Development of a machine learning approach for local-scale ozone and PM2.5 forecasting: Application to multiple AQS sites in the Pacific Northwest

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Abstract

A machine learning (ML) based modeling framework has been successfully used to provide operational forecasts of O_3 at Kennewick, WA. This paper shows its performance when applied to other observation locations to predict O_3 and PM2.5 concentrations. The 10-time, 10-fold cross-validation method was used to evaluate the model performance in the Pacific Northwest (PNW). Similar to Kennewick, ML1 captures more high-O_3 events, but also generates more false alarms, and the accuracy of ML2 is better (R^2 = 0.79), especially for low-O_3 events. Compared to AIRPACT, the combined modeling framework reduces the normalized mean bias (NMB) from 7.6% to 2.6%. In terms of Air Quality Index (AQI) forecasts, improvements occur for each AQI level which reflects more accurate O_3 predictions and better capture of more high-

O_3 events. For PM2.5, ML1 and ML2 demonstrate similar capabilities to predict high-PM2.5 events and ML2 keeps its accuracy for low-PM2.5 predictions, so there is no need to combine the two methods. During the evaluation period, AIRPACT under-predicts the wildfire season PM2.5 concentrations in the PNW (NMB = -27%) and over-predicts at some sites in the cold season up to 200%, while ML2 has a lower NMB in both seasons (NMB = 7.9% in the wildfire season and 2.2% in the cold season) and correctly captures more high-PM2.5 events. The ML modeling framework is now operational for forecasts of O_3 and PM2.5 at over 100 observation sites in the PNW.

1. Introduction

The Air-quality forecasting for the Pacific Northwest (AIRPACT) has been used for air quality forecasts in the Pacific Northwest (PNW) since May 2001 (Chen et al. 2008). A chemical transport model (CTM), Community Multiscale Air Quality (CMAQ) is used to simulate the air quality over the PNW. It provides detailed air quality forecasts, but also requires much computational power. However, it missed some unhealthy ozone events during the wildfire seasons at Kennewick. To provide more reliable ozone forecasts, a machine learning (ML) based air quality modeling forecasting system was developed to predict the ozone levels during wildfire seasons at Kennewick. Fan et al. (2022) introduced the modeling framework and evaluated its performance in the wildfire seasons during 2017 – 2020. The ML modeling framework captured 50% of unhealthy ozone events while AIRPACT missed them.

To expand the application of this ML-based modeling framework, this paper uses it at other observation sites in the PNW and modifies it to predict the PM2.5 concentrations in this region. The goal of this study is to develop a reliable air quality forecast framework using ML approaches in the PNW. The new forecast framework was tested at Kennewick, WA with a focus on the predictability of unhealthy days related to O_3. Then the modeling framework was used to predict O_3 and PM2.5 at Air Quality System (AQS) sites throughout the PNW. Section 2 presents the input data, computational requirements for the ML forecast framework, and validation methods. Sections 3 – 7 present the evaluation of the model performance using 10-time, 10-fold cross-validation to predict the O_3 and PM2.5 in the PNW. Section 8 provides a summary and conclusions.

2. Data and methods

2.1. ML predictions of O_3 and PM2.5 using observation datasets

In the PNW, there are 30 AQS sites with O_3 observations, more than 100 sites with PM2.5 observations, and 12 sites where both O_3 and PM2.5 are measured. Similar to the ML modeling framework for Kennewick, the training dataset for the multi-site machine learning models included the previous day's observed O_3 or PM2.5 concentrations, time information (hour, weekday, month), and simulated meteorology from daily WRF forecasts at each AQS site. The O_3 predictions cover May to September during 2017 – 2020 and PM2.5 predictions cover two seasons, wildfire season (May to September) and cold season (November to February) during 2017 – 2020. The wildfires affect both O_3 and PM2.5 concentrations, so the model includes periods with wildfires during the wildfire season. During the cold season, wood burning from stoves is a significant source of PM2.5 in populated areas, so the model is separately trained for PM2.5 during the cold season. The source of WRF meteorology is the daily forecasts produced by the University of Washington (Mass et al. 2003). To identify the characteristics of each individual site, the models are trained for each site with their respective meteorology and observations.

2.2. Computational requirements

Our ML modeling framework requires much less computational power than the AIRPACT CMAQ system. The ML models use a single processor to train and predict the O_3 and PM2.5 at the AQS sites throughout the PNW within 1 hour of CPU time. These requirements are much less than AIRPACT which requires 360 hours of CPU time (120 processors for 3 hours) for a single daily forecast.

2.3. Validation method and evaluation metrics

Besides the forecast verifications used in the Kennewick paper (Fan et al. 2022), a Taylor diagram is used to compare the model performance throughout the sites in the PNW (Taylor 2001). Three statistical variables, correlation (R), centered root-mean-square error (CRMSE), and the ratio of their variance, are shown in a Taylor diagram. The R and CRMSE are computed based on Equations (1) - (4), where m and o refer to the model predictions and observations.

$$\sigma_M = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(m_i - \bar{m})^2} \tag{1}$$

$$\sigma_O = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(o_i - \bar{o})^2} \tag{2}$$

$$R = \frac{1}{\sigma_O \sigma_M}\frac{1}{n}\sum_{i=1}^{n}(m_i - \bar{m})(o_i - \bar{o}) \tag{3}$$

$$CRMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}((m_i - \bar{m}) - (o_i - \bar{o}))^2} \tag{4}$$

The refined index of agreement (IOA) is used to compare the model accuracy, and its range is -1 – 1 (Willmott, Robeson, and Matsuura 2012). The IOA of a good model is close to 1. An R function *dr()* from the package *ie2misc* using Equations (5) and (6) is used to compute the IOA.

$$d_r = 1 - \frac{\sum_{i=1}^{n} |m_i - o_i|}{2\sum_{i=1}^{n} |o_i - \bar{o}|} \text{ when } \sum_{i=1}^{n} |m_i - o_i| \leq 2\sum_{i=1}^{n} |o_i - \bar{o}| \quad (5)$$

$$d_r = \frac{\sum_{i=1}^{n} |m_i - o_i|}{2\sum_{i=1}^{n} |o_i - \bar{o}|} - 1 \text{ when } \sum_{i=1}^{n} |m_i - o_i| > 2\sum_{i=1}^{n} |o_i - \bar{o}| \quad (6)$$

3. O_3 observations

This study covers the O_3 observations at the AQS sites from May to September during 2017-2020, which is a typical wildfire season in the PNW region. Table 1 summarizes the observed O_3 average values and the number of days in each year with each AQI category that is computed only with O_3: the number of days in each year is presented in the parenthesis. The daily O_3 observations in this region are mostly within lower levels: AQI category 1 (approximately 76.6% to 90.8% of total days used in this study) and AQI category 2 (approximately 8.8% to 20.1%). There is an annual variability in O_3 during this period. For example, the O_3 means are higher in 2017 and 2018 (44 and 43 ppb) than in 2019 and 2020 (39 and 40 ppb). Also, the number of days with unhealthy episodes for sensitive groups (AQI_3) and unhealthy episodes (AQI_4) are noticeably more frequent in 2017 and 2018, which could be attributed to more wildfires during these years. It is very important to predict these unhealthy events reliably as an air quality forecasting system, but AIRPACT operational air quality forecasting system failed to predict all 14 unhealthy O_3 episodes (AQI_4) during the wildfire seasons of 2017-2020.

Table 1. Summary of the O_3 observations from May to September in 2017 – 2020 at 30 AQS sites in the PNW region. Note that daily AQI is computed using O_3 only.

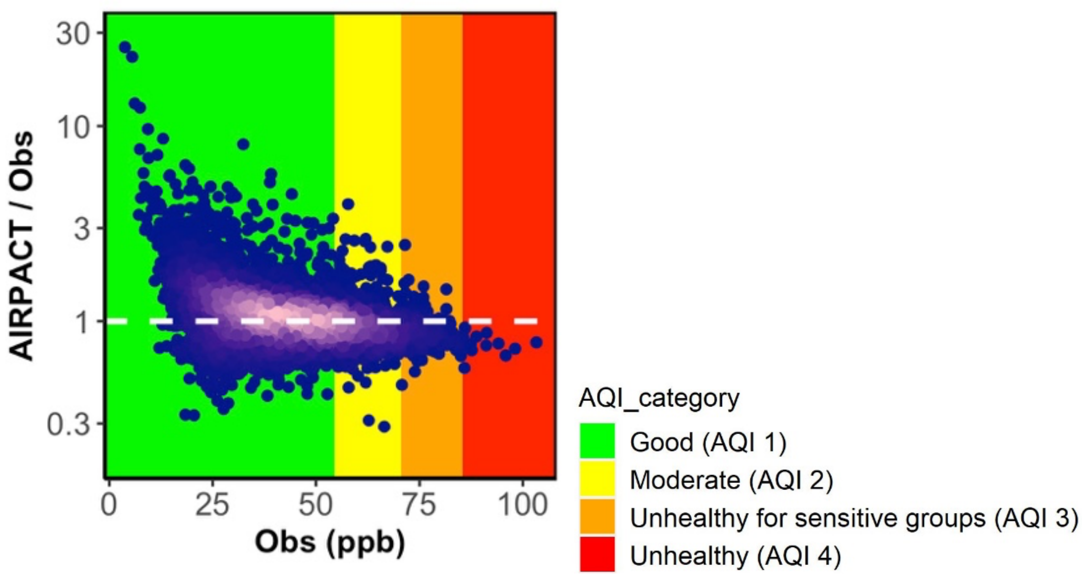
Year	Percentage and # of days for each AQI

