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A machine learning approach for ozone forecasting and its application for Kennewick, WA

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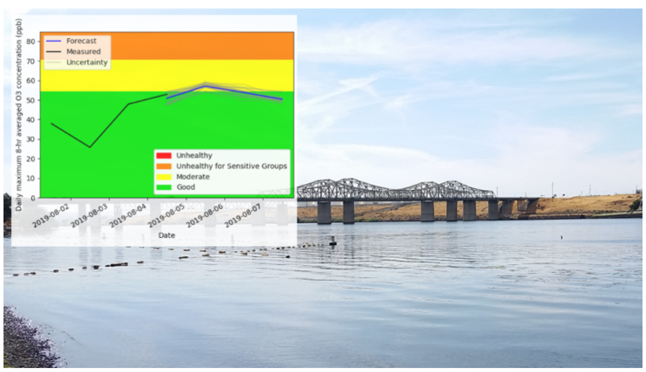
ABSTRACT:

Chemical transport models (CTM) are widely used for air quality modeling, but these models miss forecasting some air pollution events, and require a lot of computational power. In Kennewick, WA, elevated O_3 episodes can occur during the summer and early fall, but the CTM-based operational forecasting system (AIRPACT) struggles to capture them. This research used the 2015 – 2018 historical archives from the Weather Research and Forecasting (WRF) meteorological model forecasts produced daily by the University of Washington, and O_3 observation data at

Kennewick to train two machine learning modeling frameworks, ML1 and ML2 for a reliable forecasting system. ML1 used the random forest (RF) classifier and multiple linear regression (MLR) models, and ML2 used a two-phase RF regression model with best-fit weighting factors. Since April 2019, the ML modeling frameworks have been used to produce daily 72-hour O_3 forecasts and have provided the forecasts via the web for the agency and public use. For the peak O_3 days, AIRPACT showed a large variation, while ML2 underpredicted and ML1 performed the best. In the future, this dual ML forecast system will be applied to other locations within the Pacific Northwest.



1. INTRODUCTION

Chemical transport models (CTM) are widely used to simulate the temporal and spatial variation of air quality.[1] CTMs include various atmospheric physical and chemical processes as well as sources and sinks. However, not every physical and chemical process in the atmosphere has been understood.[2] Even though the accuracy of numerical models keeps improving, there are still large uncertainties and errors in the simulations. For the CTMs, the high computational cost is an additional concern.

The Air Indicator Report for Public Awareness and Community Tracking (AIRPACT) was developed for air quality forecasting in the Pacific Northwest in the U.S. AIRPACT uses the Community Multiscale Air Quality Modeling System (CMAQ) model to compute air quality with the Weather Research and Forecasting (WRF) meteorology. The AIRPACT domain mainly covers Washington, Idaho and Oregon State with 4 km horizontal grid cells and 37 vertical levels. The hourly simulations use the Carbon Bond, version 5 (CB05) as the gas chemistry mechanism and AERO6 as the aerosol module. AIRPACT 48-hour forecasts are produced daily and provided via the web to the public and local air quality agencies (http://lar.wsu.edu/airpact/).

Within the AIRPACT domain, Kennewick is part of the Tri-cities metropolitan area with a total population of about 216,000 (Estimated population of Kennewick 83,670, Pasco 75,290 and Richland 56,850 in 2019).[3] The city is 32 km north of Washington State's southern border and is in a hot dry portion of the state. Recent monitoring and a large field study have shown that a few high O_3 events typically occur during summer and early fall.[4] While AIRPACT forecasts initially predicted the Tri-cities area as an ozone hotspot, the daily forecasts struggle to forecast correctly high O_3 concentrations in this area. There were 20 days when the air quality was unhealthy for sensitive groups in 2015 – 2018, but AIPRACT only captured one of them.

