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4 REAL-TIME BIAS-ADJUSTED O<sub>3</sub> AND PM<sub>2.5</sub> AIR QUALITY  
5 INDEX FORECASTS AND THEIR PERFORMANCE EVALUATIONS  
6 OVER THE CONTINENTAL UNITED STATES  
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9 Daiwen Kang<sup>1</sup>, Rohit Mathur<sup>2</sup>, and S. Trivikrama Rao<sup>2</sup>

10  
11 <sup>1</sup> Computer Science Corporation, Research Triangle Park, 79 T.W. Alexander Drive, NC  
12 27709, USA

13 <sup>2</sup> Atmospheric Modeling and Analysis Division, National Exposure Research Laboratory,  
14 U.S. Environmental Protection Agency, Research Triangle Park, NC, USA  
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32 *Corresponding Author:* Daiwen Kang  
33 Computer Science Corporation  
34 79 T.W. Alexander Drive  
35 Building 4201 Suite 260  
36 Research Triangle Park, NC 27709  
37  
38 (919) 558-8782 Ext. 207  
39 [kang.daiwen@epa.gov](mailto:kang.daiwen@epa.gov)

40 December 2009

41 Revised: March 2010  
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1 **ABSTRACT**

2 The National Air Quality Forecast Capacity (NAQFC) system, which links NOAA's  
3 North American Mesoscale (NAM) meteorological model with EPA's Community  
4 Multiscale Air Quality (CMAQ) model, provided operational ozone (O<sub>3</sub>) and  
5 experimental fine particular matter (PM<sub>2.5</sub>) forecasts over the continental United States  
6 (CONUS) during 2008. This paper describes the implementation of a real-time Kalman  
7 Filter (KF) bias-adjustment technique to improve the accuracy of O<sub>3</sub> and PM<sub>2.5</sub> forecasts  
8 at discrete monitoring locations. The operational surface level O<sub>3</sub> and PM<sub>2.5</sub> forecasts  
9 from the NAQFC system were post-processed by the KF bias-adjusted technique using  
10 near real-time hourly O<sub>3</sub> and PM<sub>2.5</sub> observations obtained from EPA's AIRNow  
11 measurement network. The KF bias-adjusted forecasts were created daily, providing 24-  
12 hour hourly bias-adjusted forecasts for O<sub>3</sub> and PM<sub>2.5</sub> at all AIRNow monitoring sites  
13 within the CONUS domain. The bias-adjustment post-processing implemented in this  
14 study requires minimal computational cost; requiring less than 10 minutes of CPU on a  
15 single processor Linux machine to generate 24-hr hourly bias-adjusted forecasts over the  
16 entire CONUS domain.

17 The results show that the real-time KF bias-adjusted forecasts for both O<sub>3</sub> and  
18 PM<sub>2.5</sub> have performed as well as or even better than the previous studies when the same  
19 technique was applied to the historical O<sub>3</sub> and PM<sub>2.5</sub> time series from archived AQF in  
20 earlier years. Compared to the raw forecasts, the KF forecasts displayed significant  
21 improvement in the daily maximum 8-hr O<sub>3</sub> and daily mean PM<sub>2.5</sub> forecasts in terms of  
22 both discrete (i.e. reduced errors, increased correlation coefficients, and index of  
23 agreement) and categorical (increased hit rate and decreased false alarm ratio) evaluation  
24 metrics at almost all locations during the study period in 2008.

25 **Keywords:** Air quality index forecast; Bias-adjustment; O<sub>3</sub>; PM<sub>2.5</sub>; Kalman filter

1 **1. INTRODUCTION**

2 Ozone (O<sub>3</sub>) and fine particulate matter (PM<sub>2.5</sub> – particles with aerodynamic  
3 diameters less than 2.5 μm) pollution is of concern due to their adverse effects on human  
4 and ecosystem health. Ambient levels of O<sub>3</sub> and PM<sub>2.5</sub> are the two primary components  
5 used in the calculation of the Air Quality Index (AQI), a standardized indicator of air  
6 quality degradation at a given location (Federal Register, 1999). The National Oceanic  
7 and Atmospheric Administration (NOAA), in partnership with the United States  
8 Environmental Protection Agency (US EPA), has been operationally implementing the  
9 National Air Quality Forecasting Capacity (NAQFC) system. This program, which  
10 couples NOAA’s North American Mesoscale (NAM) weather prediction model with  
11 EPA’s Community Multiscale Air Quality (CMAQ) model, has provided forecasts of  
12 ozone (O<sub>3</sub>) mixing ratios since 2004 (Eder et al., 2006; Eder et al., 2010). Developmental  
13 PM<sub>2.5</sub> forecasts were initiated during the summer of 2004 (Mathur et al., 2008; Yu et al.,  
14 2008). The modeling domain for both the operational and developmental predictions  
15 currently covers the continental United States (CONUS).

16 Despite continuous refinement and improvement, all numerical models suffer from  
17 significant errors and uncertainties due to numerical solvers, emissions inventory,  
18 boundary conditions, as well as our incomplete understanding of the physical and  
19 chemical processes occurring in the atmosphere. Incorporating recent model forecasts  
20 with observations to adjust model forecasts, the bias-adjustment method has been proven  
21 to be an effective way to reduce the systematic errors in numerical model outputs (Kang  
22 et al., 2008). The implementation of bias-adjustment postprocessing for air quality  
23 forecasts relies on the availability of near real-time observations. The U.S EPA’s  
24 AIRNow measurement network, which reports near real-time hourly O<sub>3</sub> and PM<sub>2.5</sub>

1 observations nationwide, provides an ideal opportunity to perform bias-adjusted O<sub>3</sub> and  
2 PM<sub>2.5</sub> air quality forecasts for air quality forecast modeling systems.

3 Bias-adjustment techniques have been used to correct systematic biases in surface O<sub>3</sub>  
4 predictions (McKeen et al., 2005; Delle Monache et al., 2006; Wilczak et al., 2006; Delle  
5 Monache, et al., 2008; and Kang et al., 2008), and more recently have also been extended  
6 to PM<sub>2.5</sub> forecasts (Kang et al., 2009). Among these techniques, the Kalman Filter (KF)  
7 (Kalman, 1960) predictor forecast method has shown the most improvement in forecast  
8 skill. However, all previous research efforts on bias-adjustment predictions were  
9 performed on retrospective basis, i.e., the bias-adjusted predictions were formulated by  
10 using archived model predictions and observations. To test the applicability of the  
11 methods in the operational real-time setting during 2008, the KF bias-adjustment  
12 technique (Kang et al., 2008, Kang et al., 2009) was implemented, for the first time, in  
13 real-time along with the NAQFC system to provide daily bias-adjusted O<sub>3</sub> and PM<sub>2.5</sub>  
14 forecasts at all the locations where observations from EPA's AIRNOW network are  
15 available within the CONUS domain. The bias-adjusted O<sub>3</sub> forecasts were performed for  
16 the April to mid- September period covering the entire O<sub>3</sub> season while PM<sub>2.5</sub> bias-  
17 adjusted forecasts were conducted throughout the entire calendar year. This paper  
18 presents the implementation of the KF bias-adjusted forecasts and its performance  
19 evaluation for O<sub>3</sub> and PM<sub>2.5</sub> forecasts.