	Mean (ppb)	1	2	3	4	Total
2017	44	76.6% (2971)	20.1% (778)	3.1% (120)	0.2% (9)	3878
2018	43	78.3% (3195)	19.8% (808)	1.8% (75)	0.1% (4)	4082
2019	39	90.8% (3728)	8.8% (361)	0.4% (15)	0 (0)	4104
2020	40	88.8% (3361)	10.3% (390)	0.9% (35)	0 (1)	3787

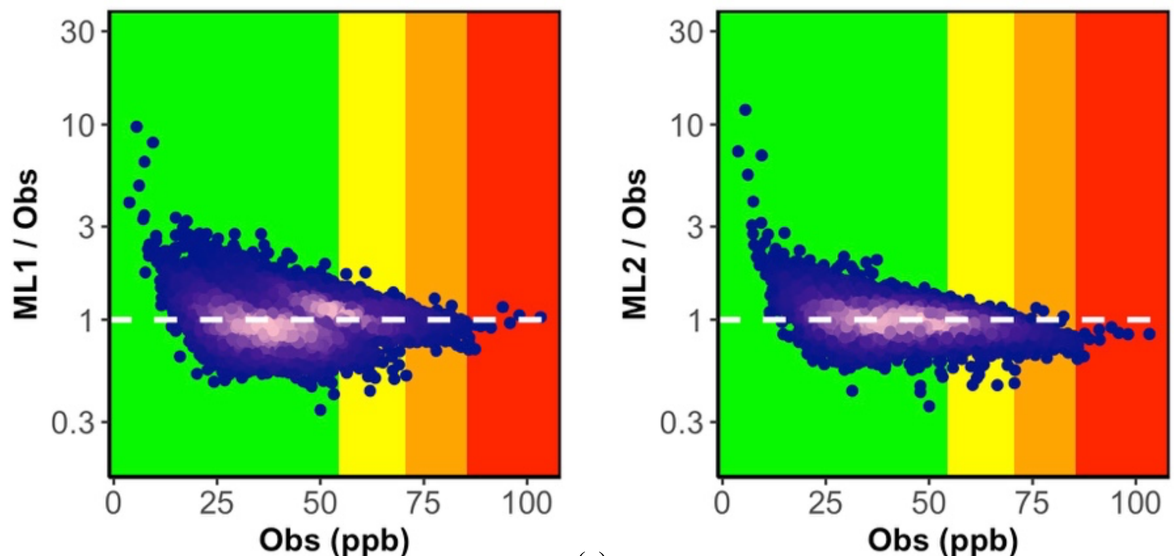
4. O_3 predictions throughout the PNW

The 10-time, 10-fold cross-validation is used to evaluate the model performance throughout the AQS sites over the PNW region. Our forecast values are initially hourly but compiled into the maximum daily 8-hour moving average (MDA8) O_3 and compare our ML performance against the CTM-based air quality forecasting system, AIRPACT.

To examine how the model performance varies by O_3 levels, we present the ratio plots of simulated to measured MDA8 O_3 against the measured MDA8 O_3 levels from the 30 AQS sites in Fig. 1, which also shows the density of the data with the bright pink color that appears around the “white” dashed line with a ratio of 1. All models have a similar issue that over-predictions seem to be worse at lower O_3 levels. For AIRPACT, the model-to-observation agreement is noticeably more scattered across the O_3 levels than the ML models, which leads to extremely under-predicted or over-predicted MDA8 O_3 forecasts that result in more misses or false alarms during the operational forecasting. It predicts 1% of good air quality events as unhealthy for sensitive groups, and predicts 7% of unhealthy air quality events as good (see S-Fig. 1). For the ML models, extremely incorrect predictions are fewer, demonstrating that our ML forecasts would be more reliable than AIRPACT. Compared to ML1, ML2 agrees better with observation as it shows the least scattered MDA8 O_3 distribution along with the O_3 levels. We can also see that the bright pink color over the AQI_1 (green) and AQI_2 (yellow) categories in Fig. 1c, where more than 95% of the O_3 observations used in this study fall into, is very close to the white dashed line with a ratio of 1. For the higher O_3 events (i.e., AQI_3 and AQI_4), ML2 under-predicts most of these events, which is concerning as it would fail to forecast a high-O_3 episode that is critical information for air quality-related public health. Our previous work that was based on a single AQS site at Kennewick, WA showed the similar prediction patterns by the ML models, indicating this is a systematic behavior in our ML models.



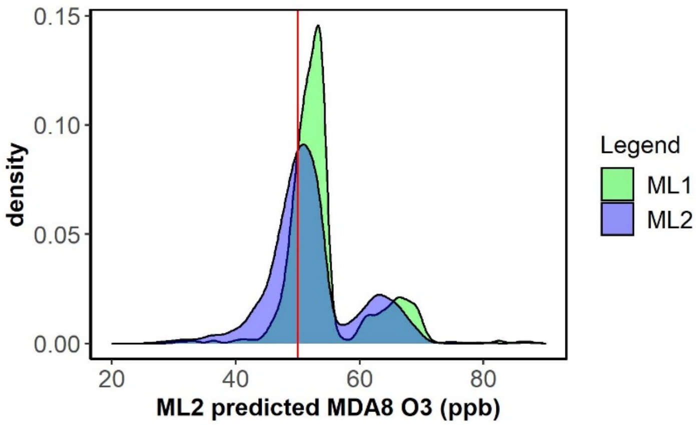
(a)



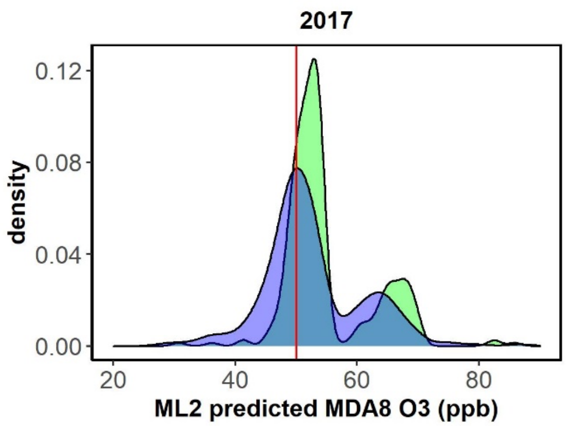
(b) (c)

Figure 1. Ratio plots of model predicted MDA8 O_3 to observations vs. observations for three models (a) AIRPACT, (b) ML1 and (c) ML2.

In order to produce the most reliable O_3 predictions with our ML models, we ran a "hybrid" ML model that used ML2 for low O_3 levels and ML1 for high O_3 levels ("ML_opr_O_3" hereafter). The ML_opr_O_3 model requires a threshold O_3 level that determines which ML prediction (ML1 or ML2) to be as a final forecast product. The threshold value should be either ML1 or ML2, as the same-day observed O_3 level is not available when the forecast is running. To find an optimal threshold O_3 level that enables either ML1 or ML2, we looked at the days with only one of the ML models capturing the observed AQI category (exclude when both models capture the observed AQI). We explored the relationship between the ML1 and ML2 O_3 predictions and find that ML2 O_3 prediction is better as it gives us a more consistent O_3 threshold (see Fig. 2). Figure 2 shows that 50 ppb is a good choice for the optimal threshold O_3 levels that switch between ML1 and ML2, and it varies only a little by year. Thus, ML_opr_O_3 uses ML2 when MDA8 O_3 predictions by ML2 are less than 50 ppb and, otherwise, uses ML1.



(a)



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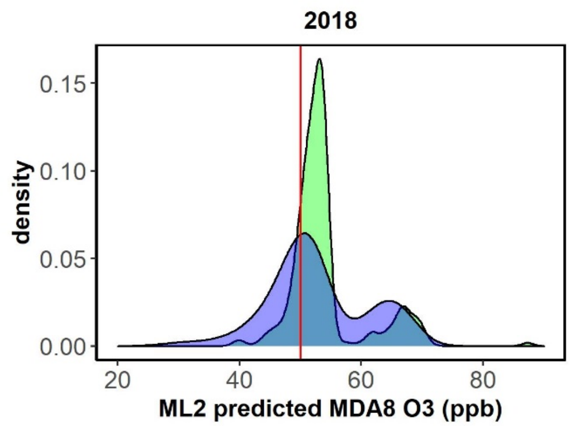
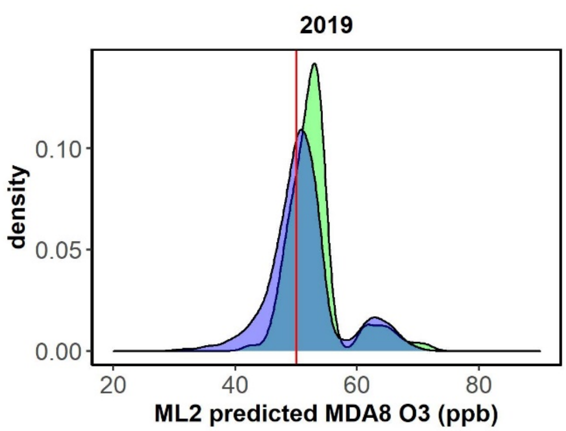


(c)



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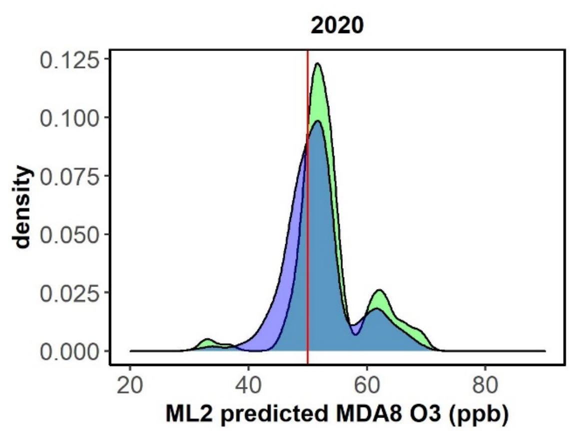


(e)

Figure 2. Distribution of better performed ML1 and ML2 in (a) 2017 -2020 and (b – e) each individual year. Notes: if ML1 and ML2 predict the same AQI category, the data are excluded in these figures.

