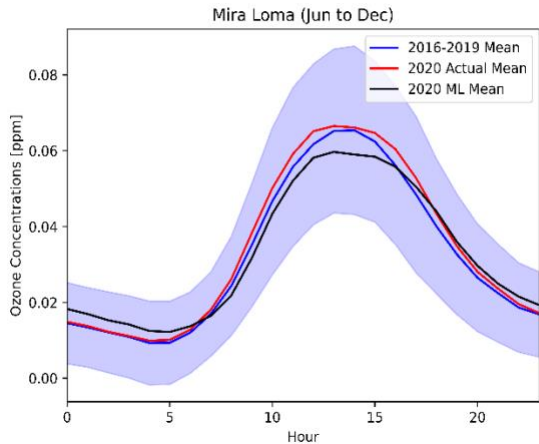
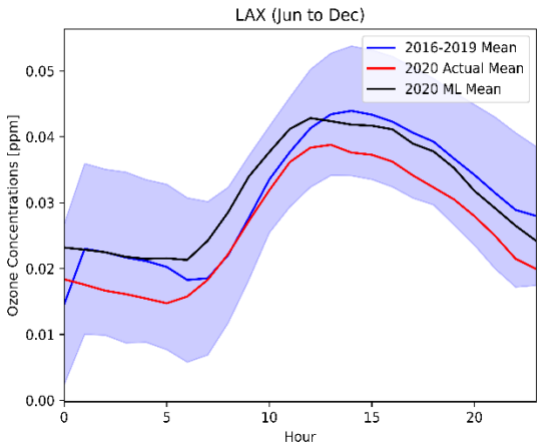
| | Jan | Feb | Mar | Apr | May | Jun | Jul | Aug | Sep | Oct | Nov | Dec |
|------------------------|------|------|------|------|------|------|------|------|------|------|------|------|
| Crestline | 0.38 | 0.67 | 0.72 | 0.52 | 0.60 | 0.63 | 0.62 | 0.62 | 0.57 | 0.57 | 0.53 | 0.51 |
| La Habra | 0.85 | 0.90 | 0.86 | 0.90 | 0.82 | 0.83 | 0.91 | 0.89 | 0.91 | 0.85 | 0.88 | 0.81 |
| Long Beach | 0.75 | 0.84 | 0.74 | 0.74 | 0.57 | 0.71 | 0.79 | 0.75 | 0.80 | 0.75 | 0.79 | 0.73 |
| Mission Viejo | 0.79 | 0.74 | 0.84 | 0.79 | 0.71 | 0.76 | 0.89 | 0.84 | 0.82 | 0.63 | 0.76 | 0.69 |
| North Hollywood | 0.84 | 0.88 | 0.89 | 0.81 | 0.88 | 0.89 | 0.94 | 0.90 | 0.94 | 0.86 | 0.91 | 0.83 |