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## **2. EXPERIMENTS AND METHODS**

### **2.1 The NAM-CMAQ Air Quality Forecast System**

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24 The NAQFC system is based on the National Centers for Environmental Prediction's  
25 (NCEP's) NAM meteorological model (Black 1994; Rogers et al., 1996) and EPA's  
26 CMAQ (Byun and Schere, 2006) air quality modeling system. A brief summary of the

1 linkage between the NAM and the CMAQ models, relevant to this study, is presented  
2 below. A more in-depth description of the NAM-CMAQ system can be found in Otte et  
3 al. (2005).

4 For this application, O<sub>3</sub> and PM<sub>2.5</sub> were forecast over the CONUS US at 12-km  
5 horizontal grids on the Lambert Conformal map projection. The vertical domain was  
6 discretized with 22 layers set on the sigma coordinate, extending from the surface to  
7 ~100 hPa. The Carbon Bond IV (CB-IV) chemical mechanism was used to represent the  
8 gas phase reaction pathways for O<sub>3</sub> forecasts and for the early part of PM<sub>2.5</sub> forecasts. The  
9 chemistry mechanism was updated to the CB05 (Yarwood et al., 2005; Sarwar et al.,  
10 2008) for the PM<sub>2.5</sub> forecasts on July 15, 2008. The AERO3 aerosol module was used  
11 with CB-IV model configuration; the module was updated to AERO4 when the chemistry  
12 mechanism was updated to CB05. Three-dimensional chemical fields were initialized  
13 from the previous forecast cycle. The primary NAM-CMAQ model forecast for next-day  
14 surface-layer O<sub>3</sub> was based on the current day's 12 UTC cycle, while for PM<sub>2.5</sub>  
15 forecasts, the 06 UTC cycle was used. The target forecast period was local midnight  
16 through local midnight next day.

17 The processing of the emission data for various pollutant sources was adapted from  
18 the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system (Houyoux et  
19 al., 2000). Emission estimates were based on the 2005 U.S. EPA National Emission  
20 Inventory. NO<sub>x</sub> and SO<sub>2</sub> emitted from elevated point sources were projected to 2008  
21 using the 2006 Continuous Emission Monitoring (CEM) data in conjunction with  
22 projections derived from the Department of Energy's Annual Energy Outlook (Pouliot  
23 and Pierce, 2003).

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## 2.2 Domain, Evaluation Regions, and Observational Data

As shown in Figure 1, the NAQFC domain covers the CONUS US. Due to large region-to-region differences in the atmospheric physical and chemical processes, the CONUS domain is divided into six subregions to facilitate the performance evaluations (see Figure 1). The four easternmost subregions, northeast (NE), southeast (SE), upper Midwest (UM), and lower Midwest (LM), are based on climatology that identified areas of homogeneous concentration variability using the Principal Component Analysis technique (Eder et al., 1993; Gogo et al., 2005). The Rocky Mountain (RM) subregion is characterized by high elevation (generally > 1000 m) and complex terrain. The Pacific Coast (PC) subregion contains the west coast states which are often under marine influence from the Pacific Ocean.

Hourly, near real-time, surface O<sub>3</sub> (ppb) and PM<sub>2.5</sub> (μg/m<sup>3</sup>) data obtained from EPA's AIRNow program were used in the KF bias-adjustment forecasts and performance evaluations. Roughly 1000 O<sub>3</sub> (crosses) and 500 PM<sub>2.5</sub> (circles) routine measurement stations, mostly in urban areas, are available (Figure 1) for the study period. For O<sub>3</sub> forecasts, the daily maximum 8-hr concentrations were calculated at each station for each day over the study period. The running 8-hr average O<sub>3</sub> concentrations were computed using the concentration at the current and succeeding 7 hours; the daily maximum 8-hr O<sub>3</sub> is the maximum of the 8-hr average values over the day. For PM<sub>2.5</sub> forecasts, the 24-h daily mean at each site was used in the performance evaluations. To facilitate performance evaluations for PM<sub>2.5</sub>, the study period is divided into a cool season (from January to April 20<sup>th</sup> and from September to December) and a warm season (from April 21<sup>st</sup> to August 31<sup>st</sup>).

### 2.3 Implementation of the KF bias-adjustment method

The KF predictor bias-adjustment algorithm (Kalman, 1960) is described in detail by Delle Monache et al. (2006). The adaptation and implementation of the technique for our applications has been presented by Kang et al., (2008). In that study, a key parameter in the KF approach which determines the relative weighting of observed and forecast values was investigated extensively with O<sub>3</sub> forecasts at over 1000 monitoring locations. Even though the optimal error ratios inherent in the KF algorithm implementation were found to vary across space, the impact of using the optimal values on the resultant bias-adjusted predictions was found to be insignificant when compared with using a reasonable single fixed value of this parameter across all locations within the modeling domain. We further tested the error ratio values in the range 0.01 to 0.10 for the entire domain, and found that the impact on the performance was relatively insignificant when the error ratios were in this range, consistent with results in Kang et al. (2008). In this study, the same single fixed error ratio value of 0.06 was used at all the locations for the real-time bias-adjusted O<sub>3</sub> and PM<sub>2.5</sub> forecasts.

The KF bias-adjustment technique was implemented for O<sub>3</sub> and PM<sub>2.5</sub> forecasts separately. First, the KF was initialized with the initial estimates of KF parameters as outlined in Kang et al. (2008) and with two days of hourly observations and raw model predictions. It then generated the third day's bias-adjusted forecasts by combining the third day's raw forecasts with the updated KF parameters. All updated KF parameters at each site for each hour were saved into a file for use in the next KF run. The KF runs then continued by reading the previous day's KF parameters and two preceding days' observations and raw model predictions to continuously generate the next day's bias-adjusted forecasts through combining with the next day's raw forecasts. The KF simulations run daily when the preceding days' observations and the raw forecasts for

1 next day (issued on current day) were available. In our implementation, if data at two  
2 consecutive days were missing at a site, the method would automatically drop this site  
3 from future bias-adjustment forecasts; however, if a new site with two consecutive days'  
4 data appeared in the observation data set, the KF would initialize the site with initial  
5 values of KF parameters and generate bias-adjusted forecasts further on. This  
6 implementation is very adaptable to the variable nature of monitoring stations reporting  
7 hourly observations to the AIRNow network, and can be easily combined with the  
8 operational AQF system to provide bias-adjusted forecasts operationally. The bias-  
9 adjusted forecasts were initialized on January 4 and April 3 for PM<sub>2.5</sub> and O<sub>3</sub> forecasts,  
10 respectively, and the programs were run daily on a Linux system; it took less than 10  
11 minutes of computation to create a bias adjusted forecast.

12

## 13 **2.4 Verification statistics**

14 To assess the performance of the KF bias-adjusted forecasts, model verification  
15 statistics commonly used by the air quality modeling community (Kang et al., 2005; Eder  
16 et al., 2006; Kang et al., 2008) are used in this study and include Root Mean Square Error  
17 (RMSE), Normalize Mean Error (NME), Mean Bias (MB), Normalized Mean Bias  
18 (NMB), and correlation coefficient (r). In addition, the index of agreement (IOA)  
19 (Willmott, 1981; Kang et al., 2008) is also calculated to specify the degree to which the  
20 observed deviations about the mean observed value agree, both in magnitude and sign, to  
21 the predicted deviations about the mean observed value. For a forecast product, another  
22 set of verification statistics is the categorical metrics (Kang et al., 2005); among those the  
23 False Alarm Ratio (FAR) and Hit Rate (H) are used in the current study.

