***Supplemental Information for*:**

A Machine Learning Approach to Quantify the Impact of Meteorology on Tropospheric Ozone in the Inland Empire, CA

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Figures

Figure S1. 8-hour ozone design value concentrations in Los Angeles. The red dash line is the National Ambient Air Quality Standard (NAAQS) for 8-hour ozone (0.070 ppm, 2015). Source: California Air Resources Board

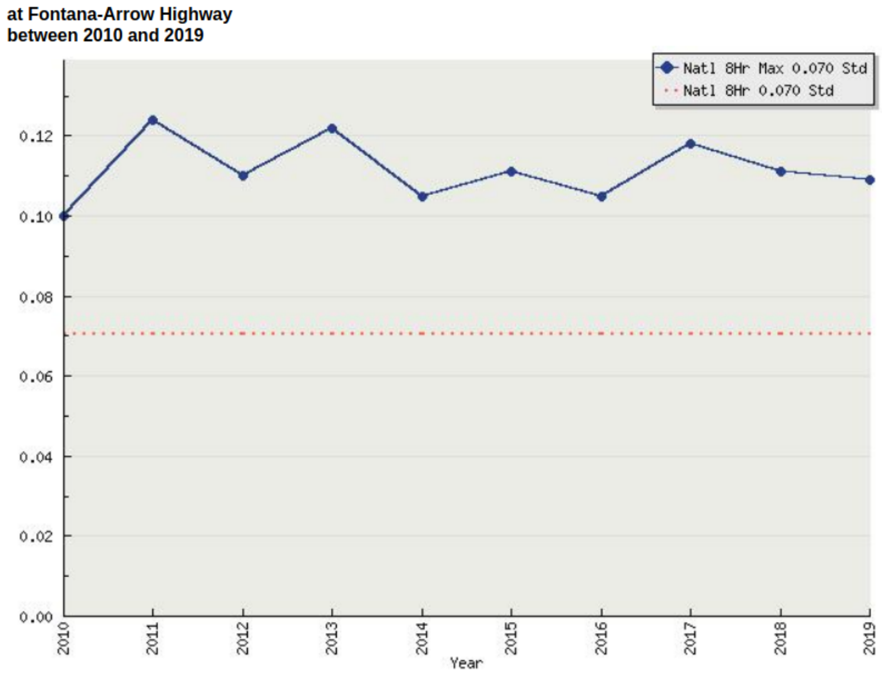


Figure S2. 8-hour ozone design value concentrations in Fontana. The red dash line is the National Ambient Air Quality Standard (NAAQS) for 8-hour ozone (0.070 ppm, 2015). Source: California Air Resources Board

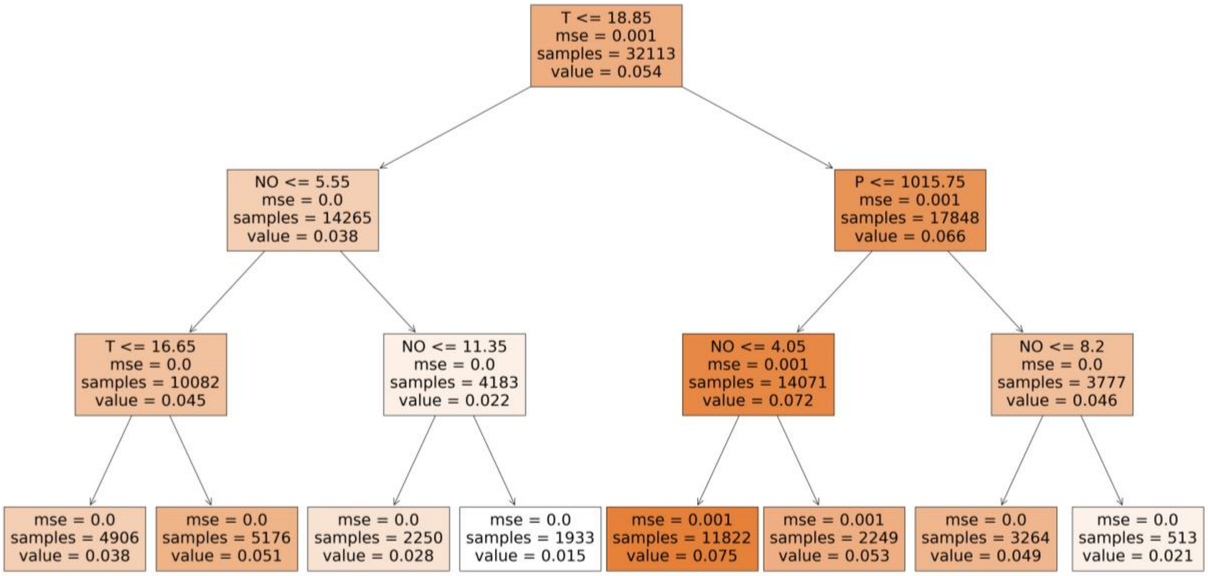


Figure S3. Three node decision trees based on air quality and meteorological input from 2014-2018. The meteorology data is from LAX, and air quality data is from Fontana. The predictions were made based on 12:00 noon to 5:00 PM training data.

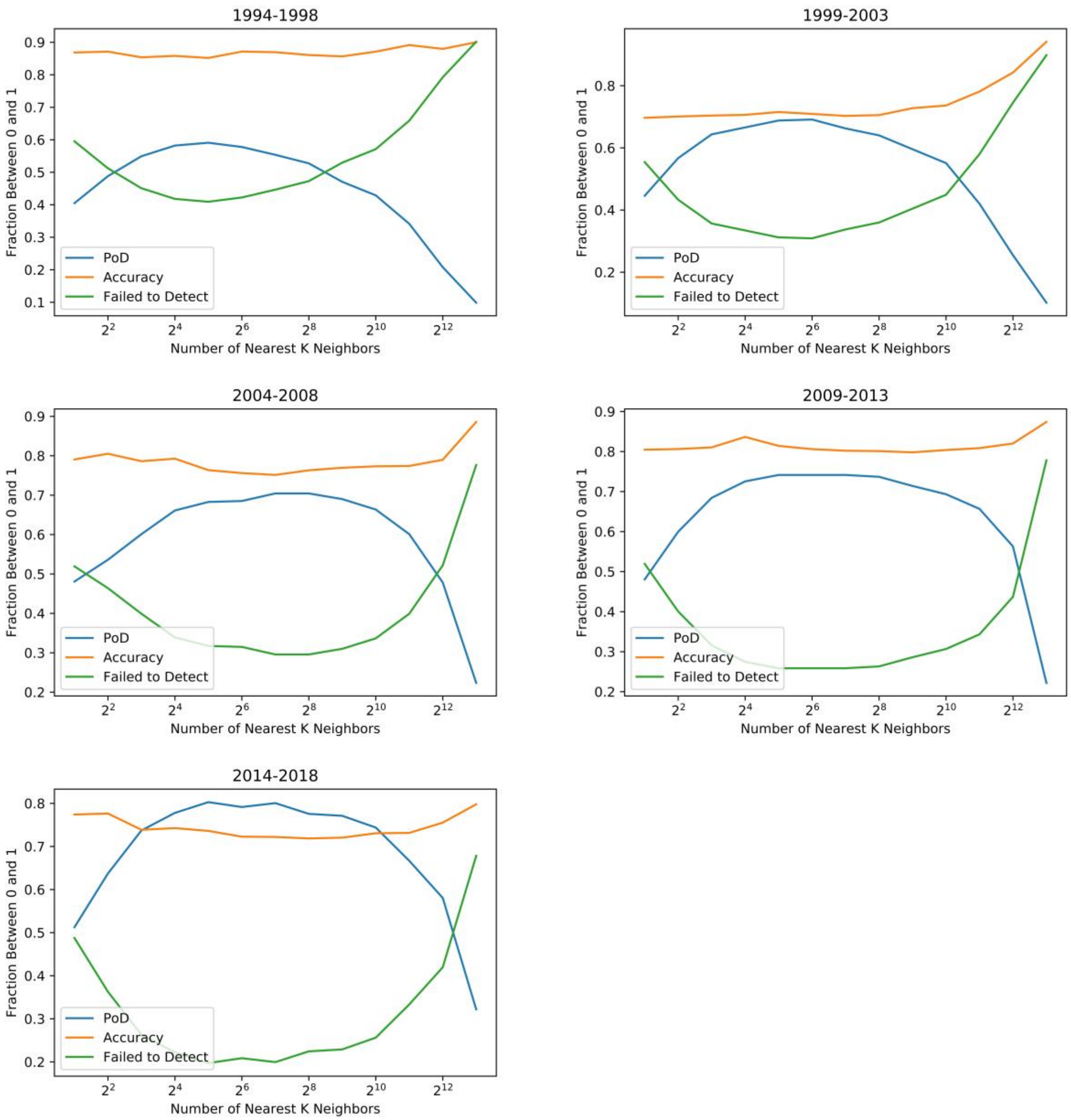


Figure S4. Testing the performance of K-NN by varying the number of nearest neighbors while keeping other parameters constant.

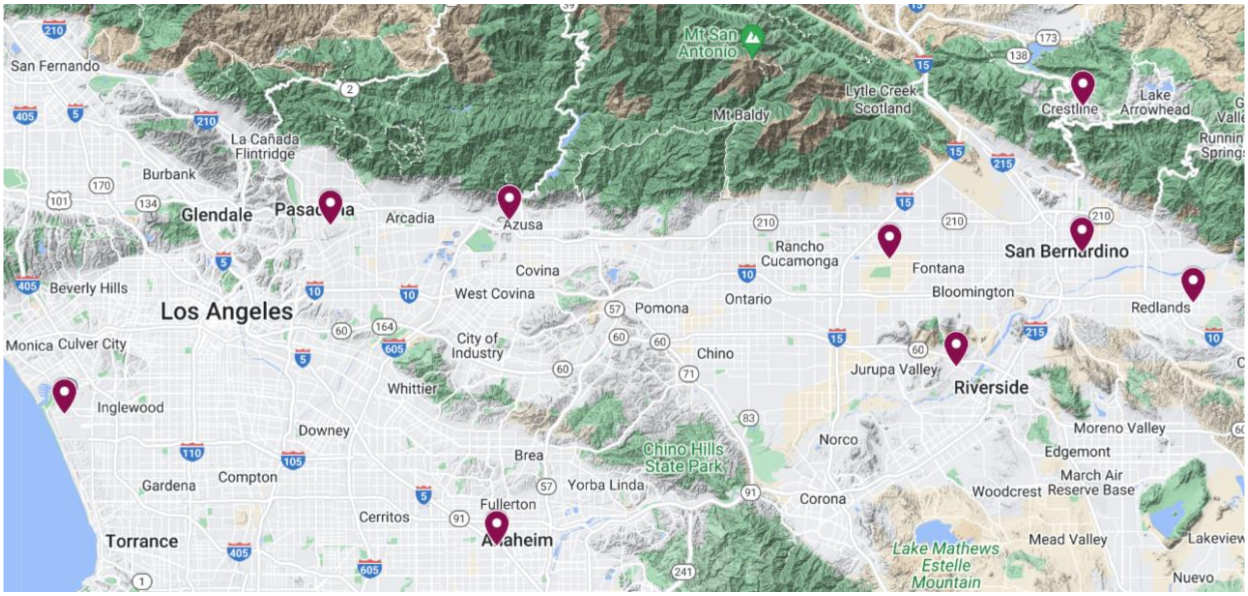


Figure S5. Nine evaluation sites from SCAQMD. From left to right, LAX, Pasadena, Anaheim, Azusa, Fontana, Riverside, San Bernardino, Crestline, and Redlands.