The model evaluation statistics of MDA8 O_3 at 30 AQS sites over the PNW region during 2017 – 2020 are summarized in Table 2. All ML models outperform AIRPACT, and ML2 is the best among the ML models: ML2 has R^2 of 0.79, NMB of -0.68%, NME of 11% and IOA of 0.79, while AIRPACT has R^2 of 0.42, NMB of 7.6%, NME of 18% and IOA of 0.64. ML_opr_O_3 performance is mostly in between ML1 and ML2, but similar statistics to ML2 as our O_3 observation data is mostly for lower O_3 levels where ML_opr_O_3 relies on ML2.

Table 2. Statistics of the 10-time, 10-fold cross-validation of the MDA8 O_3 predictions from AIRPACT and our ML models.

	AIRPACT	ML1	ML2	ML_opr_O_3
R^2	0.42	0.67	**0.79**	0.76
NMB (%)	7.6	2.2	**-0.68**	2.6
NME (%)	18	16	**11**	12
IOA	0.64	0.69	**0.79**	0.76

The model evaluation using forecast verification metrics is based on the AQI computed with only O_3 from each model and is presented in Table 3. Heidke Skill Score (HSS), a commonly used forecast verification metric, is used to evaluate the model predictability on AQI categories. Note that HSS represents the accuracy of the model prediction compared with a “random guess”-based forecast that is statistically independent of the observations, and the value less than 0 means no skill and the value close to 1 means a skillful model. Another forecast verification metric, Hanssen-Kuiper Skill Score (KSS), measures the ability to separate different categories: the value less than 0 means no skill and the value close to 1 means a skillful model. Similar to the statistics in Table 2, all ML models show higher HSS and KSS scores than AIRPACT. For HSS, ML2 and ML_opr_O_3 has the higher scores (0.59 and 0.54, respectively) than ML1 (0.47). For KSS, ML_opr_O_3 and ML1 have higher scores (0.63 and 0.61, respectively) than ML2 (0.55), because these two models distinguish the AQI categories better by predicting more days with AQI_3 and AQI_4 categories than ML2.

Table 3. Forecast verifications of the 10-time, 10-fold cross-validations using AQI computed with only O_3 from AIRPACT and our ML models.

		AIRPACT	ML1	ML2	ML_opr_O_3
HSS		0.46	0.47	**0.59**	0.54
KSS		0.49	0.61	0.55	**0.63**
CSI	1	0.83	0.80	**0.89**	0.86
	2	0.36	0.36	**0.46**	0.41
	3	0.16	**0.21**	0.038	**0.21**
	4	0	0.062	**0.12**	0.062

The Critical Success Index (CSI) scores in Table 3 measures the model’s AQI categorical forecast. ML2 has the highest CSI_1 (0.89) and CSI_2 (0.46) score, and ML1 has the highest CSI_3 score (0.21), which is consistent with what we see in Fig. 1. However, the CSI_4 score of ML1 (0.062) is lower than ML2 (0.12), despite the number of AQI_4 events captured by ML1 and ML2 are same (see S-Fig. 1). This is because ML1 tends to predict higher O_3 levels than ML2 (see Figs. 1b and 1c), which leads to more “false” AQI_3 and AQI_4 predictions. For a very rare event such as AQI_4, the CSI score is significantly influenced by having a few more false alarms. Since ML_opr_O_3 uses ML1 for higher O_3 levels, it has the same CSI_4 score (0.062).

To examine the model performance of MDA8 O_3 at each individual AQS site, we present the spatial distributions of NMB in Fig. 3 and those of IOA in Fig.4. AIRPACT tends to over-predict the MDA8 O_3 during the wildfire seasons, especially along the coast, where the NMB can be up to 28% (see Fig. 3a). ML1 performs better than AIRPACT and does not over-predict along the coast. The individual AQS site’s NMB in ML1 is mostly in the range of -6% - 8%, while that in ML2 is -4% - 0. For ML_opr_O_3, its NMB is mostly close to the NMB of ML2 except at a few sites (i.e., sites near Salt Lake City, UT) where ML_opr_O_3 performance is close to ML1. For the site-specific IOA, most ML-based models show higher values than AIRPACT, whose IOA values are mostly below 0.6 (see Fig. 4a) because AIRPACT suffers from extremely over-predicted MDA8 O_3 above 100 ppb and IOA is sensitive to them (Legates and McCabe Jr 1999). The IOA values of ML_opr_O_3 are very close to those of ML2, similar to the site-specific NMB.

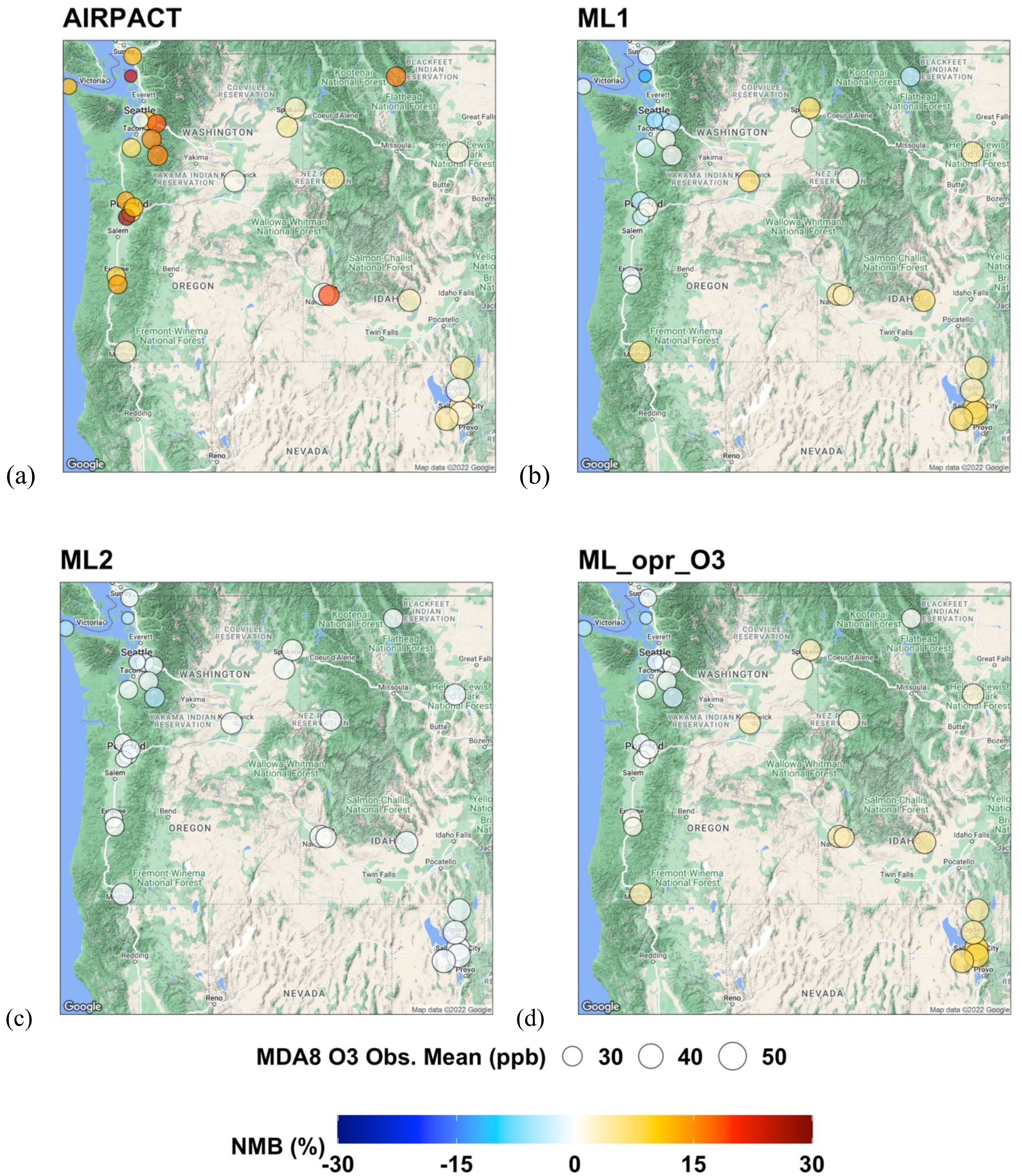


Figure 3. Maps showing NMB of MDA8 O_3 predictions from (a) AIRPACT, (b) ML1, (c) ML2 and (d) ML_opr_O_3 method at the AQS sites throughout the PNW.