24

## 25 **3. RESULTS**

### 1 **3.1 Overall Performance**

2 Table 1 presents a summary of domain (Dom) and sub-regional mean discrete  
3 statistics for the raw model and the KF forecast daily maximum 8-h O<sub>3</sub> mixing ratios  
4 during the study period. Table 2 presents similar model performance statistics for the  
5 daily average PM<sub>2.5</sub> concentrations for warm and cool seasons. As seen in Table 1, for the  
6 daily maximum 8-h O<sub>3</sub> raw forecasts, RMSE values ranged from 10.4 to 16.0 ppb. The  
7 application of the KF bias-adjustment reduced the RMSE to the range of 8.5 to 10.5 ppb,  
8 reflecting more than a 25% improvement. Similar improvement was reflected in NME.  
9 More noticeable improvement by the KF forecasts over the raw model is seen in the MB  
10 and NMB; the MB values were reduced from several ppb to about 1 ppb across all the  
11 regions, and NMB from as high as 17% to less than 2%. The correlation coefficients (r)  
12 also increased systematically from 0.5 to 0.7 range for the raw forecasts to 0.7 - 0.84  
13 range in the KF forecasts. Similar forecast skill improvement in PM<sub>2.5</sub> forecasts by the KF  
14 forecasts over raw forecasts is shown in Table 2. Compared to O<sub>3</sub> forecasts, the overall  
15 statistics for PM<sub>2.5</sub> forecasts still need to be improved due to the difficulty in simulating  
16 the complexity of PM<sub>2.5</sub> formation and distribution by the NAM-CMAQ system.

17 Figures 2 and 3 present scatter plots of selected forecast and observed percentiles for  
18 the daily maximum 8-h O<sub>3</sub> and daily mean PM<sub>2.5</sub>, respectively. In these figures, both  
19 measured and forecast time series were examined at each site and percentiles of the  
20 concentration distributions over the study period were computed for both observations  
21 and forecast values following Mathur et al. (2008). Scatter plots of specific percentiles of  
22 the concentration distributions of the modeled and observed time series are then  
23 examined to assess the ability of the model to capture the spatial variability in frequency  
24 distributions of the species of interest across the sites. As shown in Figures 2 and 3, the  
25 KF forecasts displayed a much improved match with the observed distributions as

1 reflected by the reduced and even scatter about the 1:1 line (perfect prediction) when  
2 compared to the raw forecasts. The  $r^2$  associated with the forecast and observed percentile  
3 distributions increased from 0.80 to 0.98 for the daily maximum 8-h  $O_3$  forecasts, and  
4 increased from 0.42 to 0.90 for the daily average  $PM_{2.5}$  forecasts, When the KF bias-  
5 adjustment procedure was implemented.

6 The improvement in the performance of the KF bias-adjusted forecasts over the raw  
7 forecasts is also evident in the index of agreement (IOA) comparisons (Figures 4 and 5).  
8 As seen in Figure 4, for the daily maximum 8-h  $O_3$  forecasts over the entire domain and  
9 across all the subregions, the IOA values associated with the KF forecasts increased  
10 significantly when compared with those of the raw forecasts. The median IOA values for  
11 the raw forecasts were generally less than 0.80, while the median IOA values for the KF  
12 forecasts were generally greater than 0.80. For the daily average  $PM_{2.5}$  forecasts (Figures  
13 5a and 5b), the KF forecasts again resulted in larger IOA values compared to the raw  
14 forecasts for both the warm and cool seasons as well as across all subregions.

15 Comparison of Figure 4 with Figure 5 indicates that the IOA values for both the raw  
16 forecasts and KF forecasts for  $O_3$  were larger than those for  $PM_{2.5}$ ; for the raw forecasts,  
17 the difference in IOA was about 20%, while for the KF forecasts, the difference was  
18 reduced to about 10%. Another important feature is that for  $O_3$  forecasts, both the raw  
19 forecasts and the KF forecasts performed better in the eastern portions of the domain  
20 (NE, SE, UM, and LM) than in the western regions (RM and PC). However for  $PM_{2.5}$   
21 forecasts, the raw forecasts did not perform well in SE for both seasons, though the IOA  
22 values significantly increased by the KF forecasts; both the raw forecasts and the KF  
23 forecasts displayed lower IOA values for LM and RM during both seasons than for the  
24 rest of the regions, while they performed better in PC during the cool season than during  
25 the warm season. Both raw forecasts and KF bias-adjusted forecasts displayed the largest

1 IOA values in NE for both O<sub>3</sub> and PM<sub>2.5</sub> among all the regions except that the IOA values  
2 in UM were larger than those in NE for the KF PM<sub>2.5</sub> forecasts for the cool season. It  
3 should also be pointed out that the performance of KF bias-adjusted forecasts is always  
4 dependent on the performance of raw forecasts, i.e., if the IOA values associated with the  
5 raw forecasts were lower at a region than at other regions, then the IOA values associated  
6 with the KF bias-adjusted forecasts at this region will also be lower than at other regions.

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### 8 **3.2 Temporal and Spatial Performance**

9         Figure 6 presents time-series comparisons of mean daily maximum 8-h O<sub>3</sub> mixing  
10 ratios forecast by the raw and bias-adjusted models with corresponding measurements.  
11 Figure 7 presents a similar comparison for the daily-average PM<sub>2.5</sub> forecasts. As seen in  
12 Figure 6, the NAM-CMAQ system underestimated the daily maximum 8-h O<sub>3</sub>  
13 concentrations at the beginning of the study period, then transitioned to overestimation  
14 with time; significant overestimation occurred towards the end of the study period.  
15 However, the KF forecasts were able to correct for both overestimation and  
16 underestimation and track the observed time series quite well. As noted in Figure 7, the  
17 raw model overestimated daily mean PM<sub>2.5</sub> concentrations during cool season and  
18 underestimated during warm season. Again the KF time series tracked the observed time  
19 series very well throughout the entire year and was able to reduce the systematic seasonal  
20 biases considerably.

21         To further investigate the temporal and spatial performance, boxplots of monthly  
22 RMSE values for daily maximum 8-h O<sub>3</sub> and daily mean PM<sub>2.5</sub> for each of the subregions  
23 are displayed in Figures 8 and 9, respectively. As illustrated in Figure 8, the RMSE  
24 values associated with the raw model daily maximum 8-h O<sub>3</sub> forecasts for the SE, UM,  
25 and RM subdomains exhibited a tendency to increase as the O<sub>3</sub> season progressed;

1 similar trends in the NAM-CMAQ O<sub>3</sub> forecast error were also noted for prior years (Eder  
2 et al., 2009). These trends were found to be partially related to trends in temperature  
3 forecast error in the meteorological model (NAM); the subsequent impacts on modeled  
4 emissions and chemistry are currently under investigation. Despite the systematic trend  
5 for RMSE values associated with the raw forecasts, the KF bias-adjusted forecasts were  
6 able to effectively adjust the errors and produced comparable distributions of RMSE  
7 values during the entire period.

8 For the year-long daily mean PM<sub>2.5</sub> forecasts (Figure 9), the monthly RMSE  
9 values associated with the raw forecasts started higher at the beginning months (January,  
10 February, and March). The significant decrease of RMSE values associated with the raw  
11 forecasts during the October to December period compared to the January to March  
12 period is attributable to the switch in the chemical mechanism from CB-IV to CB05 and  
13 the corresponding aerosol module from AERO3 to AERO4 on July 15, 2008. The  
14 significantly higher RMSE values during June and July in the PC region can be attributed  
15 to missing emissions from wide spread wild fires in California during these two months  
16 which resulted in elevated observed PM<sub>2.5</sub> concentrations which were not simulated by  
17 the raw model. Nevertheless, the KF bias-adjusted forecasts were able to produce  
18 significantly smaller RMSE values compared to the raw forecasts for all the regions  
19 during each of the months.