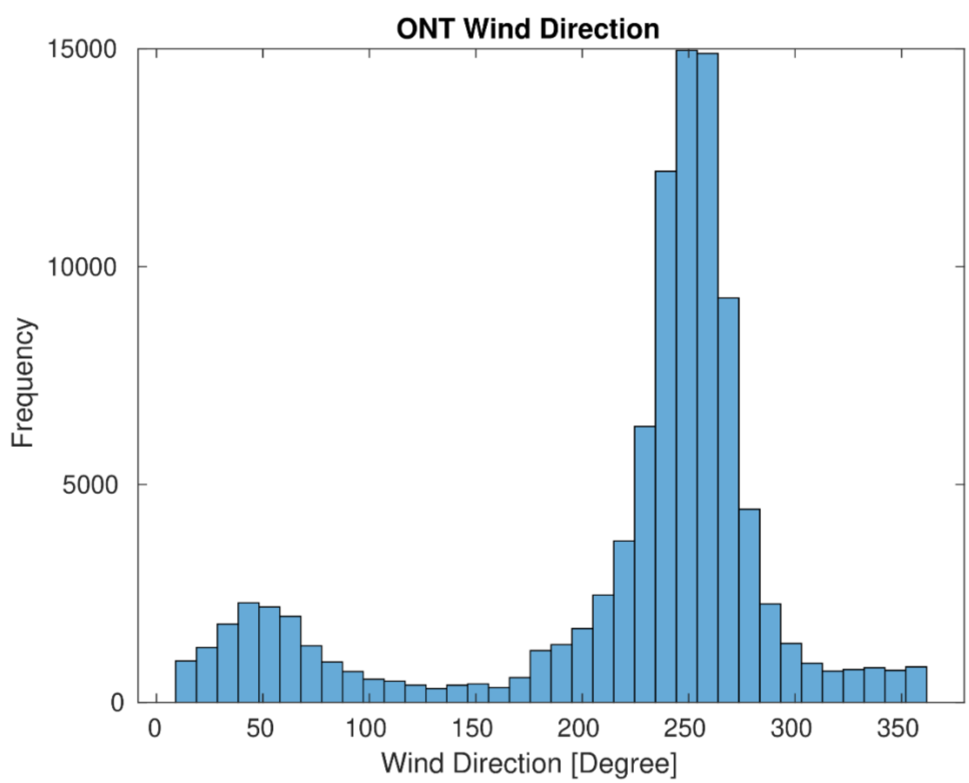


Figure S6. Wind direction in Ontario international airport. 25% of wind directions are from 254-273 degrees, and 64% of wind directions are from 225-273 degrees.

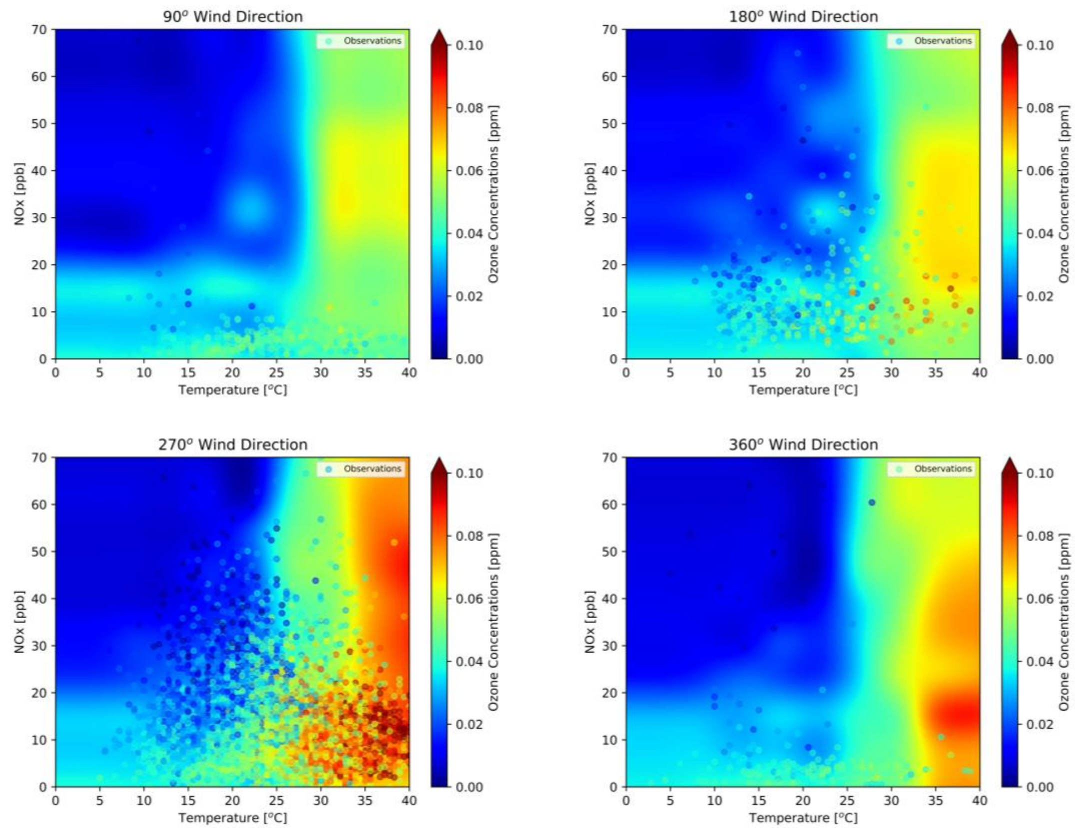


Figure S7. Contour plots generated by the RFR model trained on ONT meteorology and Fontana air quality at constant wind speed (9 m/s), visibility (16000 m), dynamic pressure, dynamic relative humidity, and at four discrete wind direction levels (90, 180, 270, 360). The dots are observational data plotted on the top of the contours.

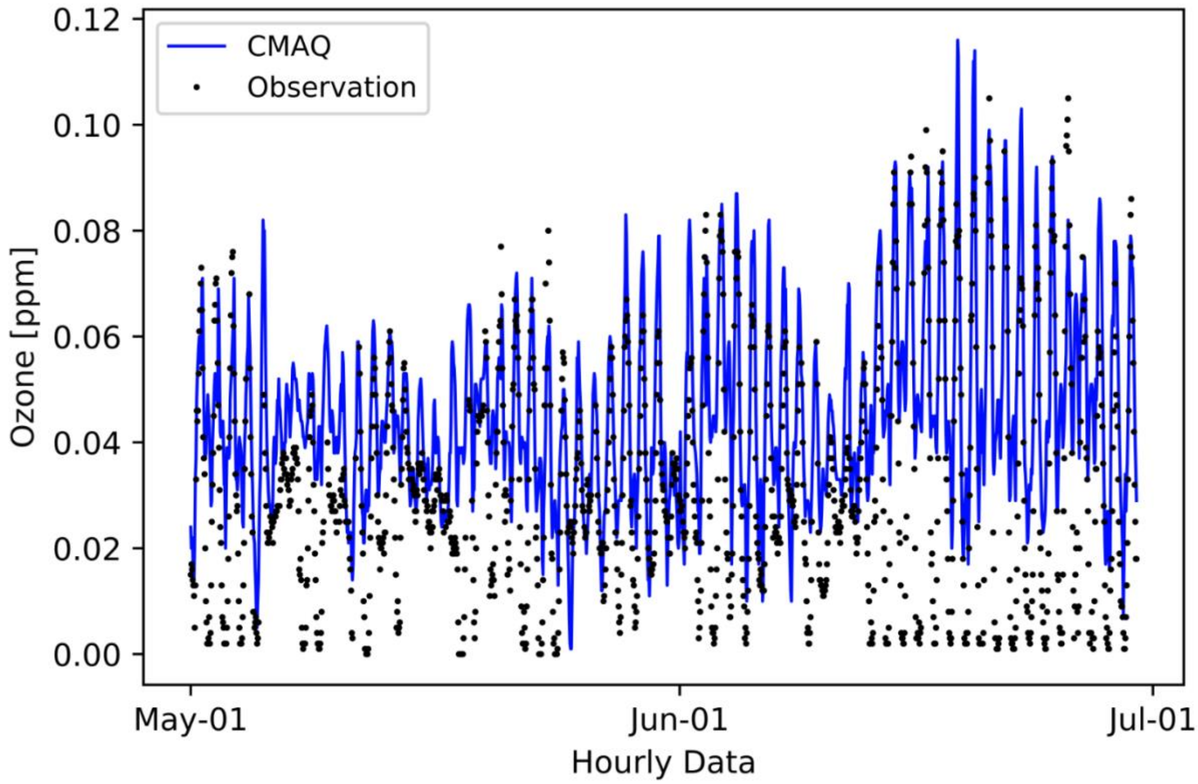


Figure S8. Time series of ozone concentration in Fontana, CA. The blue line is CMAQ simulation results, and the dots are observational data.

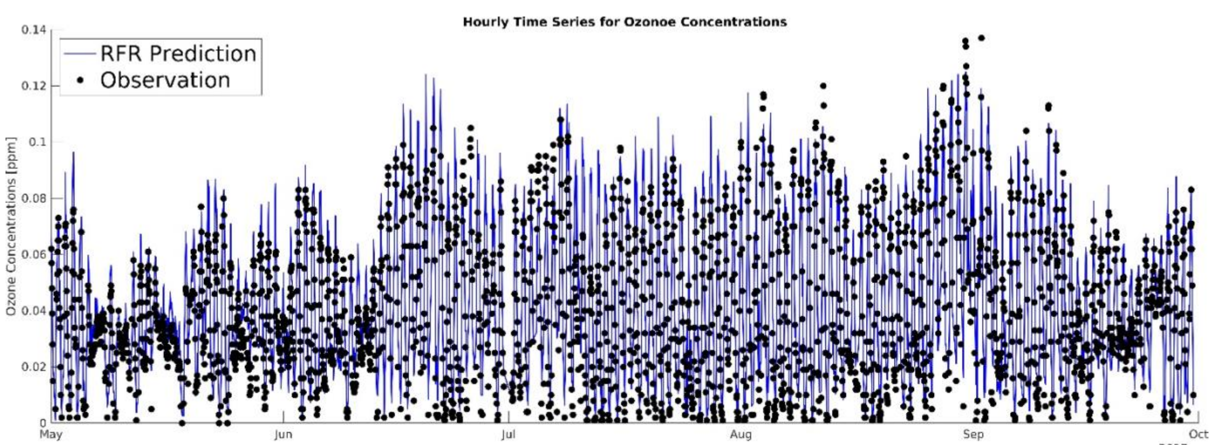


Figure S9. Time series of ozone concentration in Fontana, CA. The blue line is RFR prediction results, and the dots are observational data.

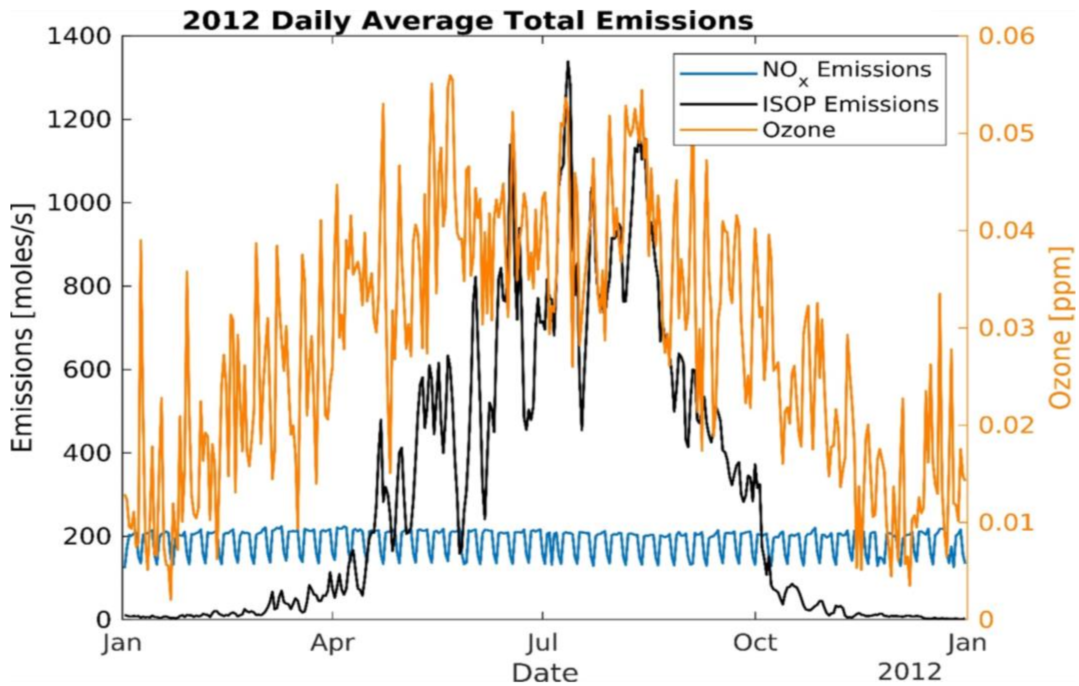


Figure S10. Daily average NO_x and isoprene (ISOP) emissions over the third model domain. The periodical oscillation of NO_x emissions (blue line) is due to weekday/weekend behavior. The black line is the total biogenic isoprene emissions of the domain. NO_x and ISOP emissions were extracted from gridded SCAQMD emissions. Twenty-four-hour ozone average is sampled from Fontana monitoring station.