Machine learning (ML) models have been used to predict air quality in recent years. These methods incorporate a variety of features, including observed pollutant levels and various meteorological variables as the basis for training and applying ML methods. For example, Feng et al.[5] input trajectory-based geographic parameters, meteorological forecasts and associated pollutant predictors to an artificial neural network to predict PM2.5 concentrations in Beijing, China. Freeman et al.[6] used a recurrent neural network with short-term memory to predict 72-hour O_3 forecasting with training via hourly air quality and meteorological data. Zamani Joharestani et al.[7] tested three machine learning approaches, random forest, extreme gradient boosting and deep learning to predict the PM2.5 concentrations in Tehran, Iran using 23 features.

A successful ML model must be trained with a large dataset. For air quality prediction, the training dataset usually includes meteorological data (temperature, relative humidity, pressure, wind speed and direction, etc.) and observed pollutant concentrations. However, compared to numerical models, ML methods tend to be more computationally efficient, require less input data, and perform better for specific events, which makes ML models popular in recent years.[5,6,8–10]

In this study, we developed ML modeling frameworks to predict O_3 mixing ratios, which were based on the following approaches: random forest (RF) and multiple linear regression (MLR). RF is one of the most popular machine learning methods and has been used in many air quality modeling and forecast studies. The RF method has been demonstrated to provide reliable forecasts for O_3 and PM2.5 with lower computational cost compared to physical models.[11–14] RF consists of an ensemble of decision trees, and decision tree learning is for approximating discrete-valued functions.[15–17] The RF model can be used for classification and regression. For our study, the RF classifier model was used to predict the O_3 Air Quality Index (AQI) categories, and the RF regression model was used to predict O_3 mixing ratios. MLR is a regression method with one dependent variable and several independent variables, which we used to predict O_3 levels. Previous studies that used MLR models to predict O_3 mixing ratios showed performance as good as more complex machine learning models.[18–21] Yuchi et al.[22] used RF and MLR for indoor air quality forecasts, and RF showed better in-sample predictions, MLR showed better out-of-sample predictions. So, this paper will discuss the application of both RF and MLR for O_3 forecasts.

The goal of this study was to provide reliable air quality forecasts using machine learning approaches, especially for high O_3 events in Kennewick, WA. Section 2 presents the two machine learning modeling frameworks we developed, including the training dataset. Section 3 presents the feature selection, evaluation of the model performance using 10-time 10-fold/walk-forward cross-validation and a summary of the forecast results in 2019.

2. DATASETS AND MODELING FRAMEWORKS

2.1. Training dataset.

The training dataset for our machine learning models includes the previous day's observed O_3 mixing ratios, time information (hour, weekday, month), and simulated meteorology from daily WRF forecasts from May to September in 2015 – 2018 at Kennewick, WA. Because the heat and sunlight favor the O_3 generation,[23] and wildfires can generate the O_3 precursors,[24] observations are only made from May to September. The training dataset covered this period. The WRF meteorology was obtained from the University of Washington,[25,26] which is used in AIRPACT as an input to generate emissions and air quality forecasting. We used the temperature, surface pressure, relative humidity, wind speed, wind direction, and planetary boundary layer height (PBL) in the training dataset. Time information was included in the training dataset due to the significant trend of O_3 variation in the diurnal, weekday and monthly scales. Table S1 summarizes the historical O_3 AQI during the training period. Here we define a high O_3 day as the day when the observed AQI category is worse than Moderate (i.e. AQI category 3 or worse). The high O_3 days in all the years used here are less than 5% of total simulated days, except for 2017. Extensive wildfires occurred in 2017, and there were 8 days that the air quality was unhealthy for sensitive groups (i.e., O_3 AQI category = 3). The days when the wildfire smoke caused excess O_3 were marked in the historical data, but it could not be involved in the training dataset because it was not predictable. And there were only four days in this case, so it would not affect the model training significantly.