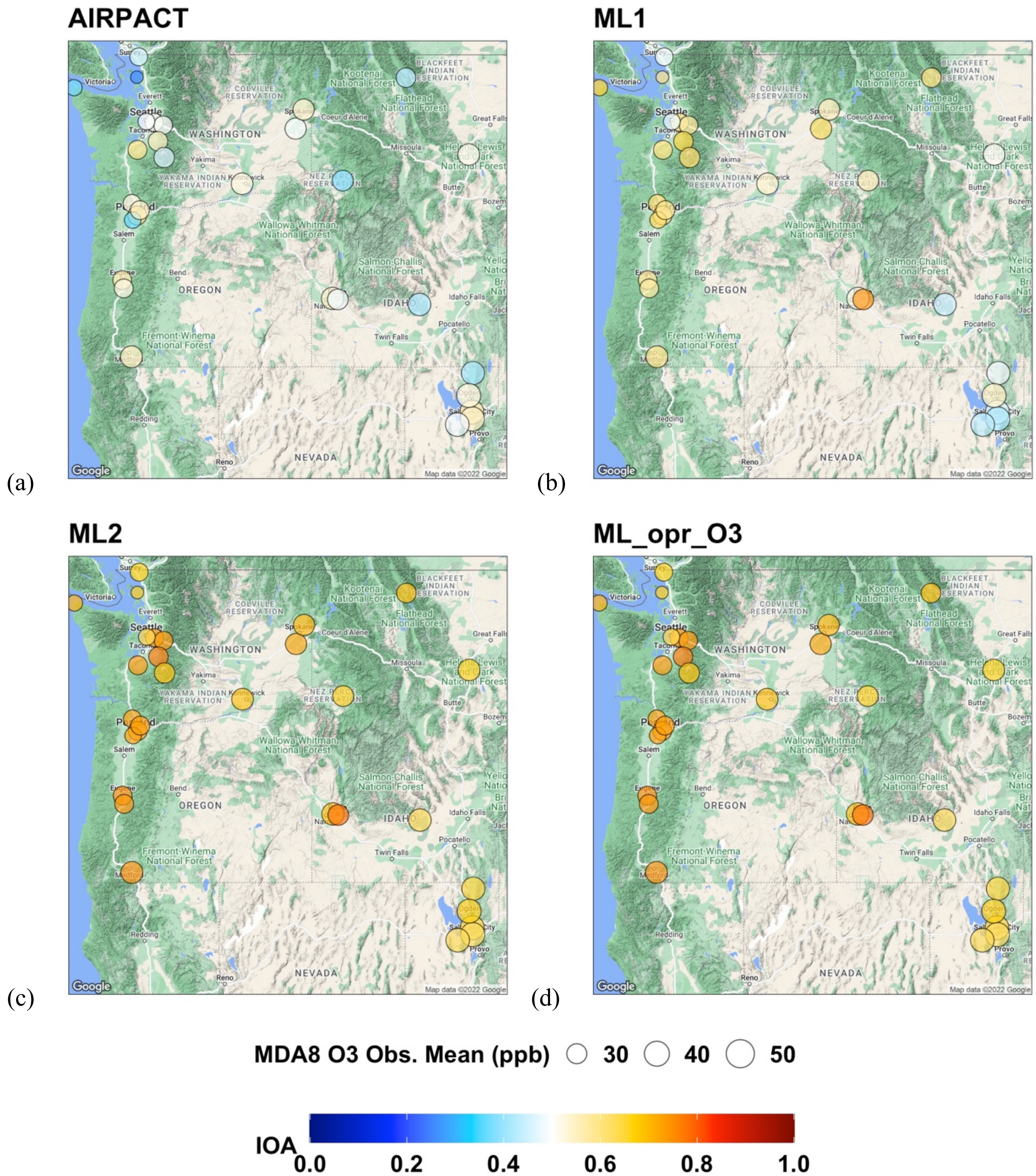


Figure 4. Maps showing IOA of MDA8 O_3 predictions from (a) AIRPACT, (b) ML1, (c) ML2 and (d) ML_opr_O_3 method at the AQS sites throughout the PNW.

We also use the Taylor diagram plots in Fig. 5 to show the model performance at the individual AQS site. Note that the statistics used in the Taylor diagram are normalized to visualize the difference among models more easily: for example, standard deviation (SD) and root mean square error (RMSE) are normalized with the observed SD at each AQS site (Taylor 2001). The Taylor diagram shows that the correlation coefficients of ML2 are within 0.6 – 0.9 and the normalized RMSE values are all within 0.5 – 0.8, while the ones of ML1 (0.5 – 1.2) and AIRPACT (0.8 – 2) are worse with a larger site-to-site variation than ML2. However, the normalized SD of ML2 is less than 1, which means the ML2 predictions have less variation than the observations. For ML_opr_O_3, it is quite like ML2 but the normalized SD is close to 1 for most sites, which means ML_opr_O_3 is better at capturing the observed variation.

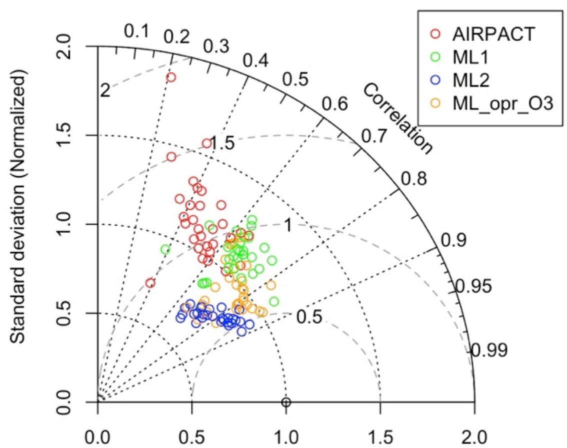


Figure 5. Taylor diagram of MDA8 O_3. Each circle symbol represents an AQS site, and the red color is for AIRPACT, green for ML1, blue for ML2 and yellow for ML_opr_O_3.

Overall, we find that ML2 predicts the low-MDA8 O_3 events best, while ML1 predicts the high-MDA8 O_3 events best. To take an advantage of both ML1 and ML2, we designed the ML_opr_O_3 model to use ML1 model when the ML2 predicted MDA8 O_3 is higher than 50 ppb and ML2 model for all other cases. The overall ML_opr_O_3 performance is close to ML2, as shown in the NMB and IOA evaluations, but it also captures the high-O_3 events like ML1. This is why we run ML_opr_O_3 as our daily O_3 forecasts at the AQS sites throughout the PNW.

5. PM2.5 observations of AQS sites

Same as O_3, we use the PM2.5 observations from 2017 to 2020. The PNW region experiences strong seasonal variations of PM2.5 due to distinct sources. For instance, wildfires are the main sources of PM2.5 from May to September, while wood-burning stoves are the main source from November to February. Based on this, our PM2.5 study is separated into the wildfire season (May to September) and cold season (November to February). We use a total of 103 AQS sites for the wildfire season and 104 sites for the cold season, which are available from 2017 to 2020.

A summary of the PM2.5 observations during these seasons is presented in Table 4. The mean PM2.5 concentrations during the wildfire season range from 4.7 to 12 $\mu g\ m^{-3}$ while those during the cold season range from 6.9 to 9.2 $\mu g\ m^{-3}$. In both seasons, daily PM2.5 concentrations are mostly in the AQI category 1 (AQI_1; corresponding to Good) and AQI_2 (Moderate). A large number of wildfires occurred in 2017, 2018 and 2020, leading to 5.0% - 5.9% of days in the wildfire season experiencing AQI_3 (unhealthy for sensitive groups) or above. The wildfires resulted in more than 1000 events with AQI_4 (unhealthy) or above at the 103 AQS sites throughout the PNW in the 2017 - 2020 wildfire season. There were few wildfires in 2019, so the mean PM2.5 concentration is particularly low and only 4 AQI_4 (unhealthy) events occurred during that 2019 wildfire season. The cold season has less variation in PM2.5 concentrations during the 2017 - 2020 period, and experiences significantly fewer unhealthy events (i.e., AQI_3 and above): only 0.1% - 1.1% of days in the cold season have AQI_3 or above.

Table 4. Summary of the daily PM2.5 observations from two seasons in 2017 – 2020 at AQS sites in the PNW region. Note that daily AQI is computed using PM2.5 only.

Season	Year	Mean	# of days for each AQI						
		($\mu g\ m^{-3}$)	1	2	3	4	5	6	Total
Wildfire season (May – Sep)	2017	11	82.4% (11442)	11.7% (1623)	2.9% (409)	2.3% (319)	0.6% (80)	0.1% (16)	13889
	2018	9.7	83.7% (11663)	11.2% (1556)	2.7% (373)	2.3% (321)	0.1% (14)	0 (2)	13929
	2019	4.7	98.4% (14144)	1.5% (211)	0.1% (16)	0 (4)	0 (0)	0 (0)	14375
	2020	12	88.9% (12556)	6.2% (871)	1.2% (163)	2.1% (296)	1.0% (143)	0.7% (100)	14129
Cold season (Nov – Feb)	2017	9.1	77.6% (7997)	21.3% (2194)	0.9% (97)	0.2% (16)	-	-	10304
	2018	7.9	82.1% (6827)	17.7% (1471)	0.3% (21)	0 (0)	-	-	8319
	2019	9.2	76.9% (8843)	22.7% (2606)	0.4% (51)	0 (3)	-	-	11503
	2020	6.9	87.1% (8647)	12.7% (1261)	0.1% (14)	0 (0)	-	-	9922

6. PM2.5 predictions during wildfire season

Similar to the O_3 prediction evaluation, 10-time, 10-fold cross-validation is used to evaluate the PM2.5 predictions. Because most daily PM2.5 concentrations are below 10 μg m^{-3}, the x-axis of ratio plots in Fig. 6 uses the log scale. It shows that AIRPACT over-predicts several events, but it mostly under-predicts the PM2.5 in the wildfire season (the bright pink region is below 1to1 line in Fig. 6a, and the NMB is -27% (shown in Table 5). ML1 and ML2 tend to over-predict some low daily PM2.5 concentrations (AQI_1 and AQI_2), but most of the predictions (bright pink regions in Fig. 6b and 6c) are close to the 1to1 line, and their NMB values (14% and 7.9%) are lower than AIRPACT. Similar to O_3 predictions, ML2 has lower NME (41%) and higher IOA (0.78) and HSS (0.59) than ML1 (NME 54%, IOA 0.70, HSS 0.53; shown in Tables 5 and 6). However, the advantage of ML1 for high-O_3 predictions is not significant for PM2.5 predictions. The KSS scores from ML1 and ML2 are the same (0.66). The CSI scores for AQI_5 and AQI_6 events from ML1 are 0.01 and 0.06 higher than ML2, but the scores for AQI_3 and AQI_4 are even 0.06 and 0.02 lower than ML2. To reduce the false alarms, ML2 has been used to forecast the daily PM2.5 at the AQS sites in the PNW.