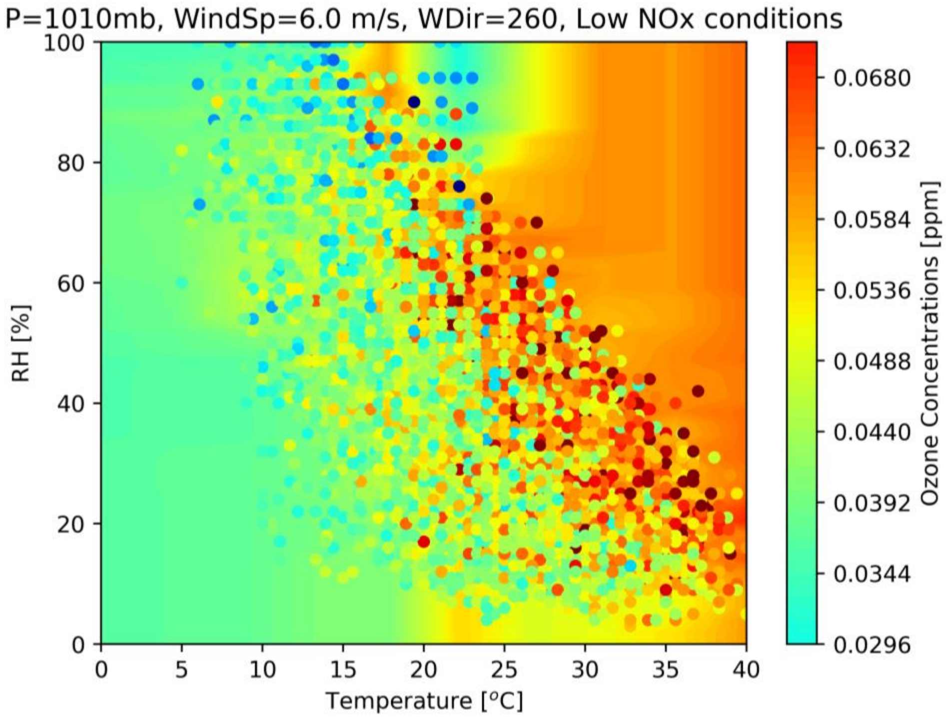


Figure S11. Contour plots generated by the RFR model trained on ONT meteorology and Fontana air quality at constant wind speed (6.0 m/s), visibility (16000 m), wind direction from 260 degree, and 1010 mb pressure. The dots are observational data plotted on the top of the contours.

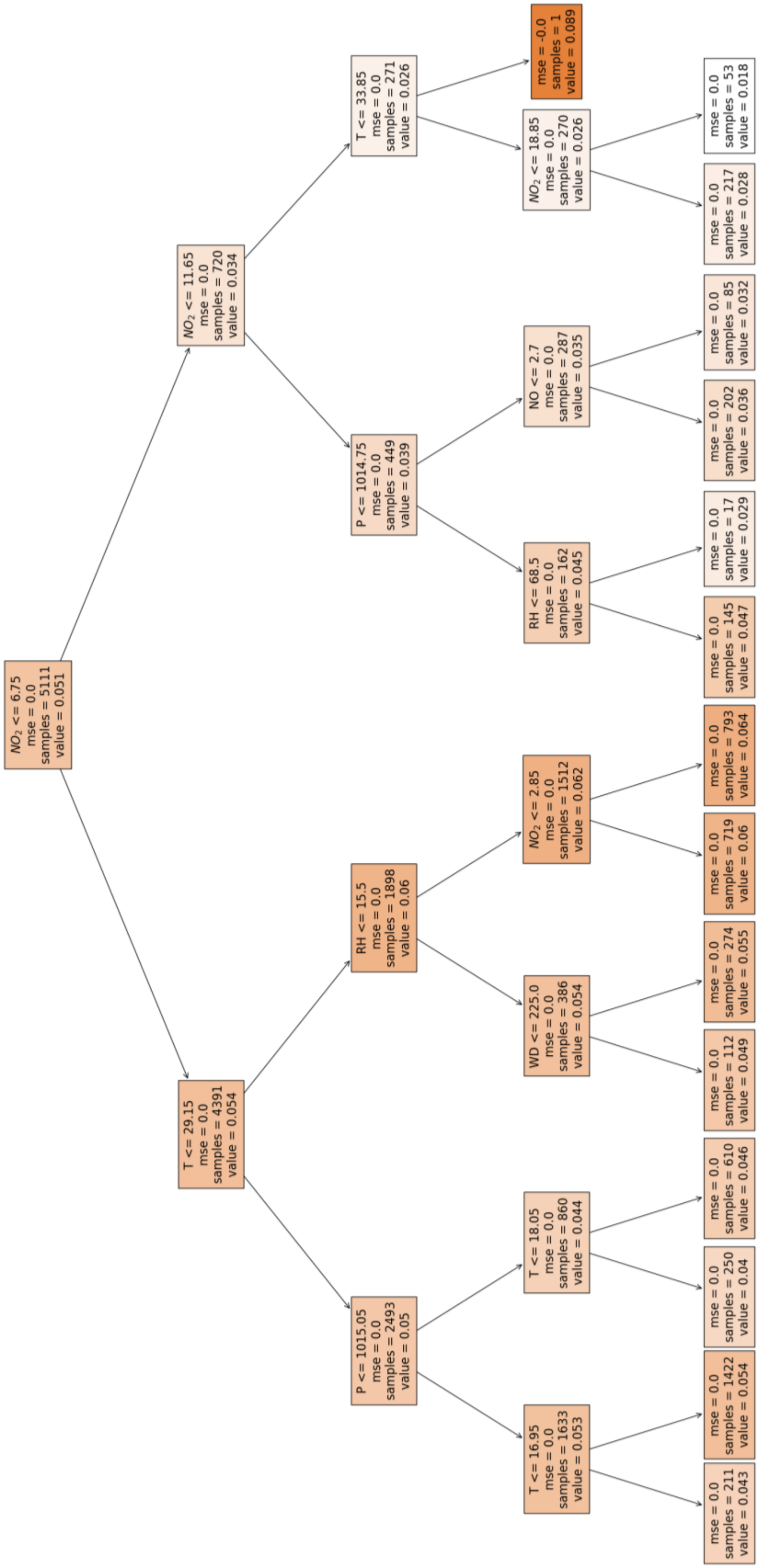


Figure S12. Four node decision trees based on air quality and meteorological input from 2014-2018. The meteorology data is from ONT, and air quality data is from Fontana. The predictions were made based on 12:00 noon to 5:00 PM training data.

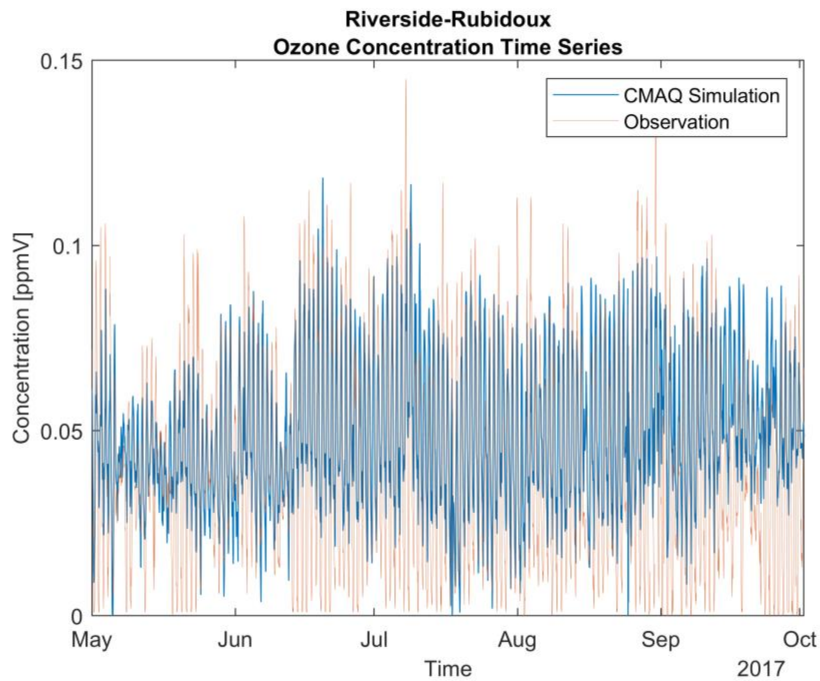


Figure S13. Riverside – Rubidoux ozone concentration time series with hourly resolution. The blue line is ozone concentration from CMAQ simulations, and orange line is observation ozone concentration.

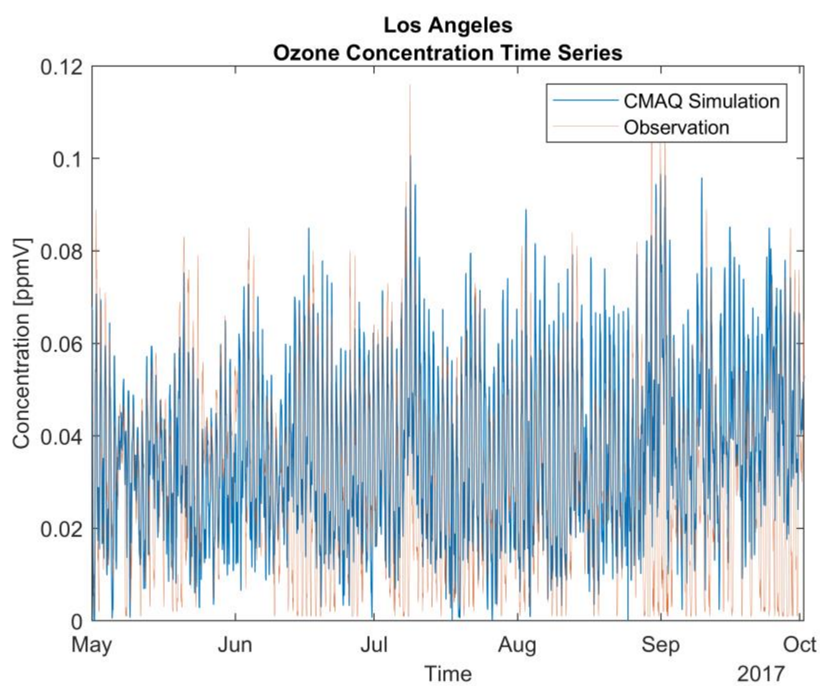


Figure S14.Los Angeles ozone concentration time series with hourly resolution. The blue line is ozone concentration from CMAQ simulations, and orange line is observation ozone concentration.

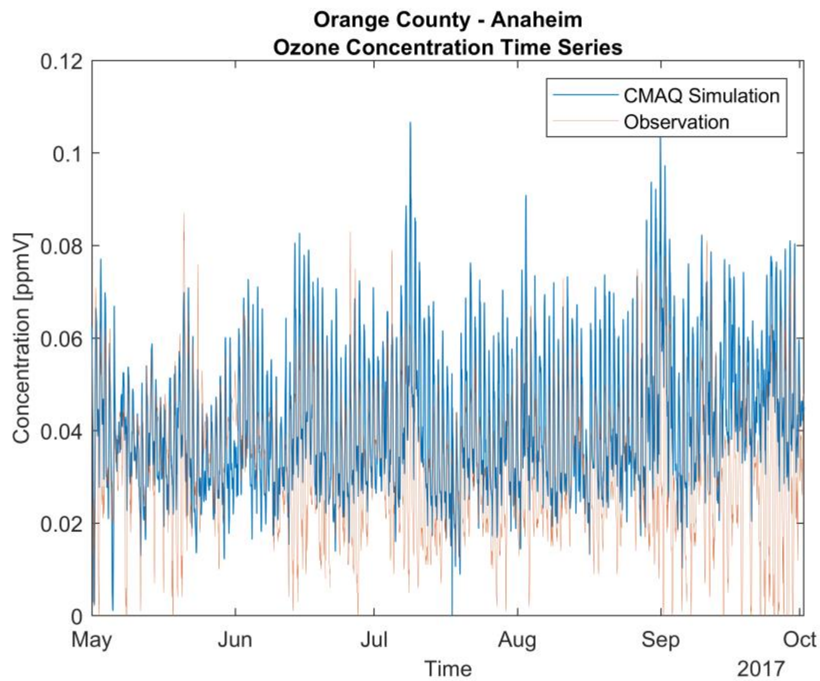


Figure S15. Orange County-Anaheim ozone concentration time series with hourly resolution. The blue line is ozone concentration from CMAQ simulations, and orange line is observation ozone concentration.