2.2. Machine learning modeling frameworks

We have developed two O_3 forecast modeling frameworks based on ML methods. The first machine learning modeling framework (ML1, hereafter; see Figure 1A) used RF classifier and MLR models. The *RandomForestClassifier* and *RFE* functions in the python module *sklearn* were used. In ML1, the WRF meteorology, time information, and previous day's 8-hour averaged O_3 mixing ratios were first used to train an RF classifier model to predict AQI categories. There are not many high O_3 cases, which makes the dataset imbalanced, and the imbalanced training data may lead the bias toward the low O_3 prediction.[27] To address the problem from the imbalanced data, the *balanced_subsample* option was turned on for the RF classifier. The *balanced_subsample* gives weights to the AQI category values based on their frequency in the bootstrap sample for each tree, so the high AQI values with low frequency in the training dataset are weighted proportionally more. Separately, the observed AQI categories were added to the training dataset to train the MLR model. When used for forecasting, the RF classifier model was first used to predict the AQI categories, which were in turn fed into the MLR model to predict the O3 mixing ratios, as the red dashed line shown in Figure 1A.

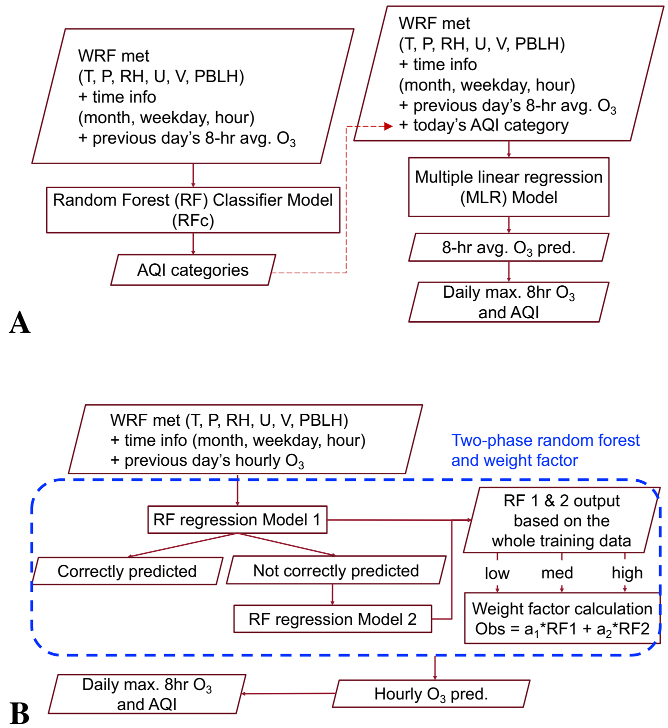


Figure 1. (A) ML1 modeling framework based on random forest (RF) classifier and multiple linear regression (MLR) models (B) ML2 based on a two-phase RF regression and weight factors

Machine Learning modeling framework 2 (ML2 hereafter; see Figure 1B) is based on a two-phase random forest regression model. The *RandomForestRegressor* function in the python module *sklearn* was used. ML2 used the WRF meteorology, time information, and previous day's hourly O_3 mixing ratios to train an RF regression model to predict O_3 mixing ratios. The whole historical dataset was used to train the first RF regression model (RF1 in Figure 1B). The training data was isolated when RF1 predicted O_3 mixing ratios differed from the observations by more than 5 ppb, and then the isolated dataset was used to train the second RF regression model (RF2 in Figure 1B). The training dataset for RF2 was a subset of the whole training data, so RF2 required more decision trees (100 trees for RF1 and 200 trees for RF2).[28] This is why it is called a two-phase RF regression model. The RF1 predicted O_3 mixing ratios were divided into three levels (low: < 30 ppb, medium: 30 – 50 ppb, high: > 50 ppb). For the data within each level, a set of weighting factors, a_1 and a_2, were computed based on a linear regression equation,

$$O_{3observed} = a_1*RF_1 + a_2*RF_2 \qquad (1)$$

When doing forecasting, RF1 and RF2 were used to provide initial predictions. The RF1 prediction determined which weighting factors would be used. The hourly O_3 prediction was computed as