20 The ability of the KF technique to improve O<sub>3</sub> and PM<sub>2.5</sub> forecast across the  
21 continental U.S. is further illustrated in Figures 10 and 11 which compare maps of mean  
22 bias in the raw and bias-adjusted forecasts. As seen in Figure 10a, the NAM-CMAQ  
23 system generally overestimated in the eastern part of the domain, especially in the  
24 northeast and southeast with MB values greater than 5 ppb. In California, the MB values  
25 indicated mixed results with both overestimation (MB ≥ 5 ppb) and underestimation (MB

1 < -5 ppb) coexisting in the same area. However, with the application of KF bias-  
2 adjustment (Figure 10b), the MB values at almost all the locations were reduced to be  
3 within  $\pm 2$  ppb, demonstrating the robustness of the KF bias-adjustment technique for O<sub>3</sub>  
4 forecasts across all locations.

5         Similar effects are also demonstrated for PM<sub>2.5</sub> forecasts over the CONUS domain  
6 (Figure 11). During warm season, underestimation of the daily average PM<sub>2.5</sub>  
7 concentrations by the raw forecasts dominated the entire domain (orange and purple  
8 squares in Figure 11a). During the cool season (Figure 11c), the raw forecasts generally  
9 overestimated in the east, and displayed mixed results in the west. However, during both  
10 warm and cool seasons, the KF forecasts were able to adjust either the overestimation or  
11 underestimation concentrations very effectively with mean bias of  $\pm 2 \mu\text{g}/\text{m}^3$  at majority  
12 of the sites (Figures 11b and 11d). Even at the sites where MB values were greater than 2  
13  $\mu\text{g}/\text{m}^3$  or less than  $-2 \mu\text{g}/\text{m}^3$ , the magnitude of the MB values was significantly reduced in  
14 the KF forecasts compared with those in the raw forecasts.

### 15 **3.3 Performance over observation concentration bins**

16         To examine the performance of the KF bias-adjustment technique over different  
17 concentration ranges, RMSE and MB for both O<sub>3</sub> and PM<sub>2.5</sub> forecasts were examined as a  
18 function of observed ambient levels. As seen in Figure 12a, the RMSE values for daily  
19 maximum 8-h O<sub>3</sub> forecasts were larger at both lower (<30 ppb) and higher ( $\geq 85$  ppb) O<sub>3</sub>  
20 levels than those in the middle. For the PM<sub>2.5</sub> forecasts, the raw forecasts displayed lower  
21 RMSE values at lower observation bins and higher RMSE values at higher observation  
22 bins for both the warm (Figure 13a) and cool seasons (Figure 13b). Compared to the O<sub>3</sub>  
23 forecasts (Figure 12b), the distribution of MB values for PM<sub>2.5</sub> forecasts (Figures 13 c and  
24 d) over concentration bins displayed very different features; during the warm season, the  
25 distribution of the MB values associated with the raw forecasts showed very little

1 variations, while when the observed concentrations were greater than  $10 \mu\text{g}/\text{m}^3$ , the raw  
2 model displayed increased underestimation with the increasing concentrations. In  
3 contrast, during the cool season (Figure 13d), the  $\text{PM}_{2.5}$  MB values associated with the  
4 raw model showed very little variation, even though the distributions became  
5 increasingly wider at higher observation bins. The KF bias-adjustment technique is able  
6 to effectively reduce the errors and biases across all concentration ranges and for both the  
7 warm and cool seasons.

### 8 **3.4 Categorical Performance**

9 It is important for an air quality forecast product to be able to accurately predict  
10 exceedance and non-exceedance events (categorical predictions). Figure 14 presents the  
11 categorical evaluations for the raw forecasts and KF bias-adjusted forecasts for daily  
12 maximum 8-hr  $\text{O}_3$  and daily mean  $\text{PM}_{2.5}$  concentrations, respectively. The statistical  
13 measures presented include the FAR and H (Kang et al., 2005). Exceedance threshold of  
14 both the 85 ppb 8-hr maximum  $\text{O}_3$  and the revised NAAQS of 75 ppb are examined; the  
15 corresponding metrics are denoted as FAR85, FAR75, H85, and H75. The threshold  
16 value for daily mean  $\text{PM}_{2.5}$  exceedance is  $35 \mu\text{g}/\text{m}^3$  and the corresponding metrics are  
17 denoted as FAR35 and H35.

18 As shown in Figure 14, the KF bias-adjusted forecasts were able to significantly  
19 reduce FAR values and increase H values for both daily maximum 8-h  $\text{O}_3$  forecasts and  
20 daily average  $\text{PM}_{2.5}$  forecasts. Comparison of the categorical metrics for the two  
21 threshold values for  $\text{O}_3$  forecasts indicates that for the new standard of 75 ppb, both the  
22 raw forecasts and the KF forecasts provide better categorical forecasts relative to those  
23 with the old standard. The KF forecasts produced an H value of 50% based on the new  
24 exceedance standard and the FAR was slightly higher than 50%, further illustrating the  
25 robustness of the KF bias-adjustment technique. For the  $\text{PM}_{2.5}$  forecasts, the FAR reduced

1 from 93% to 76% and H increased from 24% to 38% through the application of the KF  
2 bias-adjustment technique.

### 3 **3.5 Performance for Air Quality Index**

4 The air quality index (AQI) is frequently used to report daily air quality conditions.  
5 The index is an indicator of how clean or polluted the air is and what the associated  
6 health effects might be for sensitive populations. The breakpoints for converting from O<sub>3</sub>  
7 mixing ratio (ppb) or PM<sub>2.5</sub> concentrations (μg/m<sup>3</sup>) to AQI values are presented in Table  
8 3. As seen in Table 3, AQI values range from 0-500, with higher values representing  
9 greater level of air pollution and a greater associated health concern; an AQI value of 100  
10 generally corresponds to the National Ambient Air Quality Standard (NAAQS) for the  
11 pollutant. The AQI is divided into six color-coded categories; values of 0-50 (code  
12 green) represent good air quality conditions, 51-100 (code yellow ) represent moderate  
13 pollution, 101-150 (code orange) represent air pollution levels unhealthy for sensitive  
14 groups, 151-200 (code red) represent unhealthy conditions, while 201-300 (code purple)  
15 and 301-500 (code maroon) represent very unhealthy and hazardous air quality  
16 conditions, respectively. The ability of the bias correction technique to improve the AQI  
17 forecasts for O<sub>3</sub> and PM<sub>2.5</sub> at each of the monitoring locations was examined. Figure 15  
18 presents comparisons of the category hit rate for each AQI category across all monitoring  
19 locations for O<sub>3</sub> forecasts with the raw model and the KF bias-adjusted forecasts. The  
20 Category Hit Rate (cH) (Eder et al., 2009b) is defined as:  $cH_i = \frac{N_f^i}{N_{obs}^i}$ , where i is the AQI  
21 index (1, 2, 3, 4, 5), and  $N_f^i$  is the number of correctly forecast instances in the i<sup>th</sup>  
22 category and  $N_{obs}^i$  is the number of observed instances in the i<sup>th</sup> category. Figure 16  
23 presents similar comparisons for surface-level PM<sub>2.5</sub> forecasts. For forecasts of both

1 pollutants, a systematic improvement in the predictions of the different AQI categories is  
2 evident when the bias-adjustment technique was applied. The improvements in the  
3 accuracy of the AQI forecasts for the moderate to unhealthy categories, further  
4 demonstrate the applicability of the methodology and suggest the need to adopt bias-  
5 adjustment operationally for improving the reliability of model-based air quality  
6 forecasts.