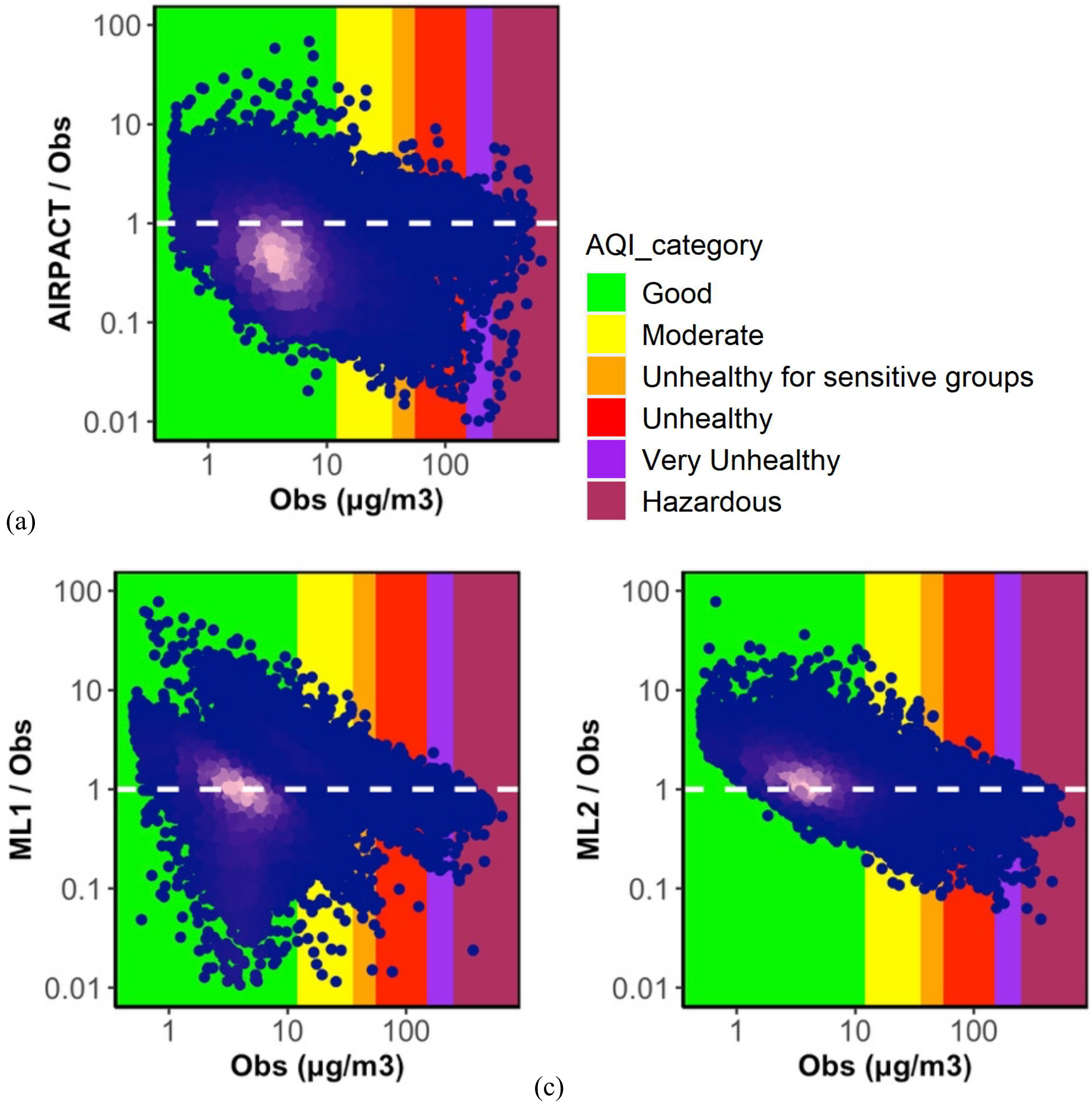


Figure 6. Ratio plots of model predicted daily PM2.5 to observations vs. observations in the wildfire season for three models (a) AIRPACT, (b) ML1 and (c) ML2.

Table 5. Statistics of the 10-time, 10-fold cross-validations of the daily PM2.5 concentrations during wildfire season from AIRPACT and our ML models.

	AIRPACT	ML1	ML2

R^2	0.51	0.69	**0.72**
NMB (%)	-27	14	**7.9**
NME (%)	59	54	**41**
IOA	0.67	0.70	**0.78**

Table 6. Forecast verifications of the 10-time, 10-fold cross-validations using AQI computed with only PM2.5 during wildfire season from AIRPACT and our ML models.

		AIRPACT	ML1	ML2
HSS		0.37	0.53	**0.59**
KSS		0.29	**0.66**	**0.66**
CSI	1	0.91	0.91	**0.92**
	2	0.17	0.31	**0.37**
	3	0.08	0.14	**0.20**
	4	0.23	0.36	**0.38**
	5	0.19	**0.24**	0.23
	6	0.30	**0.41**	0.35

AIRPACT under-predicts the daily PM2.5 at most AQS sites (94 out of 103 sites) in the PNW (see Fig. 7a), while the ML models tend to over-predict the daily PM2.5, and ML2 (-2% - 19%) performs better than ML1 (0 - 32%) because of fewer false alarms. The IOA from AIRPACT in Fig. 8a is acceptable except for the AQS sites in UT. ML1 shows better performance than AIRPACT at several sites, including the ones in UT, and ML2 generally has the highest IOA scores in the PNW.

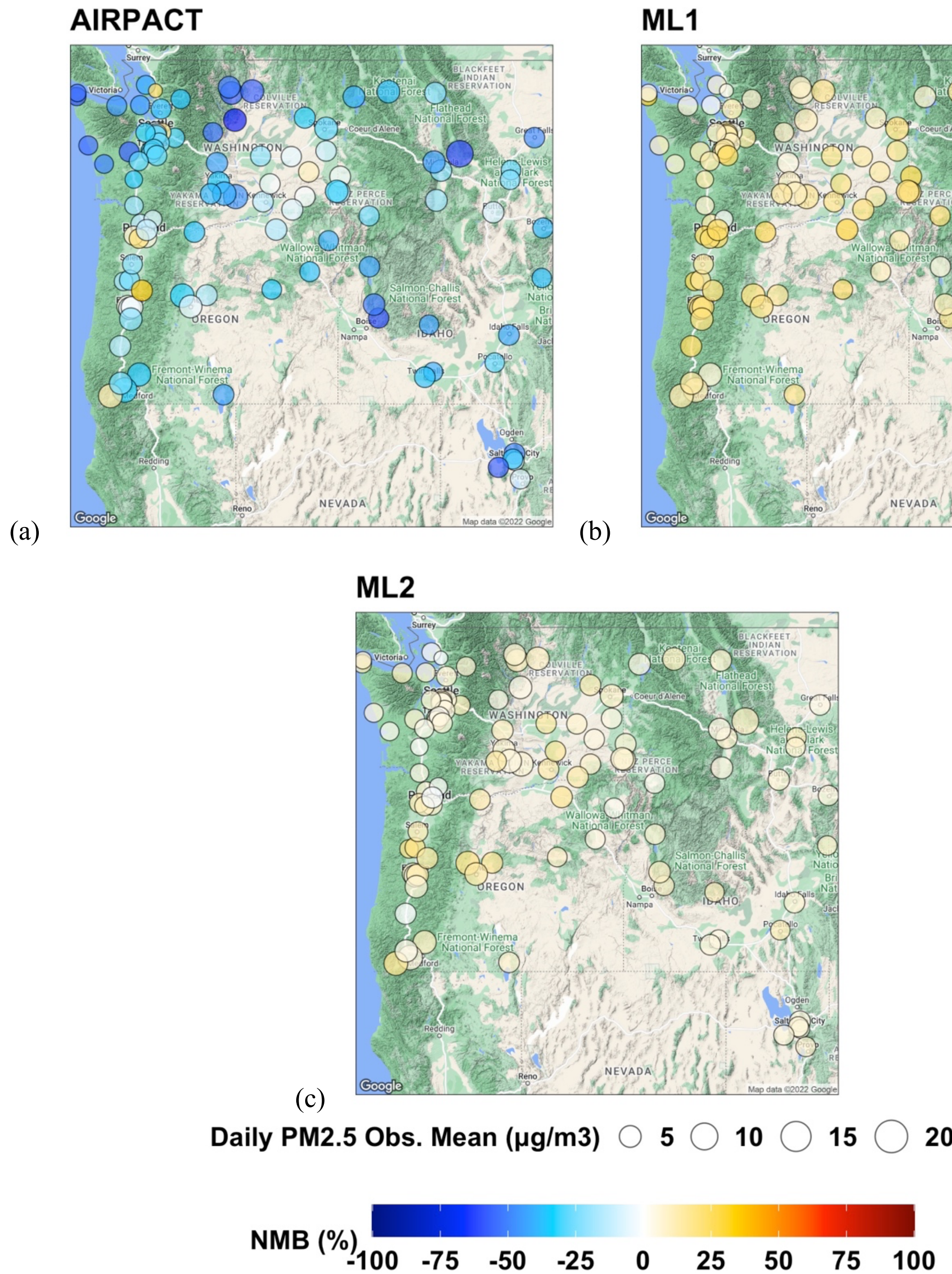


Figure 7. Maps showing NMB of daily PM2.5 predictions from (a) AIRPACT, (b) ML1 and (c) ML2 method at the AQS sites throughout the PNW.