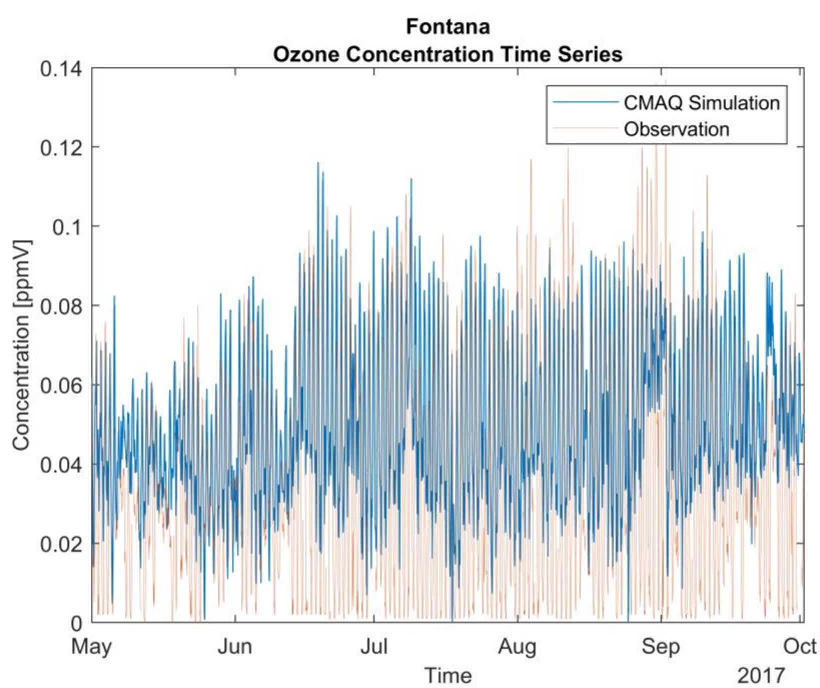


Figure S16. Fontana ozone concentration time series with hourly resolution. The blue line is ozone concentration from CMAQ simulations, and orange line is observation ozone concentration.

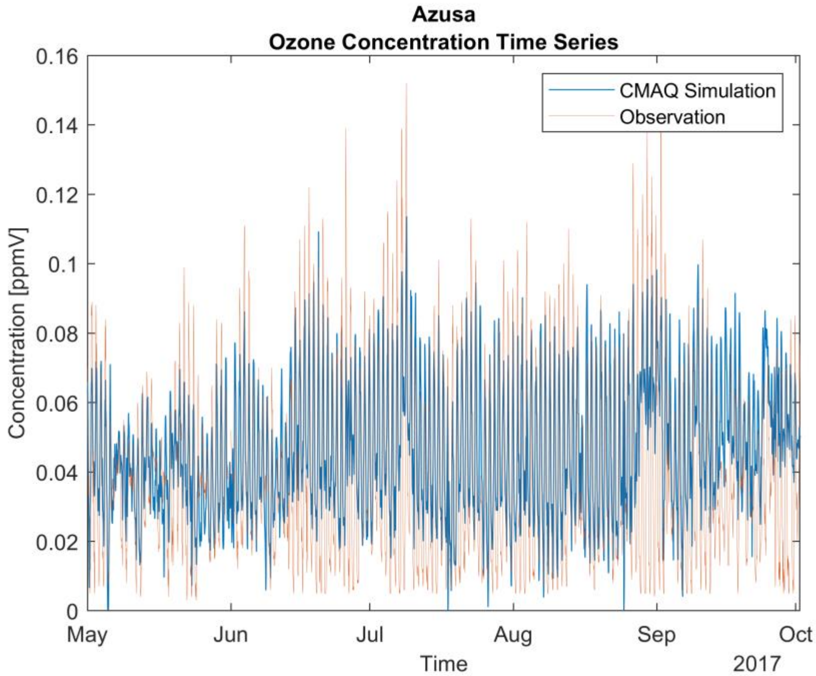


Figure S17. Azusa ozone concentration time series with hourly resolution. The blue line is ozone concentration from CMAQ simulations, and orange line is observation ozone concentration.

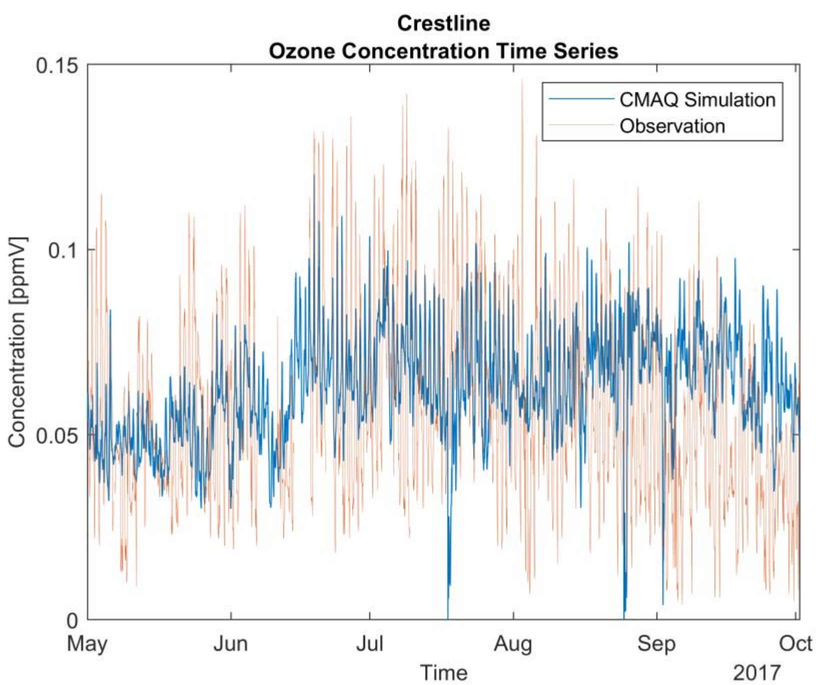


Figure S18. Crestline ozone concentration time series with hourly resolution. The blue line is ozone concentration from CMAQ simulations, and orange line is observation ozone concentration.

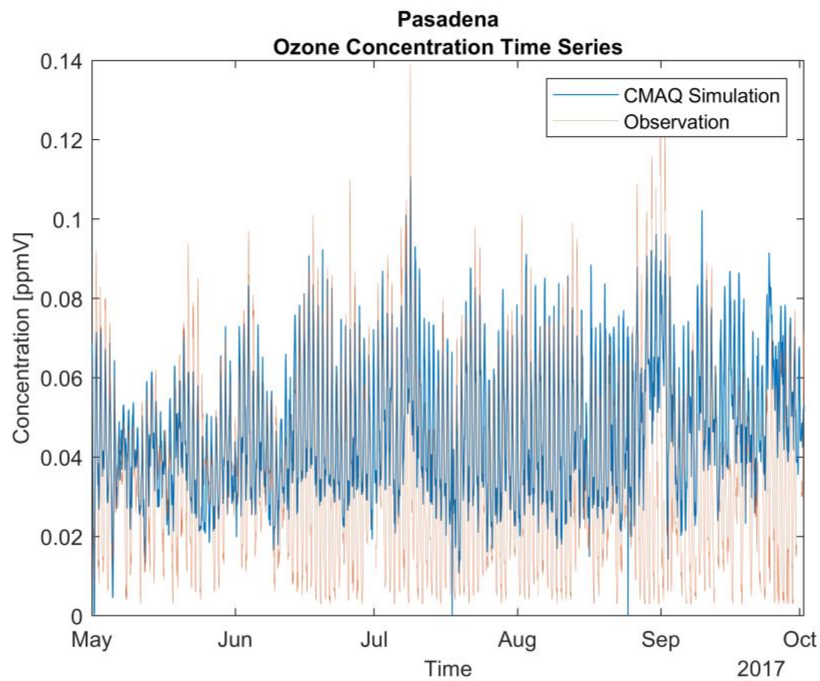


Figure S19. Pasadena ozone concentration time series with hourly resolution. The blue line is ozone concentration from CMAQ simulations, and orange line is observation ozone concentration.

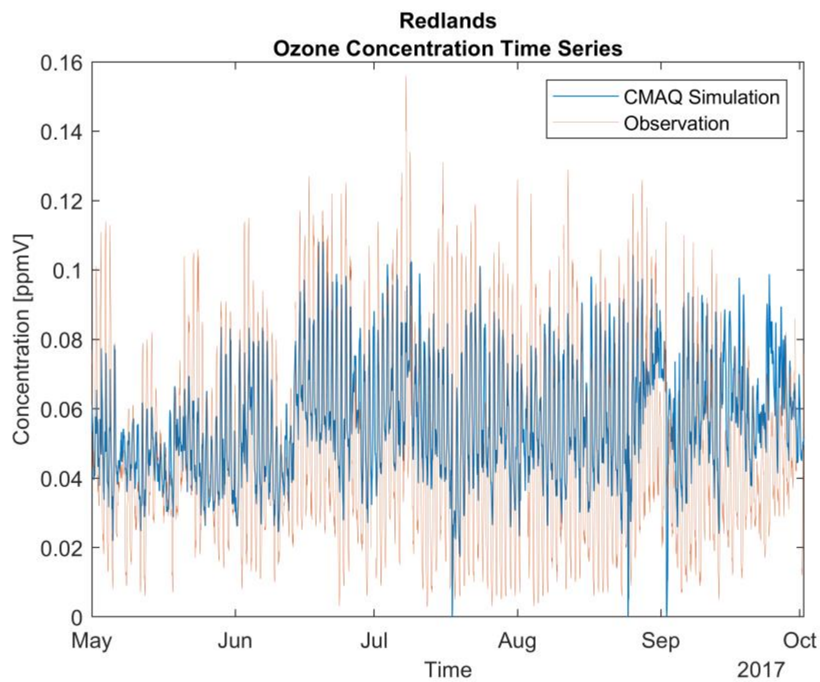


Figure S20. Redlands ozone concentration time series with hourly resolution. The blue line is ozone concentration from CMAQ simulations, and orange line is observation ozone concentration.

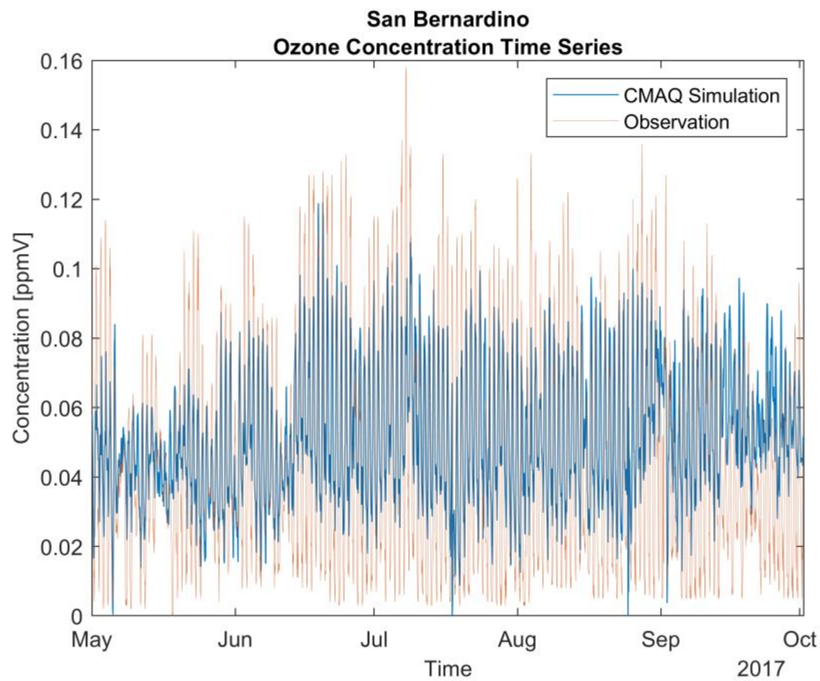


Figure S21. San Bernardino ozone concentration time series with hourly resolution. The blue line is ozone concentration from CMAQ simulations, and orange line is observation ozone concentration.