| Pasadena | 0.86 | 0.90 | 0.90 | 0.85 | 0.86 | 0.86 | 0.91 | 0.91 | 0.93 | 0.85 | 0.88 | 0.84 |
| Lake Perris | 0.86 | 0.88 | 0.96 | 0.91 | 0.86 | 0.92 | 0.84 | 0.90 | 0.88 | 0.91 | 0.87 | 0.89 |
| Pomona | 0.83 | 0.88 | 0.93 | 0.94 | 0.90 | 0.92 | 0.90 | 0.91 | 0.95 | 0.87 | 0.90 | 0.87 |
| Redlands | 0.77 | 0.80 | 0.89 | 0.83 | 0.90 | 0.92 | 0.86 | 0.88 | 0.83 | 0.61 | 0.82 | 0.71 |
| Reseda | 0.76 | 0.82 | 0.85 | 0.72 | 0.87 | 0.88 | 0.90 | 0.87 | 0.89 | 0.89 | 0.87 | 0.71 |
| West LA | 0.75 | 0.82 | 0.84 | 0.74 | 0.74 | 0.74 | 0.93 | 0.85 | 0.87 | 0.81 | 0.80 | 0.76 |
| Winchester | 0.77 | 0.71 | 0.86 | 0.73 | 0.79 | 0.78 | 0.75 | 0.69 | 0.58 | 0.56 | 0.70 | 0.71 |