$$O_3 = a_1*RF_1 + a_2*RF_2 \qquad (2)$$

2.3. Ensemble forecasting system

The ML1 and ML2 modeling frameworks have been used to provide 72-hour "ensemble" operational O_3 forecasts each day, by using more than 20 members from the University of Washington Mesoscale Ensemble system (https://a.atmos.washington.edu/wrfrt/ensembles/info.html) beginning in April 2019. We predicted the O_3 levels with each WRF member to compile a 72-hour ensemble mean forecast with an associated uncertainty range. The forecasts are available to the public on http://ozonematters.com, with the ability to sign up for email alerts if "Unhealthy for Sensitive Groups" or worse levels are forecast. To increase the size of the training dataset and improve the forecast accuracy, we included the new observational data from the previous day and re-trained the models daily. For the ensemble daily forecasts, the computational time is approximately 1 min for ML1 and less than 3 min for ML2.

2.4. Statistical methods for O_3 AQI evaluation

Two parameters, Heidke Skill Score (HSS) and the Hanssen-Kuiper Skill Score (KSS) were used to evaluate the machine learning model prediction. Table S2 is a 2x2 contingency table, which shows the simple yes or no cases.[29] For the air quality research, "yes" usually means air pollution events, and "no" means good air quality. The equations (3) and (4) show how HSS and KSS are computed.[30]

$$HSS = \frac{a + d - a_r - d_r}{n - a_r - d_r} \qquad (3)$$

Where $a_r = \frac{(a+b)(a+c)}{n}$, $d_r = \frac{(b+d)(c+d)}{n}$

$$KSS = \frac{ad - bc}{(b + d)(a + c)} \qquad (4)$$

HSS represents the accuracy of the model prediction compared with a reference forecast (r in equation 3), which is from the random guess that is statistically independent of the observations.[30,31] The range of the HSS is from -∞ to 1. A negative value means a random guess is better, 0 means no skill, and 1 means a perfect score. KSS measures the ability to separate different categories. The range is from -1 to 1 where 0 means no skill, and 1 means a perfect score.

For the multi-category case in this research with AQI 1 (Good), 2 (Moderate) or 3 (Unhealthy for Sensitive Groups), we use the 3x3 contingency table in Table S3 [32]. The skill scores are computed as follows.[30]

$$HSS = \left(\sum_{i=1}^{3} p_{ii} - \sum_{i=1}^{3} p_i\, \hat{p}_i\right) / \left((1 - \sum_{i=1}^{3} p_i\, \hat{p}_i)\right) \quad (5)$$

$$KSS = \left(\sum_{i=1}^{3} p_{ii} - \sum_{i=1}^{3} p_i\, \hat{p}_i\right) / \left((1 - \sum_{i=1}^{3} p_i\, p_i)\right) \quad (6)$$

The p_{ii} is the sample frequency when the observed and model predicted AQI is i, and p_i and $\hat{p}_i$ are the observed and model predicted sample frequency when AQI = i. The multi-category case is based on the simple yes or no case, and the skill scores, HSS and KSS have the same meaning as the simple case.

3. RESULTS AND DISCUSSION

3.1. Feature selection for machine learning models

There were 10 features for the RF classifier and regression model and 11 features for the MLR model. Too many features can cause an overfitting problem,[33] so the attributes *feature_importances_* in function *RandomForestClassifier*/*RandomForestRegressor* and *ranking_* in *RFE* were used to do the feature selection. The selected features were input to train the model.

There were two components in ML1, RF classifier and MLR model. For an RF model, the feature selection function with the default setting computed the importance weights, and the features whose weight was above the mean weight were selected. The feature weights could change in each training process, but the ranking showed very little variation. The previous day O_3 observation, temperature and hour were the primary features selected, and the relative humidity was selected in some cases. The default number of selected features for MLR was half of the total features available, so two more features were chosen by the built-in feature selection function, in addition to the three primary features: the previous day O_3 observation, temperature, relative humidity, AQI category, and surface pressure. The output of each framework was hourly O_3 mixing ratios for each 72-hour forecast. For evaluation purposes, these forecast values were compiled into the maximum daily 8-hour moving average O_3 (MDA8).