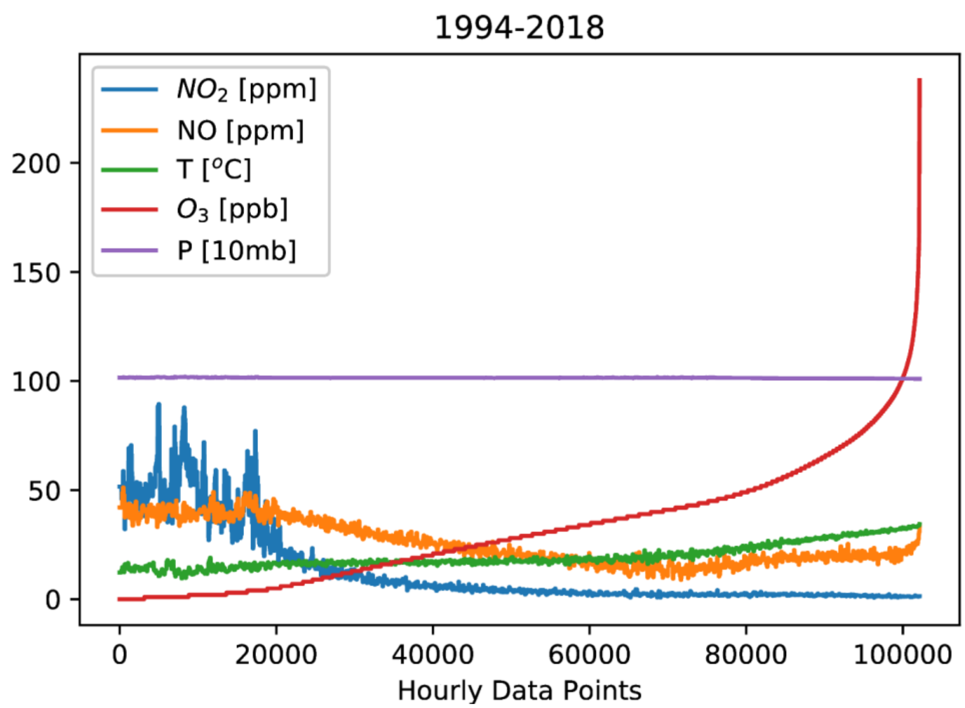


Figure S22. More than one hundred thousand hourly data from 1994 to 2018 for NO_2 (blue), NO (orange), temperature (green), ozone (red), and pressure (purple) were sorted in ascending order.

Tables

Table set S1. Wilcoxon tests for no drop feature, one drop features, two drop features, and three drop features. RFR model was trained on nine features (visibility, NO_2 (no2), NO (no), relative humidity (RH), wind speed (windSP), wind direction (windDir), dew point (dewT), temperature, and pressure). We performed the Wilcoxon tests to test the important of each feature to the model. We run the model with original nine features (no drop), eight features (drop one feature), seven features (drop two features), and six features (drop three features). The Wilcoxon tests were carried out with two scenarios. The first case was to perform the Wilcoxon tests with the actual ozone values and RFR prediction from feature drop. The second case was to perform the Wilcoxon tests with RFR prediction from all nine features and RFR prediction from feature drop.

Wilcoxon tests with the actual ozone values and RFR prediction with all nine features for five different periods from 1994 to 2018. If the output from this test was less than or equal to 0.05 (colored in red), two samples were independent of one another, indicating the significance of the dropped feature for the model prediction.

p-values	**94-98**	**99-03**	**04-08**	**09-13**	**14-18**
Without feature drop	0.17	0.30	0.10	0.10	0.25

Wilcoxon tests with the actual ozone values and RFR prediction from one feature drop for five different periods from 1994 to 2018. If the output from this test was less than or equal to 0.05 (colored in red), two samples were independent of one another, indicating the significance of the dropped feature for the model prediction.

p-values	**94-98**	**99-03**	**04-08**	**09-13**	**14-18**
drop visibility	0.01	0.75	0.02	0.07	0.29
drop no2	0.13	0.14	0.00	0.00	0.73
drop RH	0.17	0.32	0.09	0.12	0.20
drop windSp	0.06	0.92	0.00	0.06	0.57
drop windDir	0.17	0.26	0.05	0.07	0.28
drop dewT	0.17	0.28	0.09	0.20	0.20
drop no	0.00	0.49	0.11	0.11	0.09
drop temperature	0.19	0.31	0.08	0.16	0.17
drop pressure	0.17	0.30	0.08	0.16	0.27

Wilcoxon tests with RFR prediction from all nine features and RFR prediction from one feature drop for five different periods from 1994 to 2018. If the output from this test was less than or equal to 0.05 (colored in red), two samples were independent of one another, indicating the significance of the dropped features for the model prediction.

p-values	94-98	99-03	04-08	09-13	14-18
drop visibility	0.15	0.50	0.49	0.88	0.91
drop no2	0.86	0.68	0.04	0.05	0.14
drop RH	0.98	0.97	0.90	0.89	0.92
drop windSp	0.58	0.26	0.16	0.88	0.52
drop windDir	0.98	0.90	0.75	0.90	0.95
drop dewT	0.99	0.96	0.97	0.71	0.89
drop no	0.03	0.71	0.00	0.90	0.55
drop temperature	0.92	1.00	0.90	0.82	0.82
drop pressure	1.00	0.99	0.94	0.76	0.95

Wilcoxon tests with the actual ozone values and RFR prediction from two feature drop for five different periods from 1994 to 2018. If the output from this test was less than or equal to 0.05 (colored in red), two samples were independent of one another, indicating the significance of the dropped features for the model prediction.

p-values	94-98	99-03	04-08	09-13	14-18
drop temperature-windSp	0.02	0.83	0.00	0.11	0.52
drop windSp-visibility	0.00	0.34	0.00	0.06	0.88
drop dewT-no2	0.28	0.19	0.00	0.00	0.88
drop temperature-windDir	0.18	0.28	0.05	0.09	0.33
drop no2-no	0.00	0.12	0.80	0.00	0.04
drop RH-visibility	0.01	0.98	0.01	0.04	0.36
drop temperature-visibility	0.00	0.83	0.02	0.13	0.16
drop windSp-no	0.00	0.27	0.59	0.02	0.64
drop pressure-windDir	0.23	0.25	0.03	0.11	0.45
drop windDir-dewT	0.24	0.21	0.08	0.06	0.28
drop visibility-dewT	0.00	0.99	0.01	0.08	0.26

drop pressure-no	0.00	0.25	0.12	0.06	0.08
drop temperature-no2	0.15	0.10	0.00	0.00	0.97
drop windSp-no2	0.05	0.85	0.00	0.00	0.01
drop pressure-visibility	0.01	0.96	0.01	0.10	0.35
drop RH-windSp	0.06	0.74	0.00	0.07	0.57
drop RH-windDir	0.24	0.27	0.07	0.04	0.55
drop temperature-dewT	0.35	0.05	0.08	0.41	0.13
drop RH-dewT	0.02	0.90	0.01	0.00	0.93
drop visibility-no	0.00	0.97	0.67	0.06	0.11
drop windSp-windDir	0.05	0.70	0.00	0.02	0.82
drop windDir-no2	0.20	0.17	0.00	0.00	0.63
drop pressure-dewT	0.26	0.32	0.09	0.11	0.23
drop temperature-pressure	0.14	0.26	0.05	0.20	0.13
drop windDir-visibility	0.01	0.92	0.01	0.04	0.65
drop windDir-no	0.00	0.56	0.21	0.03	0.08
drop temperature-no	0.00	0.65	0.11	0.14	0.08
drop visibility-no2	0.07	0.89	0.00	0.00	0.51
drop temperature-RH	0.00	0.39	0.00	0.00	0.00
drop RH-pressure	0.21	0.31	0.06	0.13	0.27
drop dewT-no	0.00	0.73	0.11	0.06	0.13
drop RH-no2	0.24	0.21	0.00	0.00	0.71
drop RH-no	0.00	0.46	0.20	0.07	0.10
drop pressure-no2	0.19	0.24	0.00	0.00	0.72
drop pressure-windSp	0.07	0.99	0.00	0.02	0.65
drop windSp-dewT	0.07	0.88	0.00	0.07	0.67

Wilcoxon tests with RFR prediction from all nine features and RFR prediction from two feature drop for five different periods from 1994 to 2018. If the output from this test was less than or equal to 0.05 (colored in red), two samples were independent of one another, indicating the significance of the dropped features for the model prediction.

p-values	**94-98**	**99-03**	**04-08**	**09-13**	**14-18**
drop temperature-windSp	0.31	0.22	0.10	0.94	0.58

drop windSp-visibility	0.00	0.05	0.02	0.86	0.28
drop dewT-no2	0.77	0.82	0.06	0.05	0.18
drop temperature-windDir	0.96	0.97	0.78	0.97	0.86
drop no2-no	0.00	0.66	0.18	0.00	0.00
drop RH-visibility	0.20	0.29	0.31	0.72	0.78
drop temperature-visibility	0.10	0.41	0.50	0.85	0.76
drop windSp-no	0.00	0.03	0.27	0.49	0.47
drop pressure-windDir	0.85	0.89	0.64	0.96	0.66
drop windDir-dewT	0.83	0.78	0.90	0.82	0.93
drop visibility-dewT	0.10	0.30	0.41	0.97	0.97
drop pressure-no	0.03	0.91	0.00	0.84	0.52
drop temperature-no2	0.90	0.54	0.03	0.05	0.27
drop windSp-no2	0.51	0.21	0.00	0.00	0.00
drop pressure-visibility	0.26	0.35	0.33	1.00	0.81
drop RH-windSp	0.62	0.18	0.17	0.89	0.54
drop RH-windDir	0.80	0.94	0.86	0.72	0.56
drop temperature-dewT	0.67	0.38	0.97	0.01	0.73
drop RH-dewT	0.30	0.40	0.36	0.05	0.20
drop visibility-no	0.00	0.28	0.04	0.89	0.60
drop windSp-windDir	0.53	0.17	0.05	0.55	0.14
drop windDir-no2	0.96	0.78	0.04	0.01	0.10
drop pressure-dewT	0.76	0.99	0.95	0.92	0.97
drop temperature-pressure	0.89	0.90	0.75	0.71	0.73
drop windDir-visibility	0.22	0.34	0.27	0.69	0.46
drop windDir-no	0.04	0.63	0.00	0.59	0.50
drop temperature-no	0.02	0.54	0.00	0.83	0.53
drop visibility-no2	0.64	0.34	0.01	0.01	0.07
drop temperature-RH	0.00	0.04	0.00	0.00	0.00
drop RH-pressure	0.91	0.97	0.80	0.85	0.94
drop dewT-no	0.04	0.45	0.00	0.86	0.67
drop RH-no2	0.81	0.86	0.04	0.06	0.12

drop RH-no	0.03	0.74	0.00	0.91	0.59
drop pressure-no2	0.97	0.92	0.03	0.01	0.12
drop pressure-windSp	0.67	0.32	0.07	0.59	0.45
drop windSp-dewT	0.63	0.24	0.17	0.89	0.42

Wilcoxon tests with the actual ozone values and RFR prediction from three feature drop for five different periods from 1994 to 2018. If the output from this test was less than or equal to 0.05 (colored in red), two samples were independent of one another, indicating the significance of the dropped features for the model prediction.