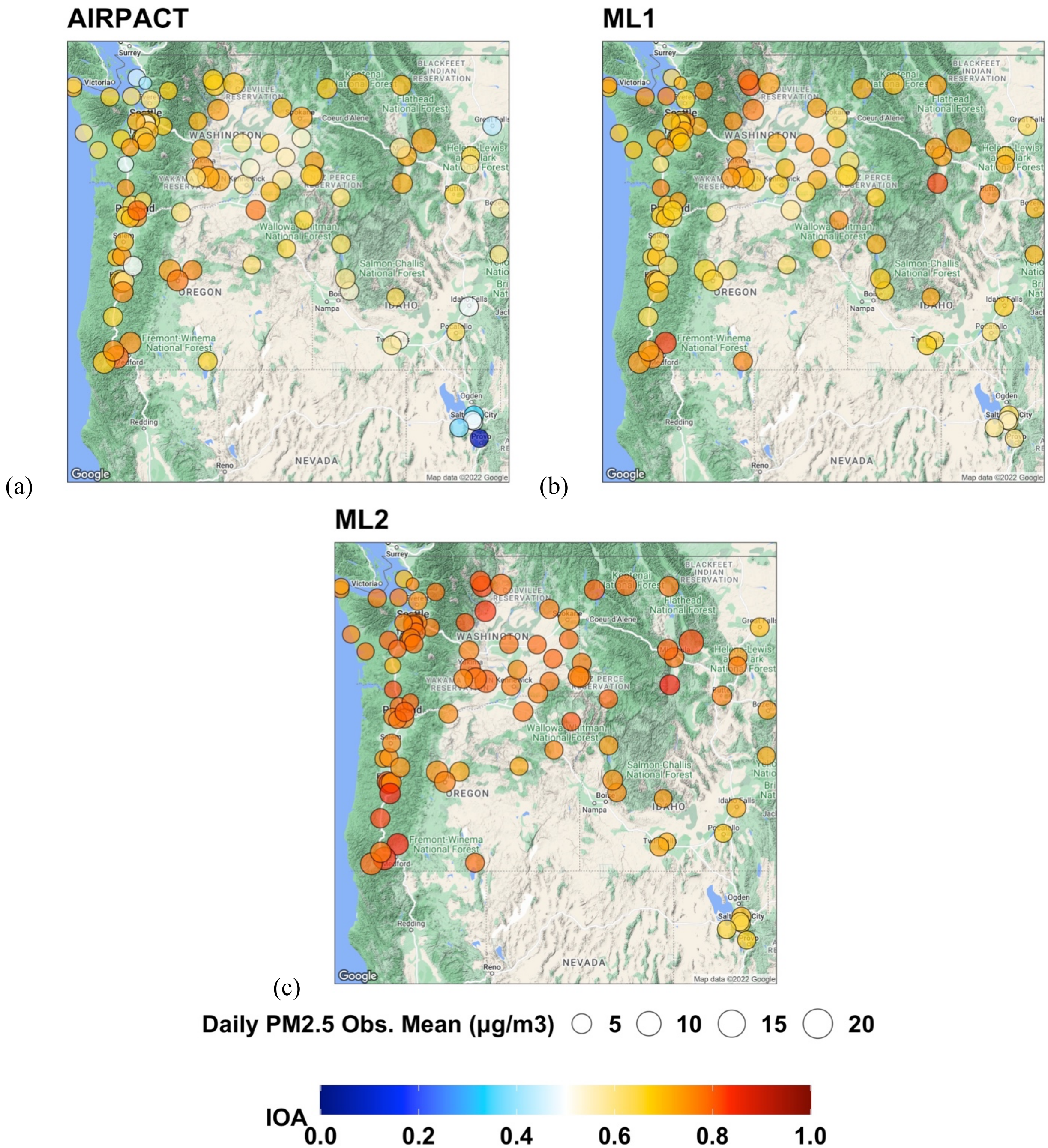


Figure 8. Maps showing IOA of daily PM2.5 predictions from (a) AIRPACT, (b) ML1 and (c) ML2 method at the AQS sites throughout the PNW.

The Taylor diagram in Fig. 9 shows that the AIRPACT performance varies among the 103 AQS sites, while ML1 and ML2 have more consistent performance. The correlation coefficients from AIRPACT range from 0.2 to above 0.9, while ML model predictions are mostly in the range of 0.6 - 0.9. ML2 shows lower normalized standard deviations than ML1. Extreme predictions still exist from AIPRACT. For example, the daily PM2.5 concentrations are below 40 μg m^{-3} during wildfire seasons of 2017 - 2020 at Lindon, UT, but AIRPACT predicts several extreme values up to 470 μg m^{-3}. The red circle outside the Taylor diagram in Fig. 9 and the deep blue circle in Fig. 8a both indicate the poor performance at this AQS site. While both ML models predict reasonable concentrations at this site.

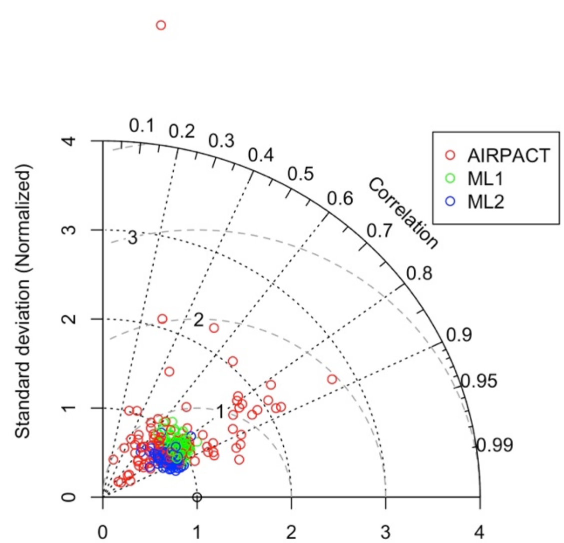


Figure 9. Taylor diagram of wildfire season daily PM2.5. Each circle symbol represents an AQS site, and the red color is for AIRPACT, green for ML1, and blue for ML2.

Like the O_3 predictions, ML1 and ML2 exhibit better performance than AIRPACT. However, ML1 does not show a significantly better capability to predict high pollution events than ML2. ML2 is the best choice due to its accuracy and capability to predict high-PM2.5 events.

7. PM2.5 predictions during cold season

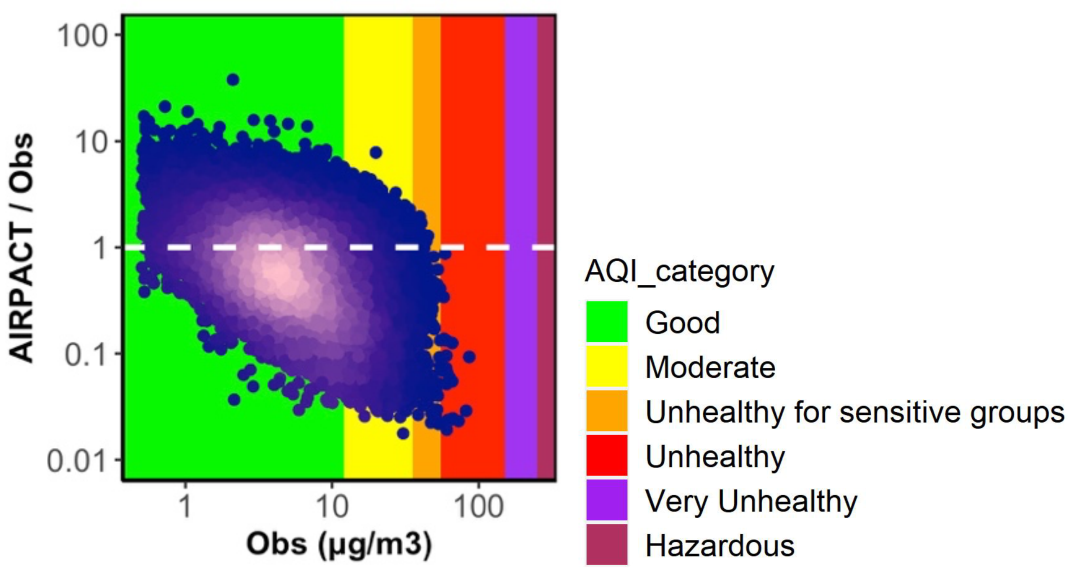
There are fewer severe pollution events in the cold season than in wildfire season (no very unhealthy or hazardous episodes in the cold season of 2017 – 2020, and only 19 unhealthy episodes), but it is difficult for the models to provide accurate PM2.5 predictions. The under-prediction of the wildfire season PM2.5 simulations from AIRPACT does not happen in the cold season, however, the lower NMB (3.4%) and higher NME (67%) in the cold season than in the wildfire season (NMB -27% and NME 59%) reveals that there is a large variation of AIRPACT predictions (shown in Table 7). Similar to the model performance in the wildfire season, ML1 and ML2 have better statistics, and ML2 shows better performance than ML1.

Table 7. Statistics of the 10-time, 10-fold cross-validations of the daily PM2.5 concentrations during cold season from AIRPACT and our ML models.