7

#### 8 **4. SUMMARY**

9       The near real-time Kalman filter bias-adjustment technique was applied to NAM-  
10 CMAQ derived O<sub>3</sub> and PM<sub>2.5</sub> air quality forecasts for the continental United States. These  
11 bias-adjustment forecasts were implemented to run daily for improving the next-day  
12 forecast. Bias-adjustment on operational basis adds minimal computational burden; on a  
13 daily-basis, it required less than 10 minutes of CPU on a single processor Linux machine.  
14 Hourly O<sub>3</sub> and PM<sub>2.5</sub> bias-adjusted forecasts have been generated for all the locations  
15 where the observations are available from the AIRNow network. The performance  
16 evaluation of the KF forecasts for both O<sub>3</sub> and PM<sub>2.5</sub> has shown significant improvement  
17 over the raw forecasts for a variety of statistical measures. Specifically, systematic errors  
18 or biases have been reduced, correlation coefficients increased, false alarm ratios  
19 reduced, while hit rates have gone up. The robustness of this bias-adjustment technique is  
20 evident for various concentration ranges over CONUS. The forecast skill has improved at  
21 all the locations within the domain during all seasons. Though the bias-adjustment  
22 technique was only applied at discrete points in this study, the bias-adjusted spatial maps  
23 of O<sub>3</sub> and PM<sub>2.5</sub> forecasts could be readily developed by using appropriate statistical  
24 methods (e.g., Hogrefe et al., 2009; Denby et al., 2009; Garcia et al., 2010). Comparison  
25 of model forecasts skills for PM<sub>2.5</sub> and O<sub>3</sub> have clearly indicated that more work needs to

1 be done to improve the accuracy of PM<sub>2.5</sub> forecasts. Improvements in the representation  
2 of fine particulate matter emissions as well as the physical and chemical processes  
3 regulating sources and sinks in atmospheric models are expected as a result of on-going  
4 research over the next several years. Nevertheless, our analysis indicates that despite the  
5 current limitations in the representation of atmospheric processes dictating the  
6 distribution of ambient PM<sub>2.5</sub>, bias-adjustment techniques can be used to help improve  
7 the accuracy and reliability of short-term PM<sub>2.5</sub> forecasts and AQI from such models.

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25 **5. ACKNOWLEDGEMENTS**

1       The authors thank Drs. Luca Delle Monache and Roland B. Stull for providing their  
2 original Kalman filter codes. The research presented here was performed under the  
3 Memorandum of Understanding between the U.S. Environmental Protection Agency  
4 (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric  
5 Administration (NOAA) and under agreement number DW13921548. Although this work  
6 has been reviewed by EPA and approved for publication, it does not necessarily reflect  
7 agency policy or views.

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**Tab Table 1. Regional summary of discrete statistics for raw model and KF bias-adjusted daily maximum 8-hr O<sub>3</sub> forecasts during 2008 summer season. RMSE: Root Mean Square Error, NME: Normalized Mean Error, MB: Mean Bias, NMB: Normalized Mean Bias, and r: Correlation Coefficient**

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<b>TYPE</b>	<b>RMSE (ppb)</b>	<b>NME (%)</b>	<b>MB (ppb)</b>	<b>NMB (%)</b>	<b>r</b>
<b>Dom-mod</b>	<b>12.5</b>	<b>20.1</b>	<b>3.2</b>	<b>6.8</b>	<b>0.65</b>
<b>Dom-kf</b>	<b>9.1</b>	<b>14.5</b>	<b>0.6</b>	<b>1.3</b>	<b>0.81</b>
<b>NE-mod</b>	<b>10.6</b>	<b>16.9</b>	<b>2.7</b>	<b>5.6</b>	<b>0.70</b>
<b>NE-kf</b>	<b>8.9</b>	<b>13.8</b>	<b>0.7</b>	<b>1.4</b>	<b>0.78</b>
<b>SE-mod</b>	<b>12.2</b>	<b>20.1</b>	<b>5.8</b>	<b>12.2</b>	<b>0.70</b>
<b>SEkf</b>	<b>9.1</b>	<b>14.7</b>	<b>0.5</b>	<b>1.1</b>	<b>0.80</b>
<b>UM-mod</b>	<b>10.4</b>	<b>17.5</b>	<b>2.5</b>	<b>5.4</b>	<b>0.59</b>
<b>UM-kf</b>	<b>8.5</b>	<b>13.7</b>	<b>0.7</b>	<b>1.5</b>	<b>0.72</b>
<b>LM-mod</b>	<b>13.6</b>	<b>27.0</b>	<b>7.0</b>	<b>16.9</b>	<b>0.64</b>
<b>LM-kf</b>	<b>9.8</b>	<b>17.7</b>	<b>0.8</b>	<b>1.9</b>	<b>0.77</b>
<b>RM-mod</b>	<b>11.4</b>	<b>16.4</b>	<b>2.7</b>	<b>5.1</b>	<b>0.50</b>
<b>RM-kf</b>	<b>8.9</b>	<b>12.8</b>	<b>0.7</b>	<b>1.3</b>	<b>0.70</b>
<b>PC-mod</b>	<b>16.0</b>	<b>21.9</b>	<b>-3.2</b>	<b>-5.9</b>	<b>0.60</b>
<b>PC-kf</b>	<b>10.5</b>	<b>14.5</b>	<b>0.2</b>	<b>0.3</b>	<b>0.84</b>

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1 **Table 2. Regional summary of discrete statistics for raw model and KF bias-**  
2 **adjusted daily mean PM<sub>2.5</sub> forecasts during 2008 warm/cool season: In each cell,**  
3 **the value on the left of slash (/) is for warm season and the value on the right of**  
4 **the slash is for the cool season. The values in the rows of each table with white**  
5 **background marked with “-mod” represent statistics associated with raw**  
6 **forecasts, while those in the rows with shaded background and with the**  
7 **extension “-kf” represent the statistics associated with the KF bias-adjusted**  
8 **forecasts.**