p-values	**94-98**	**99-03**	**04-08**	**09-13**	**14-18**
drop temperature-visibility-no	0.00	0.97	0.67	0.07	0.14
drop RH-dewT-no	0.00	0.99	0.63	0.00	0.95
drop temperature-windDir-dewT	0.48	0.01	0.02	0.86	0.54
drop pressure-windSp-windDir	0.10	0.75	0.00	0.01	0.61
drop temperature-visibility-dewT	0.03	0.25	0.00	0.52	0.45
drop windDir-visibility-no2	0.05	0.93	0.00	0.00	0.54
drop windDir-dewT-no	0.00	0.54	0.18	0.04	0.19
drop windSp-dewT-no	0.00	0.18	0.89	0.01	0.57
drop temperature-RH-pressure	0.00	0.74	0.00	0.00	0.00
drop RH-windDir-visibility	0.01	0.95	0.00	0.01	0.65
drop windSp-windDir-visibility	0.00	0.24	0.00	0.01	0.74
drop RH-pressure-dewT	0.03	0.97	0.01	0.00	0.43
drop windSp-windDir-no2	0.04	0.42	0.00	0.00	0.00
drop visibility-dewT-no	0.00	0.77	0.78	0.03	0.10
drop temperature-windSp-visibility	0.00	0.18	0.00	0.07	0.45
drop temperature-windDir-no2	0.12	0.18	0.00	0.00	0.72
drop RH-visibility-no2	0.08	0.86	0.00	0.00	0.89
drop temperature-visibility-no2	0.07	0.66	0.00	0.00	0.74
drop pressure-dewT-no	0.00	0.29	0.15	0.05	0.04
drop RH-windSp-windDir	0.06	0.70	0.00	0.01	0.98
drop windSp-dewT-no2	0.04	0.73	0.00	0.00	0.01
drop temperature-windSp-windDir	0.01	0.60	0.00	0.02	0.73

drop RH-no2-no	0.00	0.19	0.88	0.00	0.02
drop pressure-windSp-no	0.00	0.43	0.72	0.01	0.50
drop windSp-windDir-no	0.00	0.02	0.24	0.00	0.96
drop temperature-RH-windSp	0.00	0.00	0.00	0.00	0.00
drop temperature-dewT-no2	0.19	0.01	0.01	0.26	0.92
drop temperature-RH-no	0.00	0.11	0.01	0.00	0.00
drop windSp-visibility-no	0.00	0.13	0.08	0.01	0.51
drop temperature-windDir-no	0.00	0.59	0.18	0.06	0.33
drop temperature-pressure-dewT	0.69	0.00	0.02	0.42	0.11
drop pressure-no2-no	0.00	0.21	0.95	0.00	0.06
drop temperature-RH-dewT	0.00	0.55	0.00	0.00	0.00
drop pressure-dewT-no2	0.28	0.19	0.00	0.00	0.72
drop RH-windSp-dewT	0.00	0.11	0.00	0.00	0.21
drop windDir-visibility-dewT	0.01	0.81	0.02	0.03	0.65
drop windDir-no2-no	0.00	0.25	0.74	0.00	0.00
drop windSp-visibility-dewT	0.00	0.38	0.00	0.02	0.83
drop pressure-windDir-dewT	0.29	0.28	0.03	0.08	0.45
drop temperature-RH-windDir	0.00	0.17	0.00	0.00	0.00
drop RH-windDir-no	0.00	0.62	0.24	0.04	0.09
drop windDir-dewT-no2	0.15	0.23	0.00	0.00	0.38
drop temperature-pressure-no2	0.12	0.18	0.00	0.00	0.79
drop RH-windSp-no	0.00	0.23	0.64	0.02	0.72
drop dewT-no2-no	0.00	0.12	0.95	0.00	0.04
drop windSp-windDir-dewT	0.08	0.79	0.00	0.03	0.83
drop RH-pressure-windDir	0.27	0.28	0.04	0.06	0.51
drop RH-pressure-visibility	0.00	0.89	0.01	0.07	0.49
drop pressure-windSp-no2	0.01	0.30	0.00	0.00	0.01
drop pressure-windDir-visibility	0.02	0.98	0.00	0.03	0.42
drop RH-pressure-no2	0.14	0.35	0.00	0.00	0.66
drop RH-pressure-no	0.00	0.42	0.14	0.03	0.06
drop RH-dewT-no2	0.01	0.53	0.00	0.00	0.02

drop visibility-dewT-no2	0.10	0.88	0.00	0.00	0.64
drop temperature-RH-visibility	0.00	0.11	0.00	0.00	0.00
drop windDir-visibility-no	0.00	0.75	0.99	0.04	0.25
drop temperature-pressure-visibility	0.01	0.97	0.01	0.13	0.20
drop temperature-windSp-dewT	0.04	0.81	0.00	0.77	0.43
drop RH-windSp-no2	0.05	0.60	0.00	0.00	0.01
drop pressure-visibility-dewT	0.00	0.92	0.01	0.04	0.30
drop temperature-windSp-no	0.00	0.17	0.66	0.04	0.48
drop pressure-windDir-no2	0.11	0.44	0.00	0.00	0.74
drop RH-visibility-no	0.00	0.91	0.84	0.03	0.11
drop windSp-visibility-no2	0.01	0.08	0.00	0.00	0.01
drop temperature-pressure-windDir	0.21	0.20	0.03	0.07	0.23
drop temperature-windSp-no2	0.04	0.85	0.00	0.00	0.02
drop RH-visibility-dewT	0.00	0.85	0.00	0.00	0.71
drop pressure-windSp-dewT	0.06	0.92	0.00	0.03	0.53
drop pressure-windDir-no	0.00	0.33	0.29	0.02	0.16
drop visibility-no2-no	0.00	0.62	0.25	0.00	0.02
drop temperature-no2-no	0.00	0.09	0.70	0.00	0.00
drop temperature-pressure-windSp	0.03	0.90	0.00	0.07	0.45
drop windSp-no2-no	0.00	0.03	0.00	0.00	0.00
drop temperature-pressure-no	0.00	0.44	0.12	0.05	0.07
drop pressure-visibility-no2	0.11	0.88	0.00	0.00	0.66
drop pressure-visibility-no	0.00	0.80	0.65	0.03	0.06
drop temperature-windDir-visibility	0.01	0.90	0.00	0.08	0.36
drop RH-pressure-windSp	0.06	0.96	0.00	0.04	0.75
drop temperature-RH-no2	0.00	0.24	0.00	0.00	0.00
drop pressure-windSp-visibility	0.00	0.25	0.00	0.02	0.96
drop RH-windDir-no2	0.18	0.28	0.00	0.00	0.58
drop temperature-dewT-no	0.00	0.07	0.01	0.70	0.15
drop RH-windSp-visibility	0.00	0.31	0.00	0.04	0.95
drop RH-windDir-dewT	0.02	0.92	0.01	0.00	0.58

Wilcoxon tests with RFR prediction from all nine features and RFR prediction from three feature drop for five different periods from 1994 to 2018. If the output from this test was less than or equal to 0.05 (colored in red), two samples were independent of one another, indicating the significance of the dropped features for the model prediction.

p-values	**94-98**	**99-03**	**04-08**	**09-13**	**14-18**
drop temperature-visibility-no	0.00	0.32	0.03	0.94	0.69
drop RH-dewT-no	0.00	0.33	0.03	0.01	0.27
drop temperature-windDir-dewT	0.53	0.16	0.56	0.05	0.57
drop pressure-windSp-windDir	0.74	0.18	0.01	0.39	0.08
drop temperature-visibility-dewT	0.40	0.93	0.18	0.02	0.67
drop windDir-visibility-no2	0.54	0.32	0.00	0.01	0.08
drop windDir-dewT-no	0.07	0.66	0.00	0.74	0.85
drop windSp-dewT-no	0.00	0.01	0.13	0.47	0.53
drop temperature-RH-pressure	0.00	0.13	0.00	0.00	0.00
drop RH-windDir-visibility	0.16	0.34	0.23	0.39	0.46
drop windSp-windDir-visibility	0.00	0.03	0.00	0.29	0.12
drop RH-pressure-dewT	0.44	0.34	0.26	0.06	0.05
drop windSp-windDir-no2	0.48	0.06	0.00	0.00	0.00
drop visibility-dewT-no	0.00	0.45	0.05	0.67	0.60
drop temperature-windSp-visibility	0.00	0.02	0.01	0.89	0.67
drop temperature-windDir-no2	0.85	0.77	0.03	0.03	0.13
drop RH-visibility-no2	0.65	0.21	0.00	0.01	0.21
drop temperature-visibility-no2	0.61	0.56	0.00	0.02	0.15
drop pressure-dewT-no	0.04	0.99	0.00	0.81	0.33
drop RH-windSp-windDir	0.59	0.16	0.07	0.43	0.22
drop windSp-dewT-no2	0.45	0.16	0.00	0.00	0.00
drop temperature-windSp-windDir	0.24	0.12	0.02	0.53	0.11
drop RH-no2-no	0.00	0.82	0.14	0.00	0.00
drop pressure-windSp-no	0.00	0.06	0.18	0.28	0.60
drop windSp-windDir-no	0.00	0.00	0.63	0.18	0.21
drop temperature-RH-windSp	0.00	0.00	0.00	0.00	0.00
drop temperature-dewT-no2	0.99	0.16	0.30	0.58	0.30

drop temperature-RH-no	0.00	0.00	0.36	0.00	0.00
drop windSp-visibility-no	0.00	0.01	0.91	0.30	0.60
drop temperature-windDir-no	0.01	0.59	0.00	0.87	0.89
drop temperature-pressure-dewT	0.38	0.01	0.57	0.01	0.62
drop pressure-no2-no	0.00	0.82	0.11	0.00	0.00
drop temperature-RH-dewT	0.00	0.08	0.00	0.00	0.00
drop pressure-dewT-no2	0.77	0.81	0.01	0.03	0.12
drop RH-windSp-dewT	0.04	0.01	0.00	0.03	0.01
drop windDir-visibility-dewT	0.14	0.44	0.44	0.57	0.46
drop windDir-no2-no	0.00	0.94	0.18	0.00	0.00
drop windSp-visibility-dewT	0.01	0.06	0.02	0.54	0.30
drop pressure-windDir-dewT	0.73	0.95	0.61	0.92	0.68
drop temperature-RH-windDir	0.00	0.01	0.00	0.00	0.00
drop RH-windDir-no	0.05	0.56	0.00	0.74	0.57
drop windDir-dewT-no2	0.94	0.86	0.04	0.01	0.05
drop temperature-pressure-no2	0.83	0.77	0.02	0.05	0.15
drop RH-windSp-no	0.00	0.02	0.25	0.51	0.40
drop dewT-no2-no	0.00	0.60	0.12	0.00	0.00
drop windSp-windDir-dewT	0.68	0.19	0.13	0.64	0.15
drop RH-pressure-windDir	0.74	0.89	0.70	0.79	0.58
drop RH-pressure-visibility	0.07	0.39	0.22	0.87	0.60
drop pressure-windSp-no2	0.22	0.04	0.00	0.00	0.00
drop pressure-windDir-visibility	0.31	0.32	0.20	0.58	0.73
drop RH-pressure-no2	0.90	0.91	0.02	0.02	0.12
drop RH-pressure-no	0.08	0.79	0.00	0.65	0.42
drop RH-dewT-no2	0.17	0.71	0.00	0.00	0.00
drop visibility-dewT-no2	0.72	0.33	0.00	0.02	0.11
drop temperature-RH-visibility	0.00	0.01	0.00	0.00	0.00
drop windDir-visibility-no	0.00	0.17	0.09	0.68	0.94
drop temperature-pressure-visibility	0.17	0.33	0.27	0.88	0.90
drop temperature-windSp-dewT	0.40	0.17	0.07	0.04	0.67

drop RH-windSp-no2	0.57	0.11	0.00	0.00	0.00
drop pressure-visibility-dewT	0.11	0.37	0.34	0.67	0.91
drop temperature-windSp-no	0.00	0.01	0.21	0.68	0.64
drop pressure-windDir-no2	0.82	0.76	0.04	0.01	0.16
drop RH-visibility-no	0.00	0.24	0.06	0.60	0.59
drop windSp-visibility-no2	0.13	0.00	0.00	0.00	0.00
drop temperature-pressure-windDir	0.91	0.79	0.54	0.89	0.94
drop temperature-windSp-no2	0.46	0.22	0.00	0.00	0.00
drop RH-visibility-dewT	0.03	0.27	0.09	0.11	0.12
drop pressure-windSp-dewT	0.59	0.37	0.09	0.66	0.56
drop pressure-windDir-no	0.05	0.91	0.00	0.51	0.76
drop visibility-no2-no	0.01	0.53	0.67	0.00	0.00
drop temperature-no2-no	0.00	0.56	0.22	0.00	0.00
drop temperature-pressure-windSp	0.40	0.26	0.05	0.87	0.67
drop windSp-no2-no	0.00	0.00	0.01	0.00	0.00
drop temperature-pressure-no	0.03	0.77	0.00	0.84	0.49
drop pressure-visibility-no2	0.81	0.23	0.00	0.01	0.11
drop pressure-visibility-no	0.00	0.43	0.03	0.61	0.42
drop temperature-windDir-visibility	0.16	0.38	0.22	0.93	0.82
drop RH-pressure-windSp	0.60	0.35	0.09	0.75	0.36
drop temperature-RH-no2	0.00	0.02	0.00	0.00	0.00
drop pressure-windSp-visibility	0.01	0.03	0.01	0.49	0.24
drop RH-windDir-no2	0.98	0.98	0.03	0.01	0.09
drop temperature-dewT-no	0.05	0.53	0.00	0.03	0.74
drop RH-windSp-visibility	0.01	0.04	0.02	0.68	0.25
drop RH-windDir-dewT	0.33	0.39	0.25	0.03	0.09

Table set S2. Statistical evaluation for three dropped features.