The feature selection function for RF regression was the same as the RF classifier model. Temperature, previous O_3 observation, PBL height or relative humidity, were the selected features for the first phase RF regression model, and the temperature and hour were selected for the second phase.

3.2. Machine learning model evaluation

Cross-validation is commonly used for model evaluation, since it can test the subset of the dataset with an equal chance.[34] There are various cross-validation methods, such as leave-one-out, k-fold, etc. Here, the 10-time 10-fold and walk-forward cross-validation were used to evaluate the two modeling frameworks. The input data were the primary WRF output, time information and historical O_3 observations in Kennewick.

3.2.1 10-time 10-fold cross-validation

The k-fold cross-validation may be the most commonly used technique for the model evaluation.[34] It divides the dataset into k randomly chosen parts (k=10 in this research), and k-1 parts are used to train the model, the remaining portion is used to test the model, and this process is repeated k times to test all k subsets. The *RepeatedKFold* function in the python module *sklearn* was used to separate the dataset. To avoid any bias from data separation, the k-fold cross-validation was repeated 10 times in this research.

The NMB for these 10-time cross-validation was 6.3% ± 0.2% for ML1 and 0 ± 0.1% for ML2. The AIRPACT NMB was -9.3%, which was lower than ML1 and ML2. The standard deviations show that there is no significant difference among each repeat, and the model performance is stable.

The Q-Q plots in Figure 2A show the comparison between the model predictions and observations. AIRPACT underpredicted the MDA8 for MDA8 lower than 70 ppb. For MDA8 higher than 70 ppb, AIRPACT tended to predict the DMA8 close to the 1:1 line, but there were several extremely high predictions from AIRPACT which were not shown in Figure 2A. ML1 and ML2 were close to the 1:1 line when the MDA8 was lower than 45 ppb. ML1 was close to the 1:1 line for MDA8 in the 60 – 70 ppb range. For high MDA8 cases (> 70 ppb), ML1 showed the best performance.

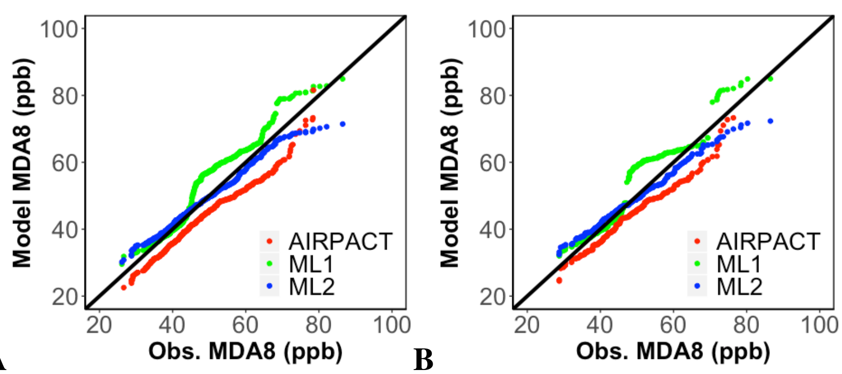
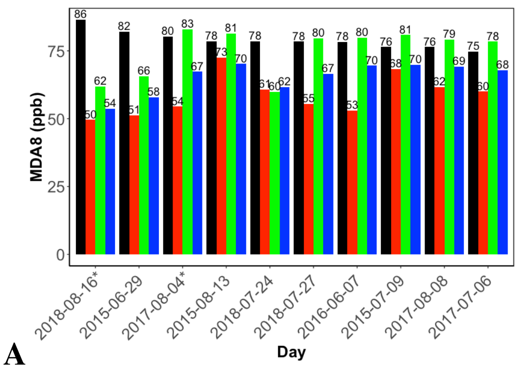
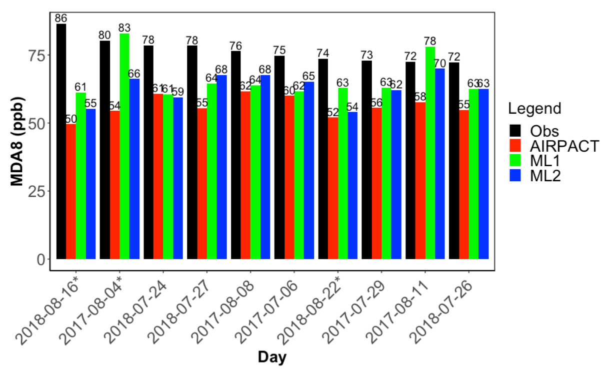