<b>TYPE</b>	<b>RMSE (<math>\mu\text{g}/\text{m}^3</math>)</b>	<b>NME (%)</b>	<b>MB (<math>\mu\text{g}/\text{m}^3</math>)</b>	<b>NMB (%)</b>	<b>r</b>
<b>Dom-mod</b>	<b>9.6/10.5</b>	<b>47.5/70.5</b>	<b>-2.3/4.5</b>	<b>-19.6/45.1</b>	<b>0.33/0.53</b>
<b>Dom-kf</b>	<b>6.6/6.4</b>	<b>32.9/42.5</b>	<b>-0.1/1.7</b>	<b>-0.4/16.5</b>	<b>0.71/0.68</b>
<b>NE-mod</b>	<b>7.5/12.3</b>	<b>39.5/76.1</b>	<b>-2.4/6.6</b>	<b>-17.8/59.9</b>	<b>0.56/0.63</b>
<b>NE-kf</b>	<b>5.5/7.3</b>	<b>29.1/44.7</b>	<b>-0.4/2.4</b>	<b>-2.7/22.1</b>	<b>0.76/0.72</b>
<b>SE-mod</b>	<b>7.8/9.1</b>	<b>41.5/62.1</b>	<b>-3.9/4.6</b>	<b>-27.5/43.8</b>	<b>0.40/0.47</b>
<b>SE-kf</b>	<b>5.3/5.4</b>	<b>27.1/37.2</b>	<b>-0.4/1.3</b>	<b>-2.7/12.8</b>	<b>0.63/0.58</b>
<b>UM-mod</b>	<b>6.0/10.7</b>	<b>36.6/68.3</b>	<b>-0.7/6.5</b>	<b>-6.0/57.4</b>	<b>0.58/0.62</b>
<b>UM-kf</b>	<b>5.0/6.1</b>	<b>30.7/37.3</b>	<b>-0.2/1.7</b>	<b>-1.7/15.2</b>	<b>0.69/0.73</b>
<b>LM-mod</b>	<b>8.7/9.4</b>	<b>52.4/67.7</b>	<b>-4.0/3.6</b>	<b>-32.9/36.8</b>	<b>0.17/0.32</b>
<b>LM-kf</b>	<b>5.8/5.9</b>	<b>34.9/42.5</b>	<b>-0.2/1.2</b>	<b>-1.5/12.2</b>	<b>0.37/0.49</b>
<b>RM-mod</b>	<b>6.4/9.3</b>	<b>50.5/75.7</b>	<b>-1.5/3.5</b>	<b>-17.2/43.1</b>	<b>0.18/0.37</b>
<b>RM-kf</b>	<b>4.6/5.6</b>	<b>33.5/44.4</b>	<b>0.0/1.3</b>	<b>0.2/16.2</b>	<b>0.57/0.62</b>
<b>PC-mod</b>	<b>15.3/10.2</b>	<b>57.9/60.2</b>	<b>-3.4/1.8</b>	<b>-30.6/15.8</b>	<b>0.23/0.53</b>
<b>PC-kf</b>	<b>10.5/7.0</b>	<b>39.0/40.9</b>	<b>0.2/1.2</b>	<b>1.9/10.4</b>	<b>0.73/0.72</b>

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1 **Table 3. Air quality index categories with their O<sub>3</sub> and PM<sub>2.5</sub> concentrations**  
2 **breakpoints**

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<b>AQI Category</b>	<b>Index values</b>	<b>Daily maximum 8-hr O<sub>3</sub> (ppb)</b>	<b>24-hr PM<sub>2.5</sub> (µg/m<sup>3</sup>)</b>
<b>Good</b>	<b>0 - 50</b>	<b>0 - 59</b>	<b>0 - 15</b>
<b>Moderate</b>	<b>51 - 100</b>	<b>60 - 75</b>	<b>16 - 35</b>
<b>Unhealthy for Sensitive Groups</b>	<b>101 - 150</b>	<b>76 - 95</b>	<b>36 - 55</b>
<b>Unhealthy</b>	<b>151 - 200</b>	<b>96 - 115</b>	<b>56 - 140</b>
<b>Very Unhealthy</b>	<b>201 - 300</b>	<b>116 - 375</b>	<b>141 - 210</b>

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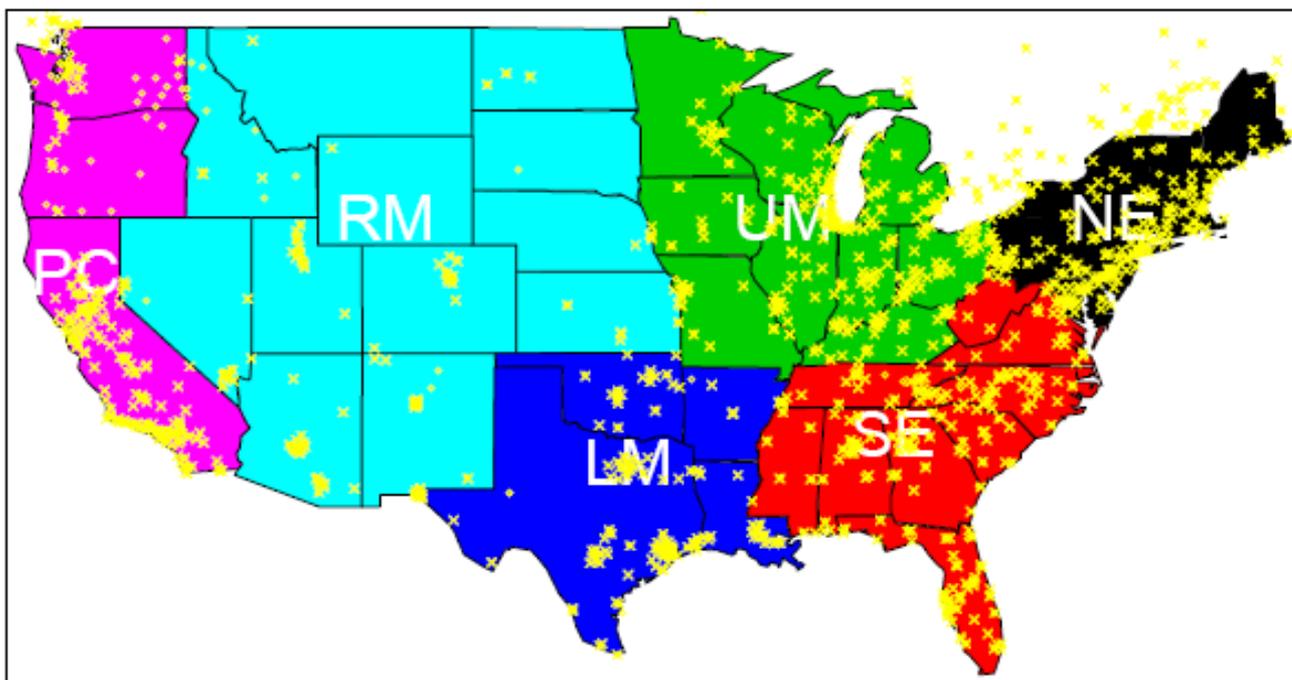


Figure 1. Model domain, evaluation regions, and observational  $O_3$  sites (crosses) and  $PM_{2.5}$  sites (circles): The regions are Northeast (NE), Southeast (SE), Upper Midwest (UM), Lower Midwest (LM), Rocky Mountains (RM), and Pacific Coast (PC)