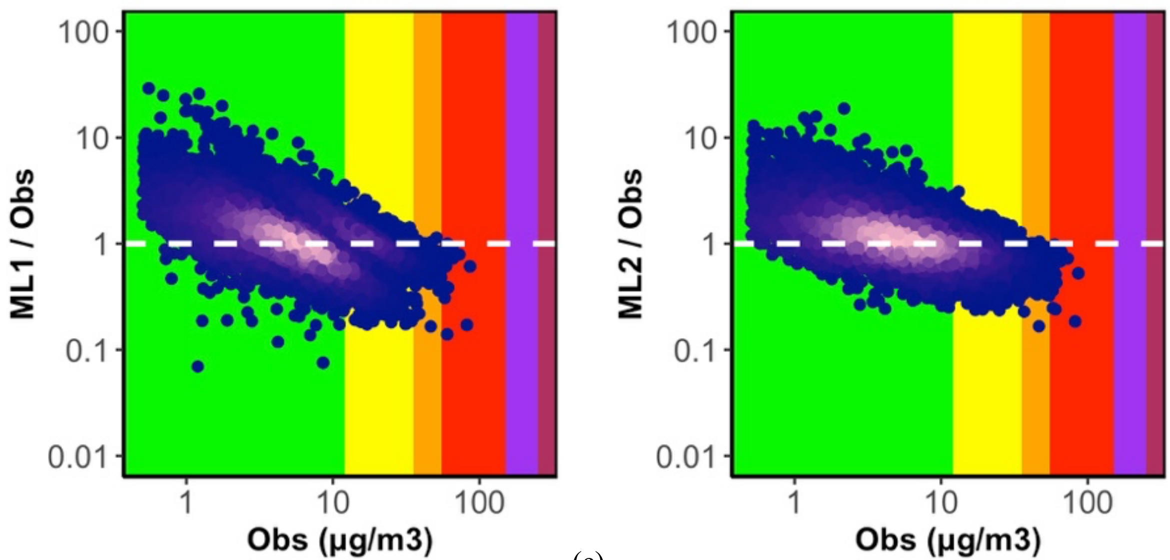
	AIRPACT	ML1	ML2
R^2	0.16	0.58	**0.70**
NMB (%)	3.4	6.7	**2.2**
NME (%)	67	36	**28**
IOA	0.40	0.68	**0.75**

The ratio plot of AIRPACT in Fig. 10a shows the densest part is below the 1to1 line, which is similar to its predictions during the wildfire season. The over-prediction mainly happens in the low PM2.5 regions and most of the unhealthy events in the red region are under-predicted.

In addition, the distribution of scatters, especially the dense part, has a wider range compared to its ratios in Fig. 6a, which also shows its large variation. The scatters in Fig. 10b and 10c are closer to the 1to1 line, and their NMB values (36% and 28%) are much lower than AIRPACT (67%). The denser scatters from ML models represent more stable model performance, and their IOA, HSS and KSS scores are also 0.28 – 0.39 higher than AIRPACT (shown in Table 8). In the wildfire season, the CSI_1 score from AIRPACT (0.91) is comparable to ML models (ML1 0.91, ML2 0.92), but the ML models show significantly better performance at all levels of PM2.5 in the cold season. ML2 has higher CSI_1 (0.87) and CSI_2 (0.53) scores than ML1 (0.83 and 0.50), and ML1 has higher CSI_3 (0.17) and CSI_4 (0.30) scores, but generally the differences are within 0.1. However, ML2 has significantly lower NMB (2.2%) and NME (28%) than ML1 (6.7% and 36%). So, ML2 provides more accurate PM2.5 predictions than ML1 in the cold season.



(a)



(b) (c)

Figure 10. Ratio plots of model predicted daily PM2.5 to observations vs. observations in the cold season for three models (a) AIRPACT, (b) ML1 and (c) ML2.

Table 8. Forecast verifications of the 10-time, 10-fold cross-validations using AQI computed with only PM2.5 during cold season from AIRPACT and our ML models.

		AIRPACT	ML1	ML2
HSS		0.23	0.58	**0.62**
KSS		0.25	**0.64**	0.61
CSI	1	0.74	0.83	**0.87**
	2	0.22	0.50	**0.53**
	3	0.018	**0.17**	0.11
	4	0	**0.30**	0.21

Compared to the AIRPACT performance in the wildfire season, the variation among the AQS sites is more significant in the cold season as shown in Fig. 11a. It largely over-predicts the

PM2.5 concentrations along the coast in the cold season, where the NMB can be above 100%, while it under-predicts at several inland sites, where the NMB is down to -85%. The largely over-predictions and under-predictions lead to the low IOA (<0.1) in Fig. 12a. The ML model performance is significantly better than AIRPACT. The NMB values from ML1 and ML2 are mostly in the range of -10% - 20% and -1% - 10%, which is even better than their performance in the wildfire season. ML2 has lower NMB, and also higher IOA at most sites than ML1. The unhealthy event prediction is a difficult task for both AIRPACT and ML models. However, there are fewer unhealthy events in the cold season, so ML models take the advantage of their capability of low-PM2.5 accurate prediction and show great model performance (the IOA is mostly above 0.5 at the AQS sites in the PNW).

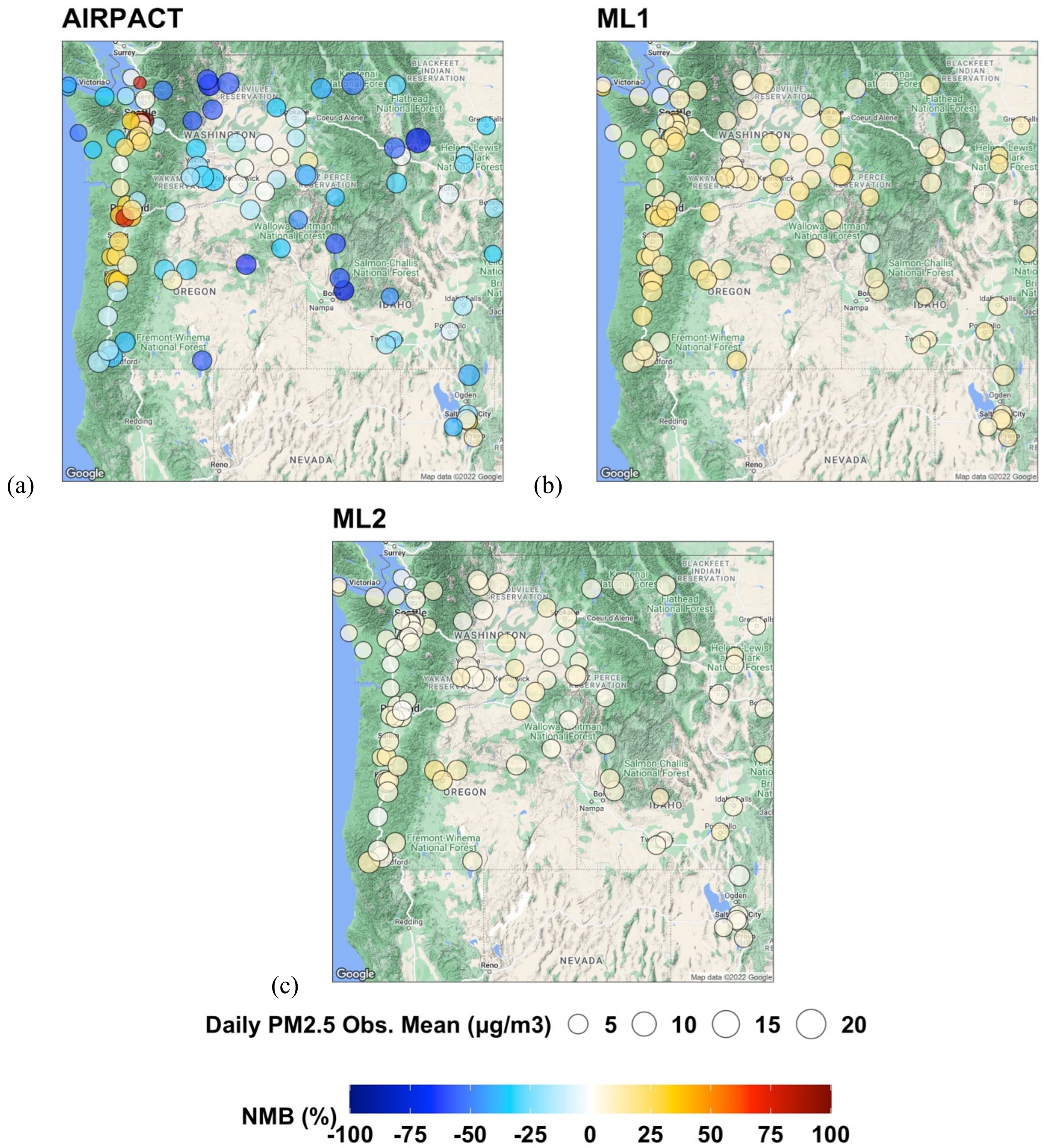


Figure 11. Maps showing NMB of cold season daily PM2.5 predictions from (a) AIRPACT, (b) ML1 and (c) ML2 at the AQS sites throughout the PNW.