Figure 2. Q-Q plots of averaged model vs. observed MDA8 (A) during May – September 2015 – 2018 based on the 10 times 10-fold cross-validation (B) during May – September 2017 – 2018 based on the walk-forward cross-validation

The highest 10 observed MDA8 during 2015 – 2018 and their model predictions were selected and shown in Figure 2B. ML2 and AIRPACT underpredicted all 10 cases, and ML1 provided close predictions for 7 out of 10. These results show that ML1 performs better for high O_3 events, and results from the Q-Q plot also confirms this. The two ML models showed a similar trend, and they both largely underpredicted 3 cases. So, they may miss the same factor which led to the high MDA8. The highest O_3 day was affected by the wildfire smoke, and all models missed it.



A



B

Figure 3. Top 10 observed MDA8 and model predictions from (A) 10-time 10-fold cross-validation (B) the walk-forward cross-validation

* means that the wildfire smoke caused excess ozone on that day

3.2.2 Walk-forward cross-validation

The 10-time 10-fold cross-validation does not consider the temporal order of the data, which is important for the time-series data. Walk-forward cross-validation is a technique for time-series data.[35] For this evaluation, the 2015 and 2016 data were used to train the model and predict the first day in the 2017 dataset (May 1st, 2017). Then the May 1st, 2017 data was included in the training dataset and the models were used to predict O_3 for May 2nd, 2017. This process was repeated for each additional day of the 2017 and 2018 ozone seasons.

When a new day's MDA8 was predicted by the ML models, the NMB was recomputed by including the new prediction. The change of NMB was shown in Figure 3A. In the beginning, there was no clear trend for the NMB values for both ML models. The NMB from ML1 prediction sharply increased after June 2017 (Day 50 in Figure 3A) when more high O3 events occurred, slowly increased after August 2017 (Day 100 in Figure 3A), and slowly decreased after July 2018 (Day 200 in Figure 3A). The overprediction from ML1 during the low O3 periods (May and June) could lead to the NMB increasing, while the NMB values were stable or even decreasing during the high O3 period (July and August). For ML2, there were some fluctuations before August 2018, and the NMB was stable after that. For both ML1 and ML2, the NMB values were getting stable when more data got involved. The final NMB of two ML models were 5.6% and -0.9%, which were lower than the 10-time 10-fold cross-validation.

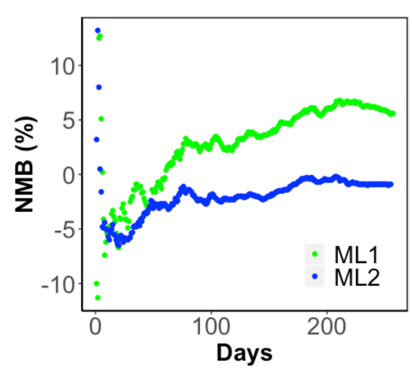


Figure 4. The walk-forward NMB of each time step for ML1 and ML2

The walk-forward cross-validation provided two-year MDA8 predictions (2017 and 2018), and the Q-Q plots were similar to the 10-time 10-fold cross-validation. The two breakpoints of ML1 distribution were clearer in Figure 3B. Ten highest MDA8 in 2017 and 2018 were shown in Figure 4. ML1 only captures 2 out of the top 10 observed MDA8 and ML2 captured 1. In some cases, ML1 was even lower than ML2. Three high O_3 days with stars (*) in Figure 4 were affected by the wildfire smoke, and ML1 captured two of them. The two ML models still performed better than AIRPACT.