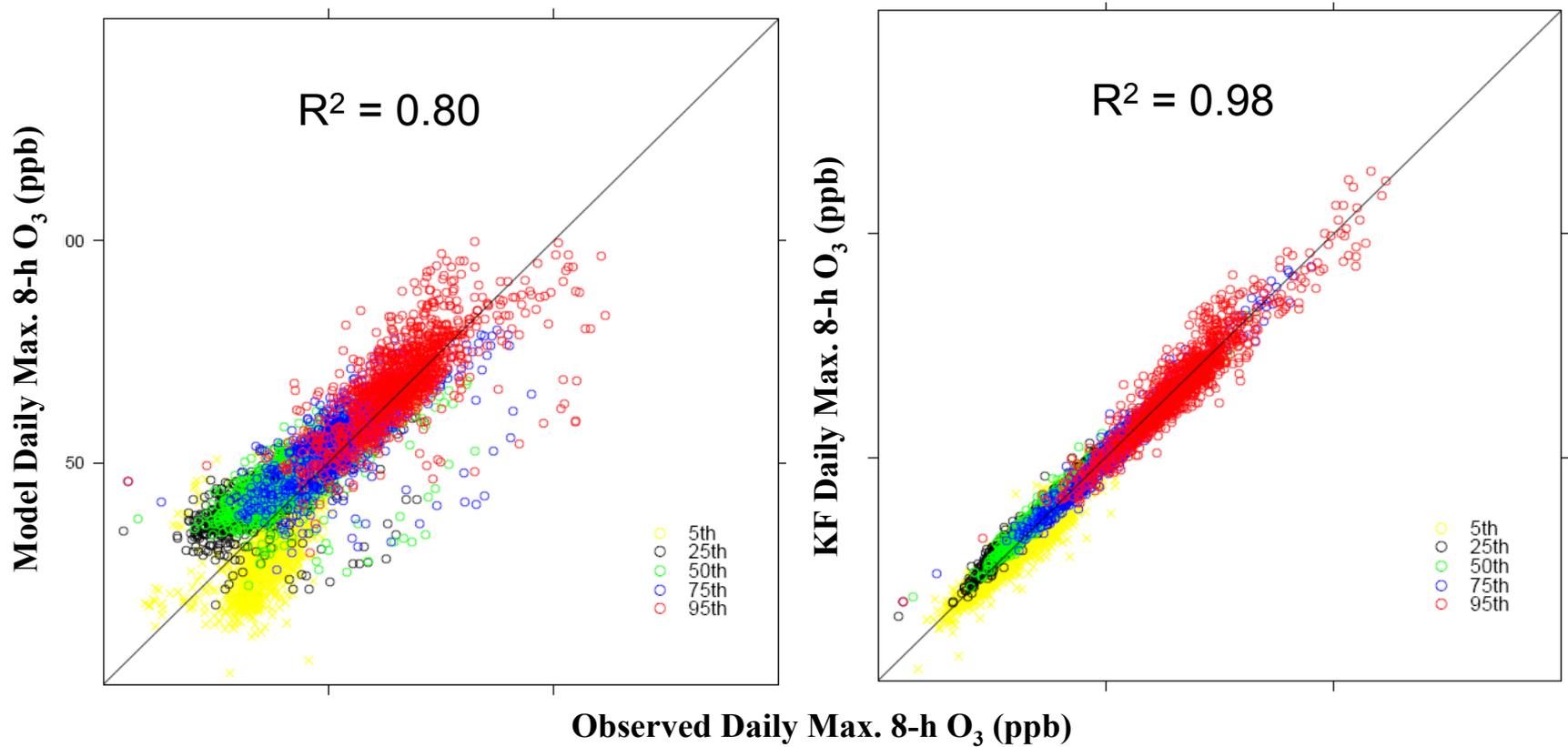


Figure 2. Scatterplots between forecasts and observations for selected percentiles for daily maximum 8-h O<sub>3</sub> mixing ratios (ppb).

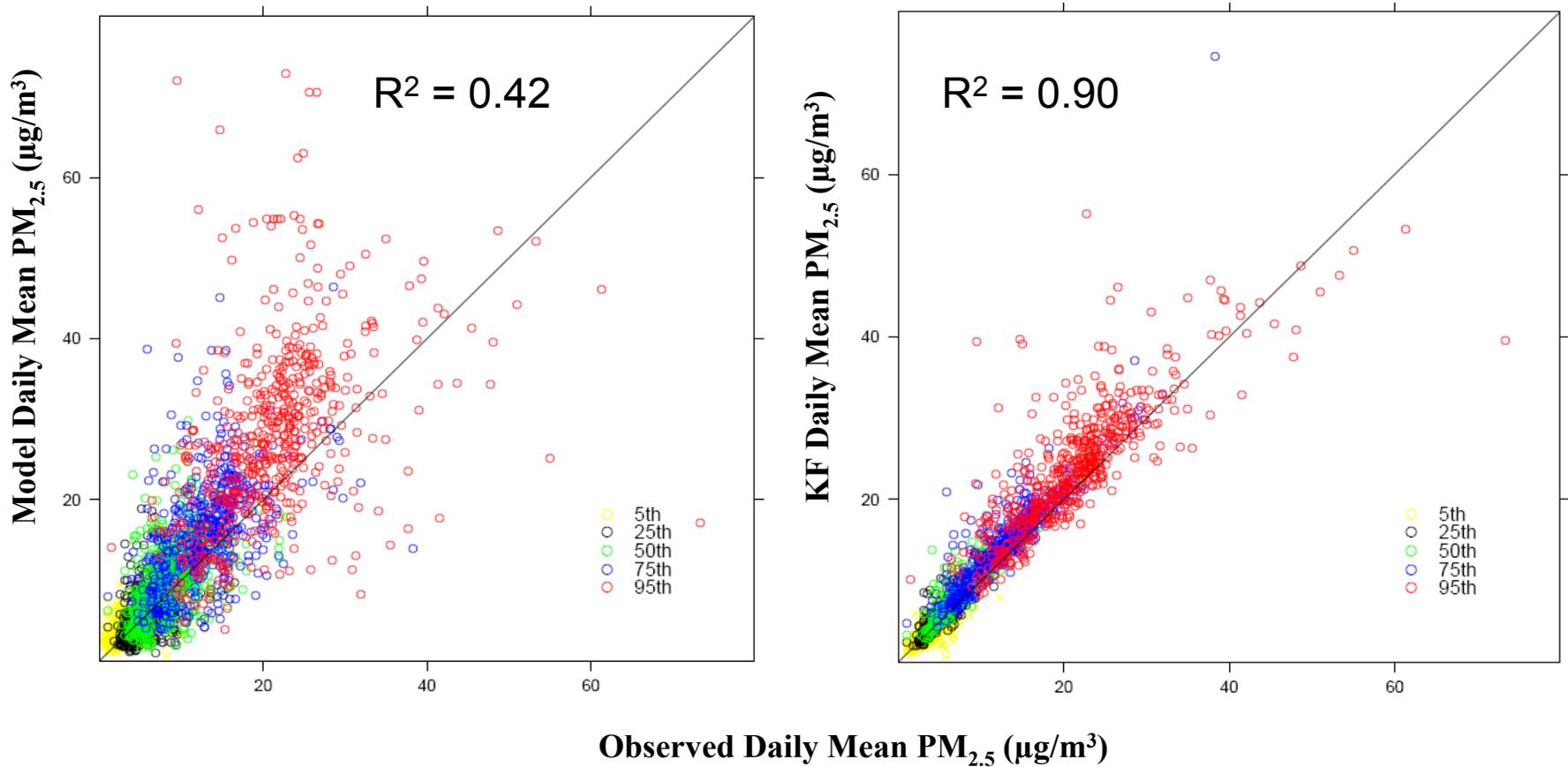


Figure 3. Scatterplots between forecasts and observations for selected percentiles for daily mean PM<sub>2.5</sub> concentrations (µg/m<sup>3</sup>).