Statistical evaluation for three dropped features from 1994 to 1998. P-value (p) and h were from Wilcoxon test with actual ozone values and RFR prediction from three feature drop. h is 1 when p is less than or equal to 0.05. CC is the correlation coefficient, and NMB is the normal mean bias.

Features Drop	**p**	**h**	**CC**	**NMB**

drop temperature-visibility-no	7.00E-06	1	0.801784	-0.14274
drop temperature-windDir-dewT	0.45695	0	0.783211	-0.07695
drop temperature-visibility-dewT	0.031928	1	0.683842	-0.1173
drop temperature-RH-pressure	3.93E-10	1	0.671577	-0.18099
drop temperature-RH-windSp	1.04E-28	1	0.601521	-0.2818
drop temperature-dewT-no2	0.181967	0	0.759473	-0.09037
drop temperature-RH-no	1.44E-17	1	0.626231	-0.23009
drop windSp-visibility-no	3.62E-10	1	0.782998	-0.17465
drop temperature-pressure-dewT	0.664721	0	0.739901	-0.07331
drop pressure-no2-no	1.97E-06	1	0.793104	-0.13027
drop temperature-RH-dewT	3.45E-11	1	0.662465	-0.19932
drop windDir-no2-no	1.50E-05	1	0.804392	-0.12553
drop temperature-RH-windDir	9.89E-11	1	0.685107	-0.18846
drop temperature-RH-visibility	3.48E-12	1	0.666221	-0.19847
drop windDir-visibility-no	1.42E-05	1	0.796187	-0.13747
drop temperature-windSp-dewT	0.033606	1	0.743337	-0.10844
drop visibility-no2-no	0.000221	1	0.78021	-0.1251
drop temperature-no2-no	2.53E-06	1	0.80524	-0.13841
drop windSp-no2-no	3.36E-10	1	0.791098	-0.16675
drop pressure-visibility-no	9.97E-06	1	0.795026	-0.13594
drop temperature-RH-no2	2.95E-10	1	0.683469	-0.18164
drop temperature-dewT-no	0.001461	1	0.734516	-0.13513

Statistical evaluation for three dropped features from 1999 to 2003. P-value (p) and h were from Wilcoxon test with actual ozone values and RFR prediction from three feature drop. h is 1 when p is less than or equal to 0.05. CC is the correlation coefficient, and NMB is the normal mean bias.

Features Drop	**p**	**h**	**CC**	**NMB**
drop temperature-windDir-dewT	0.012967	1	0.787945	0.024295
drop temperature-visibility-dewT	0.262872	0	0.783029	-0.00334
drop temperature-RH-pressure	0.711	0	0.735766	-0.04654
drop RH-no2-no	0.202349	0	0.765157	0.000328
drop pressure-windSp-no	0.41427	0	0.807998	-0.04159
drop temperature-RH-windSp	2.80E-14	1	0.669267	-0.19542
drop temperature-dewT-no2	0.01234	1	0.770627	0.02407
drop temperature-RH-no	0.099614	0	0.710964	-0.07459
drop temperature-pressure-dewT	0.000216	1	0.745702	0.048967
drop pressure-no2-no	0.218405	0	0.747899	0.003472
drop temperature-RH-dewT	0.526379	0	0.697282	-0.04446
drop windDir-no2-no	0.258033	0	0.765861	-0.00022
drop temperature-RH-windDir	0.161704	0	0.754945	-0.06661
drop dewT-no2-no	0.122467	0	0.762824	0.007162
drop temperature-RH-visibility	0.106475	0	0.762941	-0.06819

drop temperature-windSp-dewT	0.780732	0	0.760772	-0.03486
drop visibility-no2-no	0.639241	0	0.744436	-0.01202
drop temperature-no2-no	0.096085	0	0.767118	0.00764
drop windSp-no2-no	0.030094	1	0.725952	-0.06466
drop pressure-visibility-no	0.824903	0	0.808422	-0.01421
drop temperature-RH-no2	0.231534	0	0.733835	-0.05912
drop temperature-dewT-no	0.072791	0	0.74421	0.000943

Statistical evaluation for three dropped features from 2004 to 2008. P-value (p) and h were from Wilcoxon test with actual ozone values and RFR prediction from three feature drop. h is 1 when p is less than or equal to 0.05. CC is the correlation coefficient, and NMB is the normal mean bias.

Features Drop	**p**	**h**	**CC**	**NMB**
drop temperature-RH-pressure	9.15E-09	1	0.691019	-0.11974
drop RH-no2-no	0.851888	0	0.789129	-0.01003
drop temperature-RH-windSp	8.93E-33	1	0.638616	-0.21775
drop temperature-RH-no	0.008522	1	0.667063	-0.06782
drop temperature-pressure-dewT	0.021587	1	0.778933	-0.05898
drop pressure-no2-no	0.92948	0	0.770663	-0.00919
drop temperature-RH-dewT	8.00E-10	1	0.708957	-0.128
drop windDir-no2-no	0.713252	0	0.778714	-0.01301
drop temperature-RH-windDir	7.14E-09	1	0.734965	-0.1192
drop dewT-no2-no	0.925348	0	0.786617	-0.00787
drop temperature-RH-visibility	6.06E-09	1	0.737463	-0.12258
drop visibility-no2-no	0.239182	0	0.779829	-0.02533
drop temperature-no2-no	0.674961	0	0.787052	-0.01177
drop windSp-no2-no	6.79E-05	1	0.759365	-0.0697
drop temperature-RH-no2	5.96E-13	1	0.717344	-0.13626
drop temperature-dewT-no	0.014611	1	0.753523	0.018978

Statistical evaluation for three dropped features from 2009 to 2013. P-value (p) and h were from Wilcoxon test with actual ozone values and RFR prediction from three feature drop. h is 1 when p is less than or equal to 0.05. CC is the correlation coefficient, and NMB is the normal mean bias.

Features Drop	p	h	CC	NMB
drop temperature-windDir-dewT	0.886059	0	0.79726	-0.01132
drop temperature-visibility-dewT	0.539812	0	0.802949	-0.00061
drop RH-no2-no	3.53E-07	1	0.780223	-0.07705
drop temperature-RH-windSp	2.09E-23	1	0.603255	-0.16104
drop temperature-dewT-no2	0.250885	0	0.76968	-0.02417
drop temperature-RH-no	1.48E-10	1	0.646956	-0.10852

drop temperature-pressure-dewT	0.434343	0	0.775243	-0.00507
drop pressure-no2-no	6.43E-07	1	0.767951	-0.07716
drop temperature-RH-dewT	1.15E-12	1	0.66335	-0.1142
drop windDir-no2-no	3.26E-07	1	0.777546	-0.08089
drop temperature-RH-windDir	1.62E-11	1	0.675657	-0.1131
drop dewT-no2-no	1.87E-07	1	0.785766	-0.07794
drop temperature-RH-visibility	4.33E-11	1	0.670451	-0.1106
drop temperature-windSp-dewT	0.797974	0	0.790291	-0.00799
drop visibility-no2-no	7.29E-09	1	0.774264	-0.08313
drop temperature-no2-no	9.26E-07	1	0.787752	-0.07393
drop windSp-no2-no	2.23E-14	1	0.750573	-0.10816
drop temperature-RH-no2	2.27E-17	1	0.646149	-0.13188
drop temperature-dewT-no	0.726114	0	0.755332	-0.00863

Statistical evaluation for three dropped features from 2014 to 2018. P-value (p) and h were from Wilcoxon test with actual ozone values and RFR prediction from three feature drop. h is 1 when p is less than or equal to 0.05. CC is the correlation coefficient, and NMB is the normal mean bias.

Features Drop	**p**	**h**	**CC**	**NMB**
drop temperature-windDir-dewT	0.561955	0	0.769046	-0.0127
drop temperature-visibility-dewT	0.464277	0	0.771125	-0.01168
drop temperature-RH-pressure	0.000239	1	0.633839	-0.06806
drop temperature-RH-windSp	5.46E-13	1	0.623159	-0.11354
drop temperature-dewT-no2	0.948555	0	0.734269	-0.01476
drop temperature-RH-no	2.63E-05	1	0.632899	-0.07046
drop temperature-pressure-dewT	0.112191	0	0.721429	-0.00148
drop pressure-no2-no	0.053613	0	0.772973	-0.02917
drop temperature-RH-dewT	5.74E-07	1	0.643603	-0.08532
drop windDir-no2-no	0.004348	1	0.776112	-0.04655
drop temperature-RH-windDir	0.000919	1	0.656068	-0.06274
drop dewT-no2-no	0.035604	1	0.802024	-0.03372
drop pressure-windSp-no2	0.004735	1	0.800965	-0.04549
drop temperature-RH-visibility	0.000253	1	0.655908	-0.06693
drop temperature-windSp-dewT	0.445095	0	0.742402	-0.0126
drop visibility-no2-no	0.019345	1	0.785613	-0.0343
drop temperature-no2-no	0.004275	1	0.800114	-0.04446
drop windSp-no2-no	2.45E-08	1	0.769147	-0.07873
drop temperature-RH-no2	1.11E-07	1	0.618039	-0.0844
drop temperature-dewT-no	0.15424	0	0.74638	0.002089

Table S3. CMAQ MDA8 Fontana

Month	MBE	NMB	MAE	MFB	MFE
5	6.059286	0.125268	8.270714	0.133177	0.173034
6	8.99	0.141363	11.56667	0.145812	0.179497
7	9.504032	0.140691	13.125	0.138504	0.192391
8	-3.76042	-0.04737	13.84077	-0.03533	0.175221
9	13.95382	0.235017	15.64347	0.225449	0.247755

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 error:

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

Mean absolute error:

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

Root mean square error:

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

Relative root mean square error:

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

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:

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

We evaluated the regression algorithms using the intrinsic metrics of linear fit (e.g., R^2, slope, and intercept), CC, RMSE, and MAE. We evaluated different classification algorithms based on probability of detection (PoD), accuracy, model error, and failure to predict (Eqs. 14-17).

Probability of detection:

$$PoD = \frac{True\ predicted\ exceedances}{Observed\ exceedances} = \frac{d}{b + d} \quad (14)$$

Accuracy:

$$Accuracy = \frac{a + d}{a + b + c + d} \quad (15)$$

Model Error:

$$Error = \frac{b + c}{a + b + c + d} \quad (16)$$

Failure to predict:

$$Failture\ to\ predict = 1 - PoD \quad (17)$$

In Eqs. 15 and 16, a is the number of correct non-exceedance predictions; b is the number of incorrect non-exceedance predictions; c is the number of incorrect exceedance prediction; and d is the number of correct exceedance predictions.