Table 1 summarizes the HSS and KSS of the two machine learning models and AIRPACT from the two cross-validation methods. Both machine learning models show better performance with higher HSS and KSS values than AIRPACT. ML2 shows higher HSS than ML1 for both cross-validation results, which means ML2's prediction is generally more accurate. ML1 shows higher KSS in 10-time 10-fold cross-validation due to its better performance of high O_3 predictions. The statistics from AIRPACT and ML2 are close between two cross-validations, but HSS and KSS from walk-forward are lower than 10-time 10-fold cross-validation.

Table 1. HSS and KSS from two cross-validations

		AIRPACT	ML1	ML2
10-time 10-fold	HSS	0.32	0.44	0.55
	KSS	0.25	0.62	0.50
Walk-forward	HSS	0.34	0.37	0.57
	KSS	0.27	0.53	0.51

3.3. O_3 ensemble forecasting in 2019

Since April 2019, our machine learning models have been used for operational O_3 ensemble forecasting for Kennewick, WA. The ensemble forecasting to predict O_3 levels was based on more than 20 WRF ensemble members provided by the University of Washington. The difference among the predicted MDA8 from the ensemble members was not significant (within 5%). To better compare with the evaluation in the previous section, this section only covers the data from May to September in 2019. The ML1 and ML2 results are the ensemble means of the MDA8 values from more than 20 ML forecasts. The Q-Q plot in Figure 5 shows that the ML1, ML2 and AIRPACT model forecasts are close for O_3 lower than 40 ppb. For the O_3 in 40 – 60 ppb, ML1 tends to overpredict, while AIRPACT and ML2 are closer to observations. When the O_3 mixing ratio is higher than 60 ppb, ML1 slightly overpredicts, ML2 underpredicts, and AIRPACT varies in cases. For the highest 5 MDA8 points in Figure 6, the observed values were 62 – 66 ppb, while ML1's predictions were closer to the observations than AIRPACT and ML2. AIRPACT showed larger variation (48 – 70 ppb) compared to two ML models.

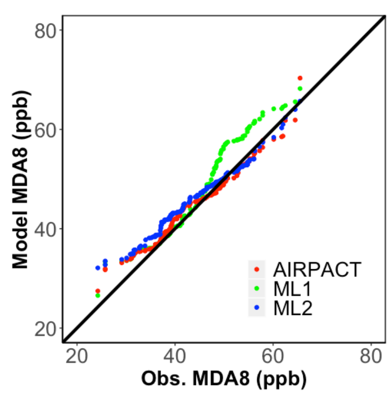


Figure 5. Q-Q plots of ensemble mean model vs. observed MDA8 during May - September 2019