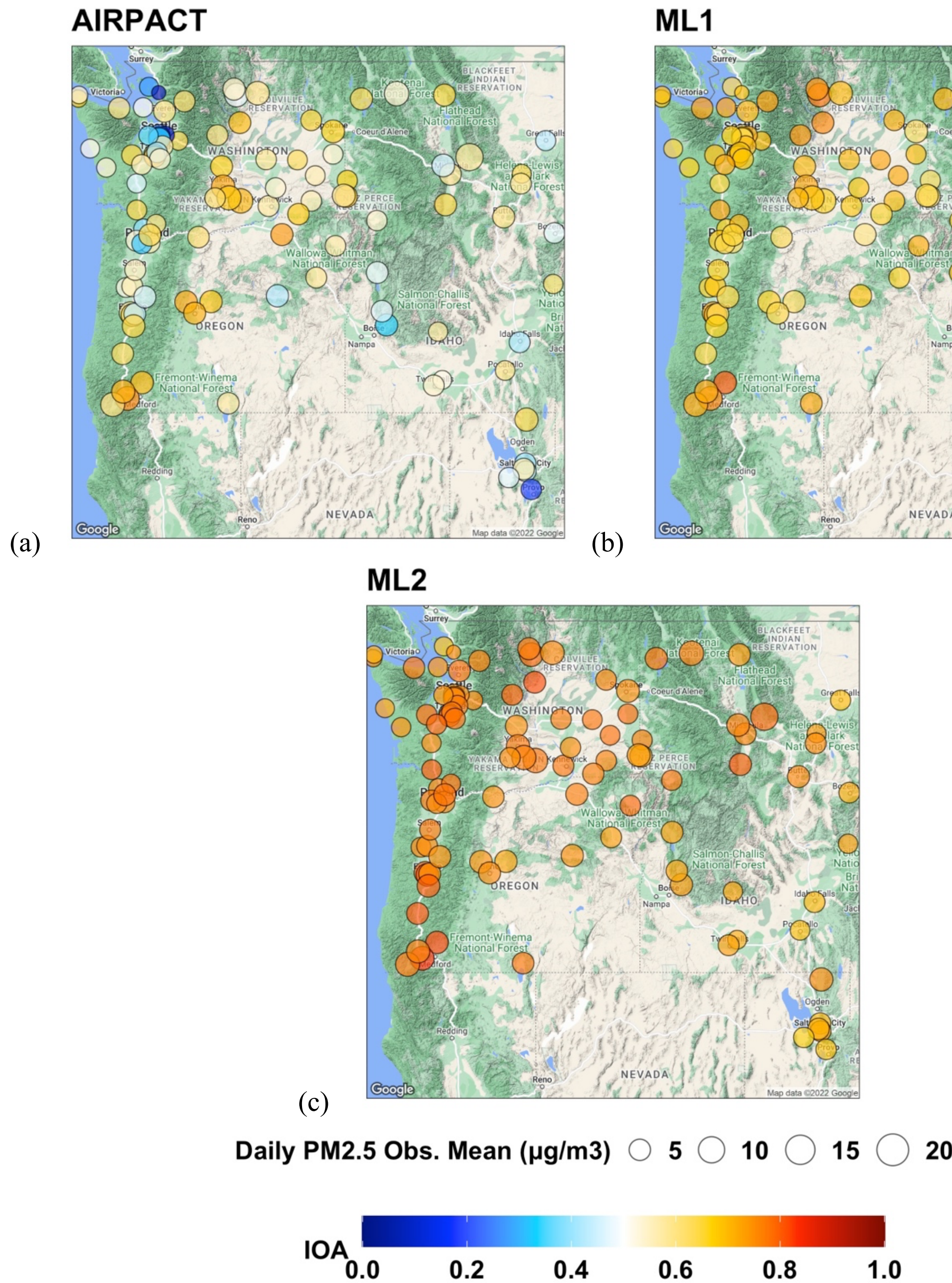


Figure 12. Maps showing IOA of cold season daily PM2.5 predictions from (a) AIRPACT, (b) ML1 and (c) ML2 at the AQS sites throughout the PNW.

Compared to the Taylor diagram of wildfire season PM2.5 predictions in Fig. 9, the normalized root-mean-square-error values from AIPRACT are higher than 2 at more sites, and the correlation coefficients decrease from 0.2 – 0.95 to 0 – 0.85. The normalized standard deviation values also show a large variation, and one value is even above 4 (the red circle outside the Taylor diagram in Fig. 13), which represents the AQS site in Bellevue, WA. The observed mean PM2.5 at Bellevue is 4.0 μg m^{-3}, but the mean prediction from AIRPACT is 14 μg m^{-3}, and it predicts several high PM2.5 events up to 67 μg m^{-3}. The ML models keep their consistently stable performance, and ML2 has more correlation coefficients in the range of 0.8 – 0.9. With the better performance at most sites from ML2 than ML1, the ML2 is also used for the operational PM2.5 forecasts in the cold seasons.

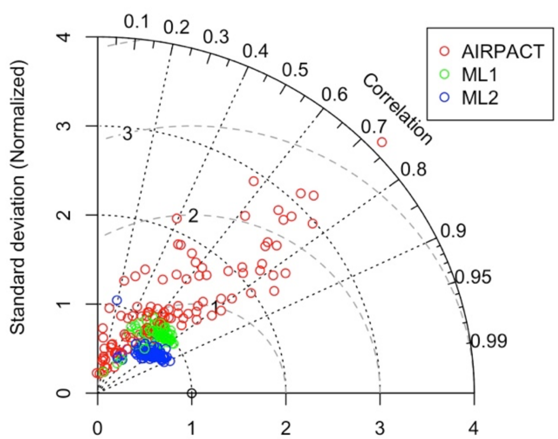


Figure 13. Taylor diagram of cold season daily PM2.5. Each circle symbol represents an AQS site, and the red color is for AIRPACT, green for ML1, and blue for ML2.

8. Conclusions

CTMs are widely used for air quality modeling and forecasting, but they may fail to properly forecast pollution episodes, plus they are computationally expensive. AIRPACT is a CTM-based operational forecasting system for the PNW, but it has a history of failing to correctly predict the air quality levels in the PNW. An ML modeling framework is presented in the previous paper, which is used to predict the O_3 level at Kennewick, WA. After the ML modeling framework performed successfully using for operational forecasts at Kennewick, WA, it was then extended to predict the air quality at the AQS sites throughout the PNW.

There are 30 AQS sites with available O_3 observations in the wildfire season. AIRPACT fails to capture the unhealthy episodes in the high-O_3 year, 2017 and 2018, but it performs well in 2019 and 2020. ML1 is capable of capturing the high-O_3 episodes, and ML2 shows its accuracy for low MDA8 O_3. The combined approach uses the advantages of the two ML methods and improves the model performance significantly over AIRPACT. The NMB and NME decrease from 7.6% and 18% to 2.6% and 12%. The statistical parameters, IOA, HSS, KSS and CSI, are larger than AIRPACT, and the higher CSI_3 and CSI_4 scores indicate that the model identifies more high-O_3 events.

There are 103 sites with available wildfire season PM2.5 observations and 104 sites with cold season data. ML1 and ML2 are trained for two seasons, respectively. AIRPACT under-predicts the wildfire season PM2.5 due to the missing the high-PM2.5 days. In the cold season, the NMB from AIRPACT is lower than during the wildfire season, but NME is higher. This is because AIRPACT struggles to predict the accurate low-PM2.5 concentrations, with a large variance, and the over-predictions and under-predictions cancel each other. ML1 does not perform significantly better than ML2 for the high-PM2.5 predictions, so ML2 can be used to predict the PM2.5 without combining the ML1 results. Compared to AIRPACT and ML1, ML2 has lower NMB and NME and higher IOA in both seasons. The associated HSS and KSS values are 0.22 – 0.39 higher than those for AIRPACT. The CSI (from CSI_3 to CSI_6) values from ML2 are close to or even higher than ML1, which shows its capability of capturing the high-PM2.5 events.

Within about 1 hour of CPU time, the ML modeling framework could finish training and provide the ensemble forecast of O_3 and PM2.5 levels at the AQS sites throughout the PNW, while AIRPACT needs 120 processors for 3 hours (360 hours of CPU time). Compared to AIRPACT, the ML model provides more accurate forecasts (most $R^2 > 0.7$) and captures 70% more high pollution events. Overall, the ML modeling framework requires much fewer computational sources and provides more reliable air quality forecasts at the selected locations than AIRPACT. It has been used to provide the daily air quality (O_3 and PM2.5) at the AQS sites in the PNW.

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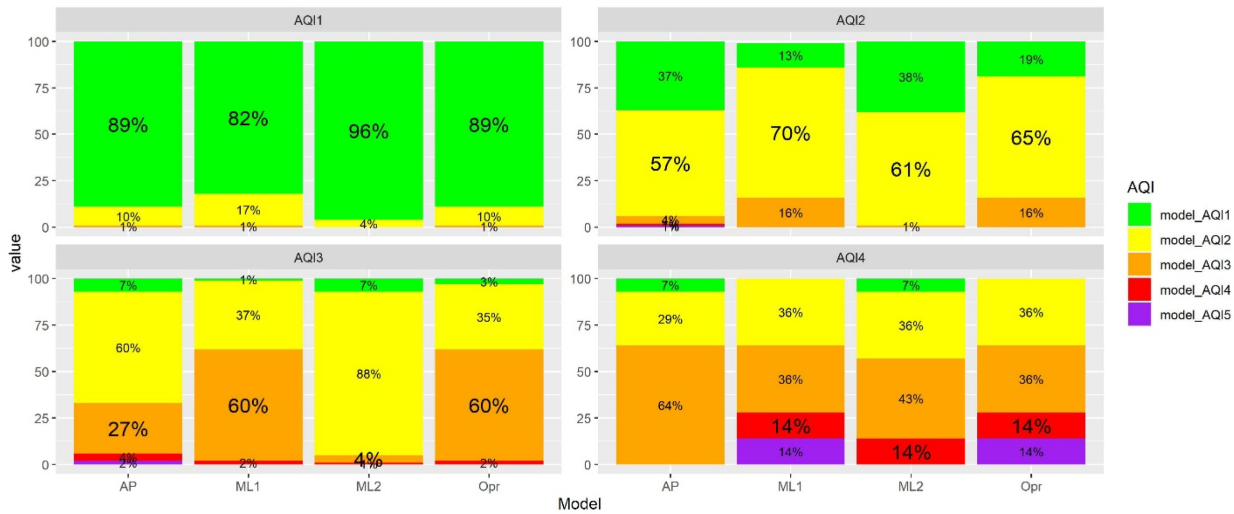
Supplementary Materials

Supplementary Figure



Supplementary Figure 1. Percentage of model predicted AQI at each observed AQI group. Note that daily AQI is computed using O_3 only.