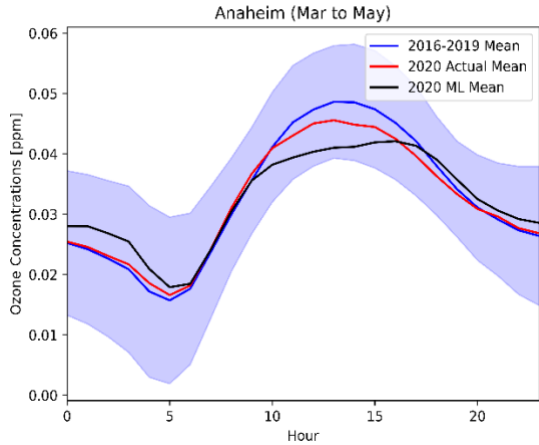
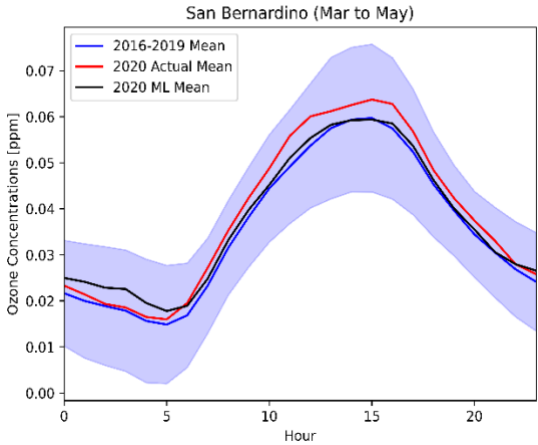
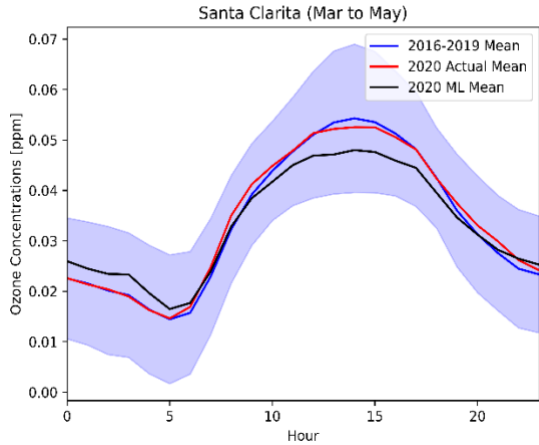
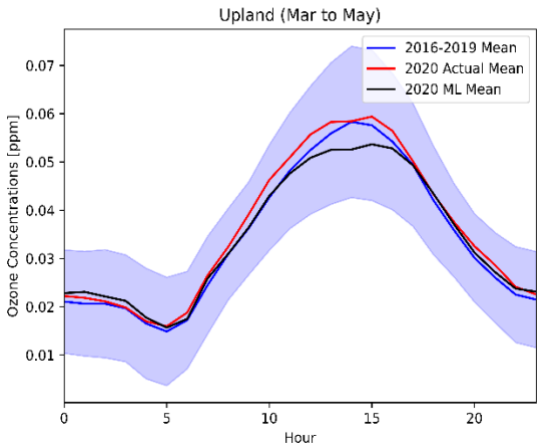
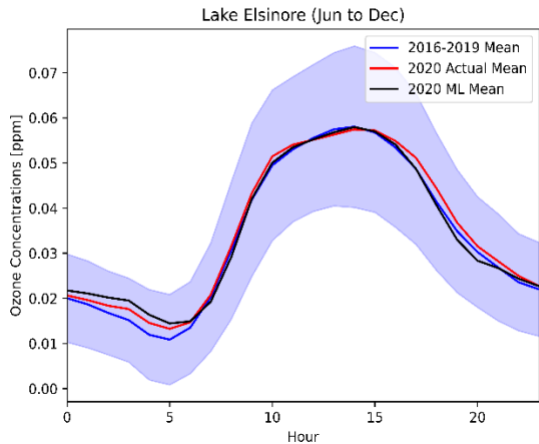
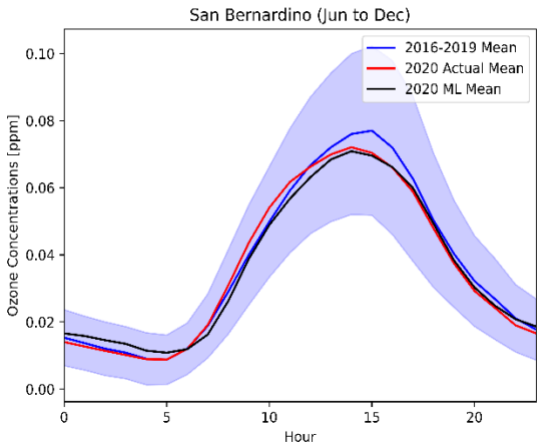












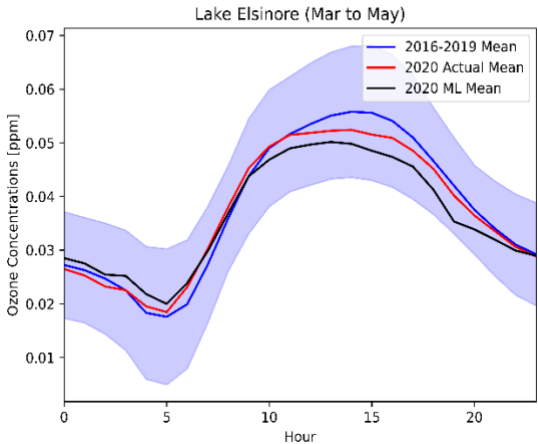
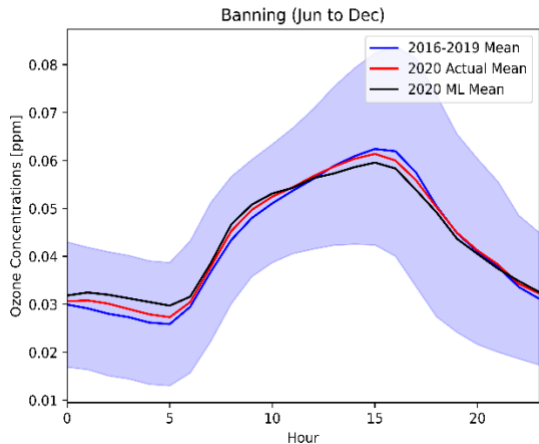
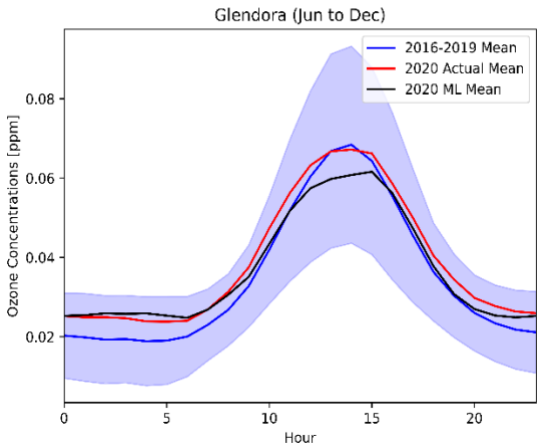


Figure S12. Averaged diurnal profiles of 2016 - 2019 (blue), actual 2020 (red), and ML predicted 2020 (black) ozone concentrations (ppm) for three different periods, the pre lockdown (Jan to Feb), the lockdown (Mar to May), and the post lockdown period (after May). The shaded area is the standard deviation of the 2016 - 2019 measurements.