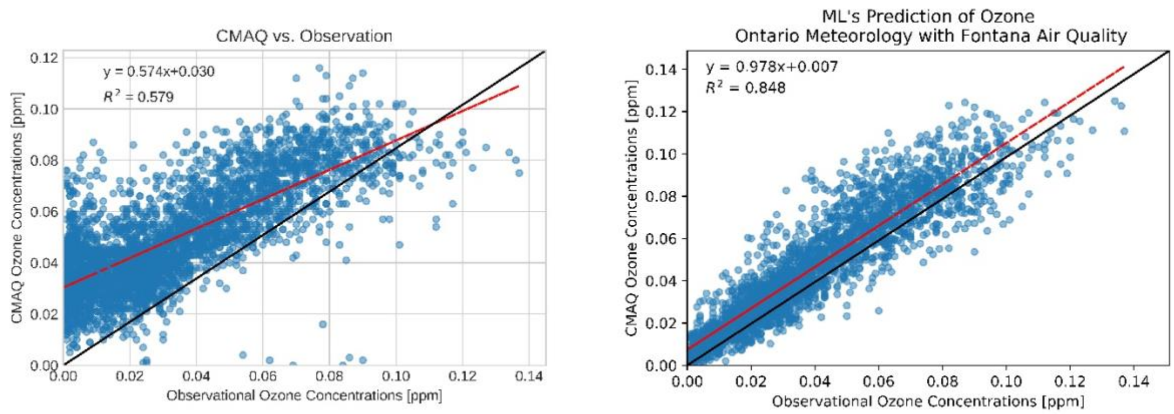
A Direct Comparison between ML and CMAQ

We compared the performance between the ML prediction and CMAQ simulation for ozone concentrations. We used the ML model that was trained on ONT meteorology with Fontana air quality to predict the ozone concentrations for the period from May to October of 2017. Figure S25 shows a time series of daily average ozone concentrations which were predicted by RFR model (red line). The RFR model well captured the ozone trends throughout the ozone season. The highest daily average ozone days can be seen in late August of 2017 and are strongly correlated with high temperatures. The RFR model was also able to reconstruct the ozone peaks (high and low ozone levels). It has done a better job to capture the nighttime ozone concentrations, which CMAQ greatly overestimated (Figure S8). The statistical summary for CMAQ and RFR model is shown in Table S4. Overall, the RFR model had better statistical evaluation metrics (NMB, MB, and MAE) for the 2017 ozone season. Both CMAQ and RFR overestimate ozone levels; however, the RFR model has a smaller bias, which ranges from 3.9 ppb to 10 ppb while CMAQ outputs' MB ranges from 11 ppb to 22 ppb.

Table S4. Statistical summary of CMAQ and ML for the period from May to September 2017. The units are in ppm.

Month	NMB		MB (ppm)		MAE (ppm)	
	CMAQ	RFR	CMAQ	RFR	CMAQ	RFR
May	0.382	0.202	0.0111	0.00683	0.0134	0.0077
June	0.473	0.160	0.0161	0.00665	0.0178	0.00987
July	0.526	0.250	0.0175	0.0102	0.0199	0.0129
August	0.354	0.084	0.0136	0.00391	0.0207	0.00870
September	0.651	0.122	0.0216	0.00489	0.0235	0.00857

Figure S23a and Figure S23b show scatter plots of observation and model for CMAQ simulation and RFR model, respectively. The R^2 for CMAQ simulation was 0.58, and most of the data points lie above the 1:1 line indicating that ozone concentrations were overestimated. The CMAQ scatter plot's linear equation also shows that CMAQ greatly overestimated low ozone concentrations (nighttime ozone). The RFR model gave a better performance with the R^2 of 0.85, the slope of 0.98, and the intercept of 7 ppb. The small value of intercept and the slope, which is closed to one, specify the good achievement from the RFR model, and the data of scatter plot were distributed more evenly around the 1:1 line.



(a) (b)

Figure S23. Scatter plots of CMAQ simulation (a) and RFR predictions (b) for Fontana for 2017 ozone season.

CMAQ Model Descriptions

The second part of our study uses a chemical transport model to provide evaluation data from a deterministic model. CMAQ was run in parallel on a dual Xeon workstation with 16 processing units on an Ubuntu server operating system and compiled with GFortran. Meteorological and atmospheric simulations were carried out at 4 km horizontal resolution with 11 vertical layers over SoCAB. The mechanism configuration used for the 2017 simulation was SAPRC07tc_ae6_aq (SAPRC07tc photochemical mechanism, aerosol module 6, and aqueous chemistry). Gridded 4 km emissions inputs of

73 air pollutants were provided by SCAQMD as daily emission files with hourly temporal resolution, and emissions estimates were based on their 2016 Air Quality Management Plan[1]. At the end of every simulated day, CMAQ generated daily NetCDF output files, and those results were used as inputs for the following day's initial conditions. CMAQ's governing processes and the details of SAPRC-07 may be found in the work of Byun and Schere and William P.L. Carter, respectively [2,3]. The boundary conditions were extracted from a CMAQ simulation over the U.S from a previous study.[4] The Weather Research and Forecasting (WRF) model version 3.9 was used to generate meteorological data. The optimal options for WRF and the WRF Preprocessing System (WPS) specific to SoCAB are USGS land use, thermal diffusion surface layer scheme [5], and Yonsei University planetary boundary layer scheme [6]. We combined the North American Mesoscale (NAM) Forecast System initialization data with NOAA high-resolution sea surface temperature (SST) nudging [7] to improve the accuracy of meteorological inputs for SoCAB. The SCAQMD region, shown in thick black lines, was selected as the target study area (Figure S24). The finest domain has a horizontal grid resolution of 4 km (Domain 3), fully covering the SCAQMD region, and the domain consisted of 156 (east west) x 102 (north-south) grid cells.

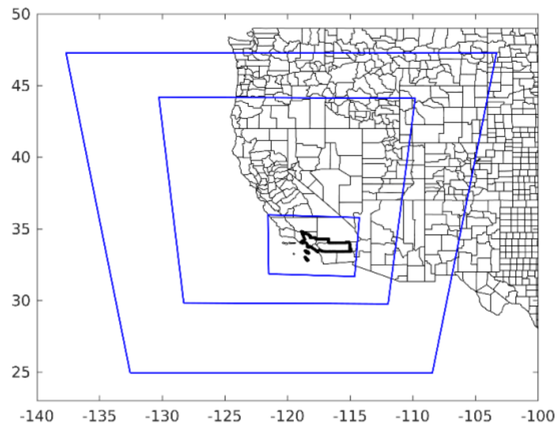


Figure S24. Nesting of model domains for WRF. The outer most domain has 36 km horizontal resolution, and the first and second inner domains have 12 and 4 km resolution, respectively. The South Coast Air Quality Management District boundary is in bold.

CMAQ Evaluation

The positive MBs for all evaluation sites suggest the overall overestimates of the model with a maximum MB of 16 ppb (Fontana) and a minimum of 6 ppb (Crestline and LA). The overestimation occurred because the model did not capture the low ozone concentrations at night (Figure S8), which significantly increased the CMAQ daily average ozone concentrations. Figure S shows the daily average temperature with daily average ozone levels in Fontana. The dots and solid line represent observations and model outputs, respectively. Ozone concentrations are simulated by CMAQ v5.2 (Figure S25). The temperature profile was well-represented by the WRF model in Fontana. The minimum average temperature was 13.1^{o}C for WRF model and 11.3^{o}C for observations on May-07, and the maximum was 33.8^{o}C for WRF model and 31.1^{o}C for observations on Jul-07. The minimum and maximum temperature days matched for the observations and model. Over the period, the model overestimates ozone by a factor of 1.52. However, the simulated ozone well-captured the historical temporal trends and peaks. Ozone trends are shown in Figure S8 for the two months from May-01 to July-01. The model matches the observation for the peak ozone of the day; however, it did not represent the lowest ozone level resulting in the overall overestimates of the daily average ozone concentrations. Simulated ozone exhibited the expected response to the high-temperature days, and the highest daily average ozone (0.077 ppm) was obtained on the day with the highest daily average temperature.

Table S5. CMAQ benchmarking statistical summary of ozone simulation for nine SCAQMD air monitoring stations. Units are in ppm.

Stations	Max	Min	Mean	Median	Q1	Q3	RMSE	rRMSE	MAE	MBE
Anaheim	0.107	0	0.037	0.041	0.032	0.053	0.014	0.391	0.012	0.009
Azusa	0.114	0	0.042	0.046	0.033	0.060	0.017	0.402	0.014	0.008
Crestline	0.12	0.004	0.060	0.062	0.055	0.069	0.023	0.499	0.020	0.006
Fontana	0.116	0	0.045	0.050	0.036	0.065	0.022	0.567	0.019	0.016
LA	0.101	0	0.033	0.037	0.023	0.051	0.015	0.757	0.013	0.006
Pasadena	0.111	0	0.043	0.046	0.035	0.058	0.018	0.433	0.016	0.012
Redlands	00.108	0	0.053	0.056	0.046	0.067	0.021	0.413	0.018	0.008
Rubidoux	0.118	0	0.045	0.049	0.035	0.065	0.018	0.762	0.015	0.009
SB	0.119	0	0.047	0.052	0.038	0.066	0.020	0.449	0.017	0.007

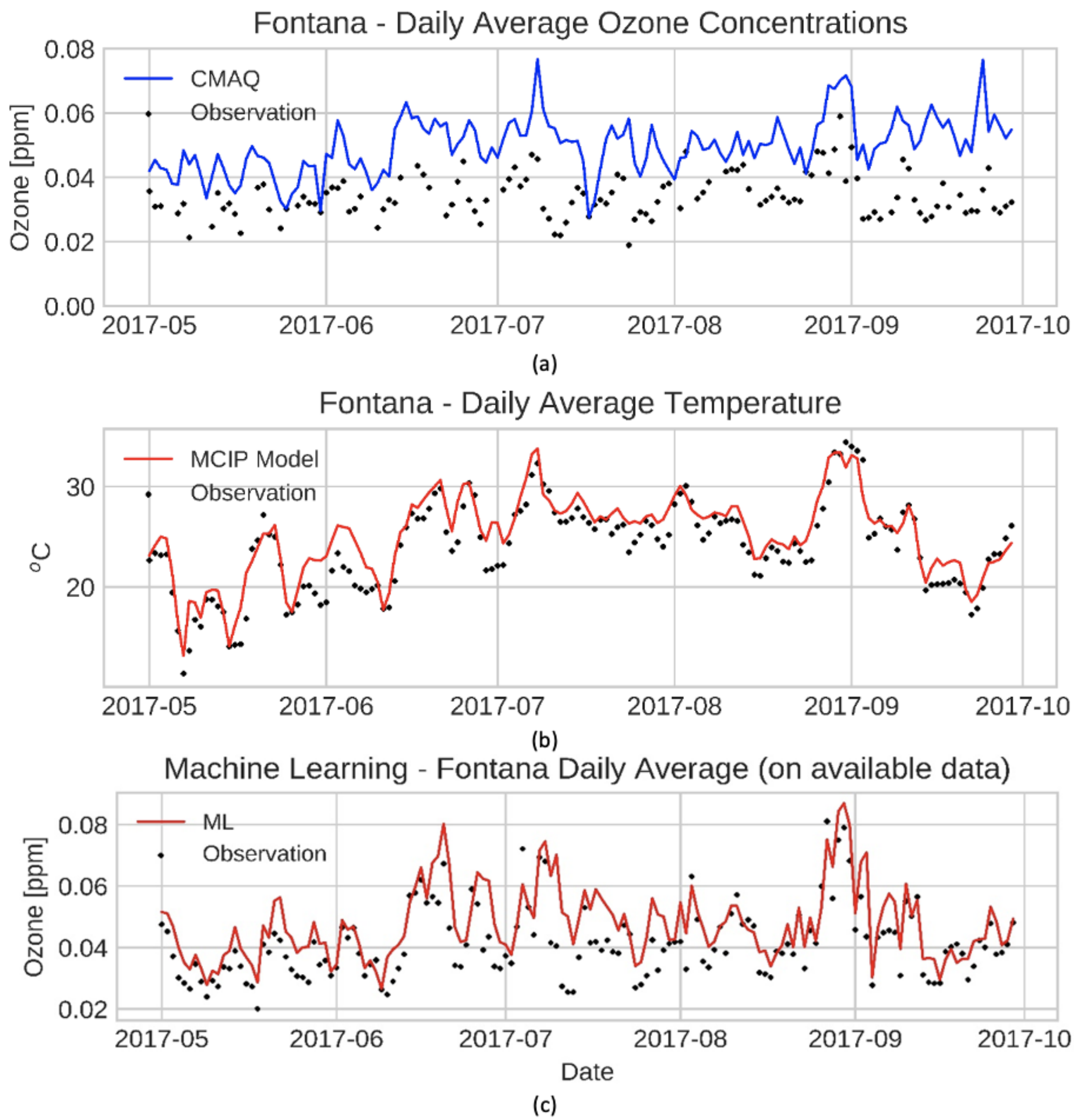


Figure S25. Time series of daily average ozone concentrations (a) of CMAQ outputs (blue line) and observation (black dots), daily average temperature (b) from WRF (red line) and observation (black dots), and (c) ML predictions (red line) and observation (black dots) in Fontana, CA. The Fontana daily average calculation for ML was based on available data, which was not restricted to twenty-four data points per day. Due to the missing data, the ML outputs were sparser than the CMAQ outputs. Therefore, the computed daily average observations from hourly data were the different between (a) and (c).

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