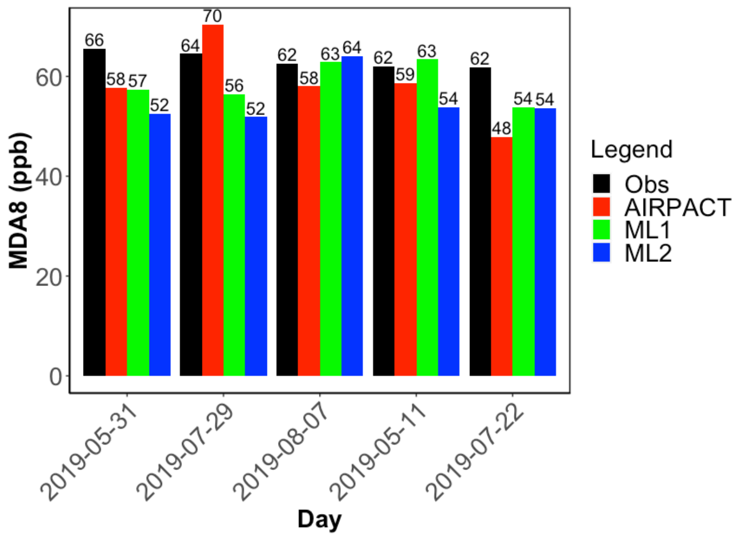
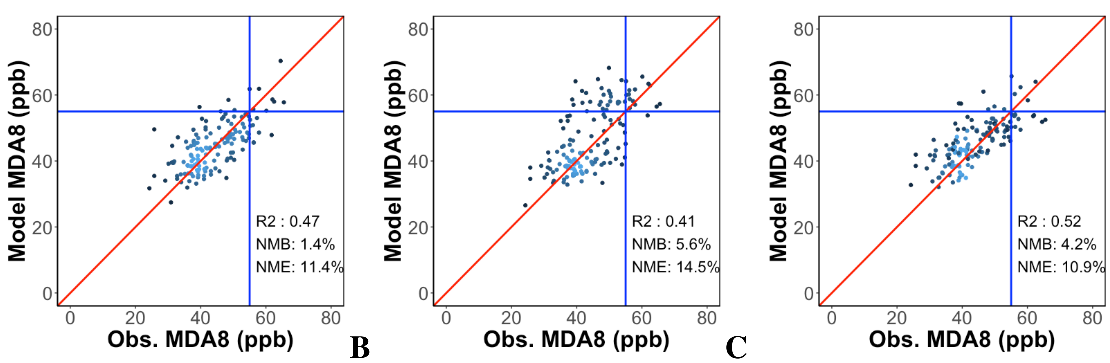


Figure 6. Top 5 observed MDA8 and model predictions in 2019

The scatter plots in Figure 7 show the ensemble mean MDA8 from May to September in 2019. ML2 shows relatively higher R^2 value (0.52) than ML1 (0.41) and AIRPACT (0.47). The NMB of AIRPACT is lowest (1.4%), but its NME (11.4%) is higher than ML2 (10.9%). The low NMB is due to the offset of overprediction and underprediction. ML1 tended to overpredict the MDA8 O_3 especially when it was higher than 40 ppb. Because of mostly favorable meteorological conditions and few wildfires in the Pacific Northwest, the O_3 mixing ratios were not very high in 2019 and the model performance of ML2 was the best.



A **B** **C**

Figure 7. Scatter plots of observed vs. ensemble mean MDA8 of AIRPACT in (A), ML1 in (B) and ML2 in (C) at Kennewick from May to September in 2019

The model performance statistics are presented in Table 2, the blue cells show misses, and red cells show false alarms. In 2019, all the AQI_{obs} at Kennewick were less than 3. Compared to AIRPACT, ML1 captured high O_3 days better (15 events vs. 7 events for AQI_{obs}2) but tended to overpredict the O_3 AQI (26 false alarm events vs. 3 false alarm events). ML2 predicted similar AQI days to AIRPACT. Based on the analysis above, we decided to use ML1 to provide the daily forecasting for Kennewick when the predicted AQI was above 2, and ML2 when the predicted AQI was 1 or 2.

Table 2. Number of days for each AQI during May – September 2019

		Observation							
		AQI 1	AQI 2		AQI 1	AQI 2		AQI 1	AQI 2
AQI 1	AIRPACT	122	11	ML1	99	3	ML2	119	13
AQI 2		3	7		26	15		6	5

ML1 and ML2 are the ensemble mean results using 20 WRF ensemble members.

The blue cells mean the model misses high O_3, and the red cells mean the model raises false alarms.

Acknowledgement

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