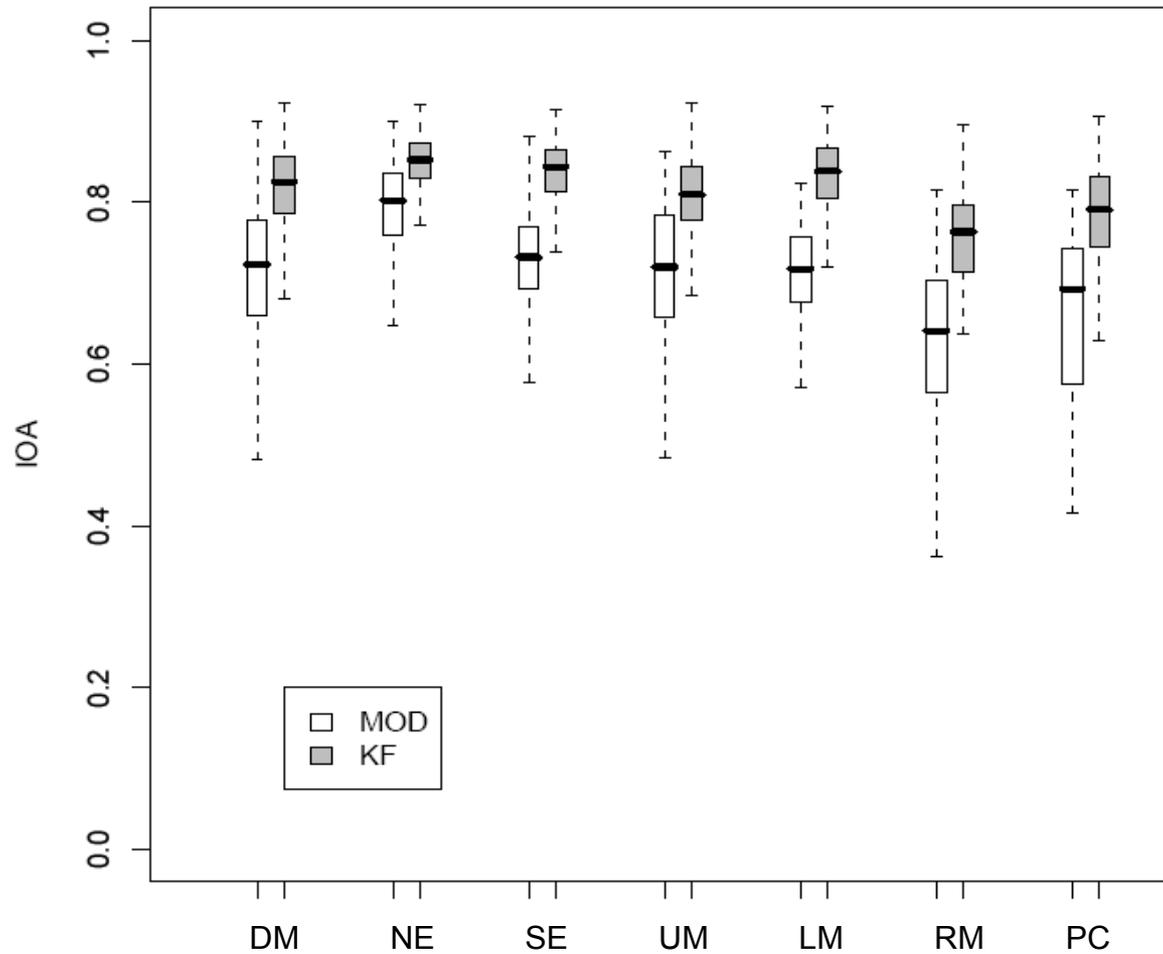


Figure 4. Box plots of index of agreement (IOA) of daily maximum 8-h  $O_3$  (ppb) for the raw model (MOD) forecasts and KF bias-adjusted forecasts over the domain (DM) and across all subregions

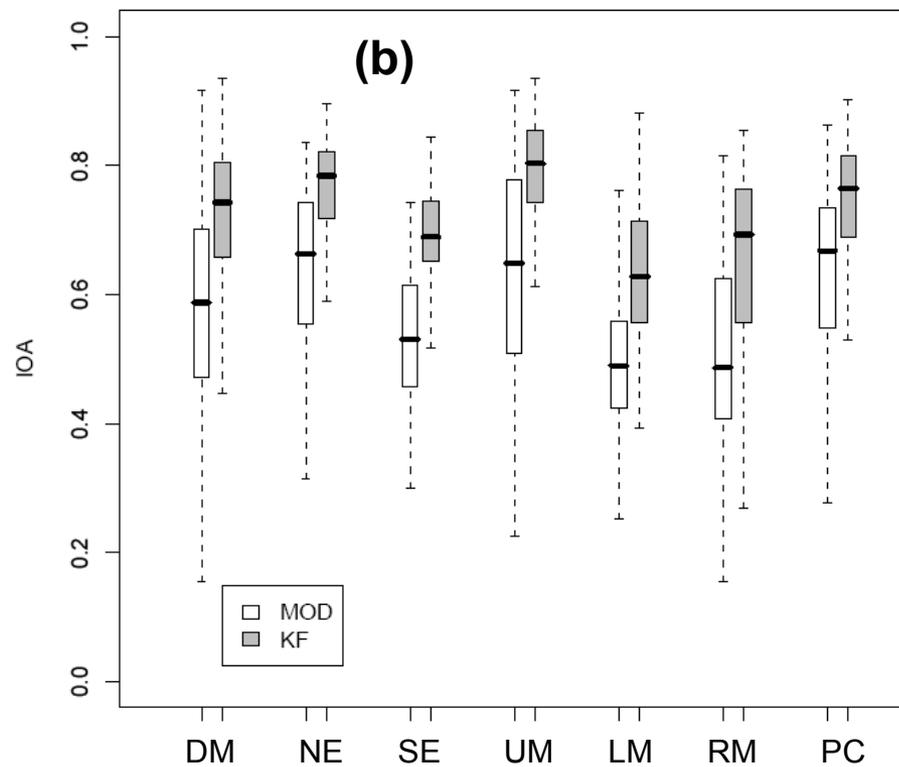
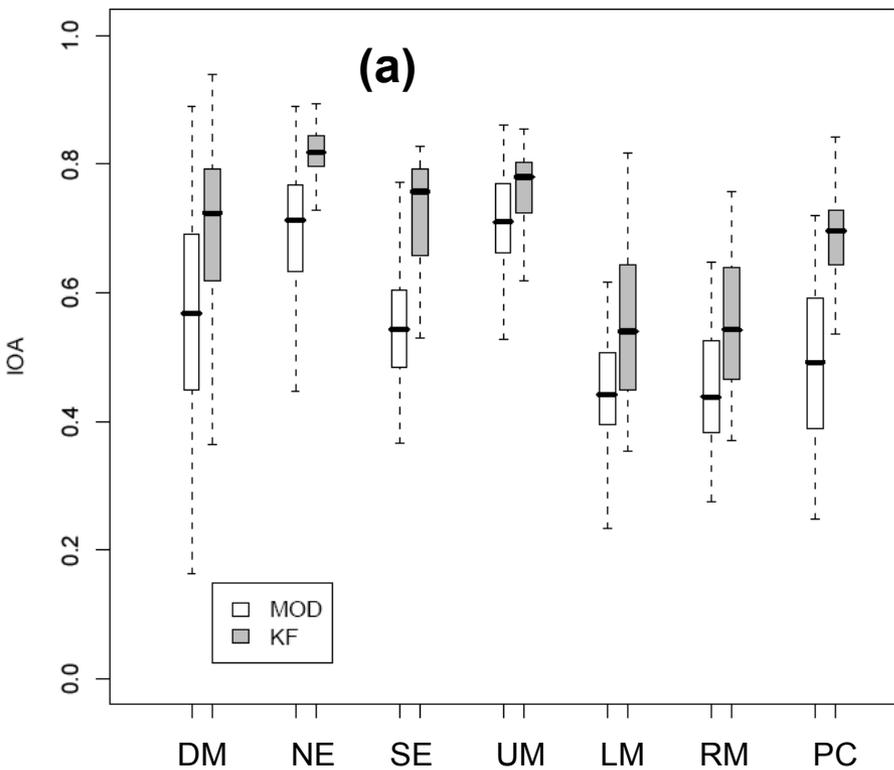


Figure 5. Box plots of index of agreement (IOA) of daily mean  $\text{PM}_{2.5}$  ( $\mu\text{g}/\text{m}^3$ ) for the raw model (MOD) forecasts and KF bias-adjusted forecasts over the domain (DM) and across all subregions during (a) warm season and (b) cool season

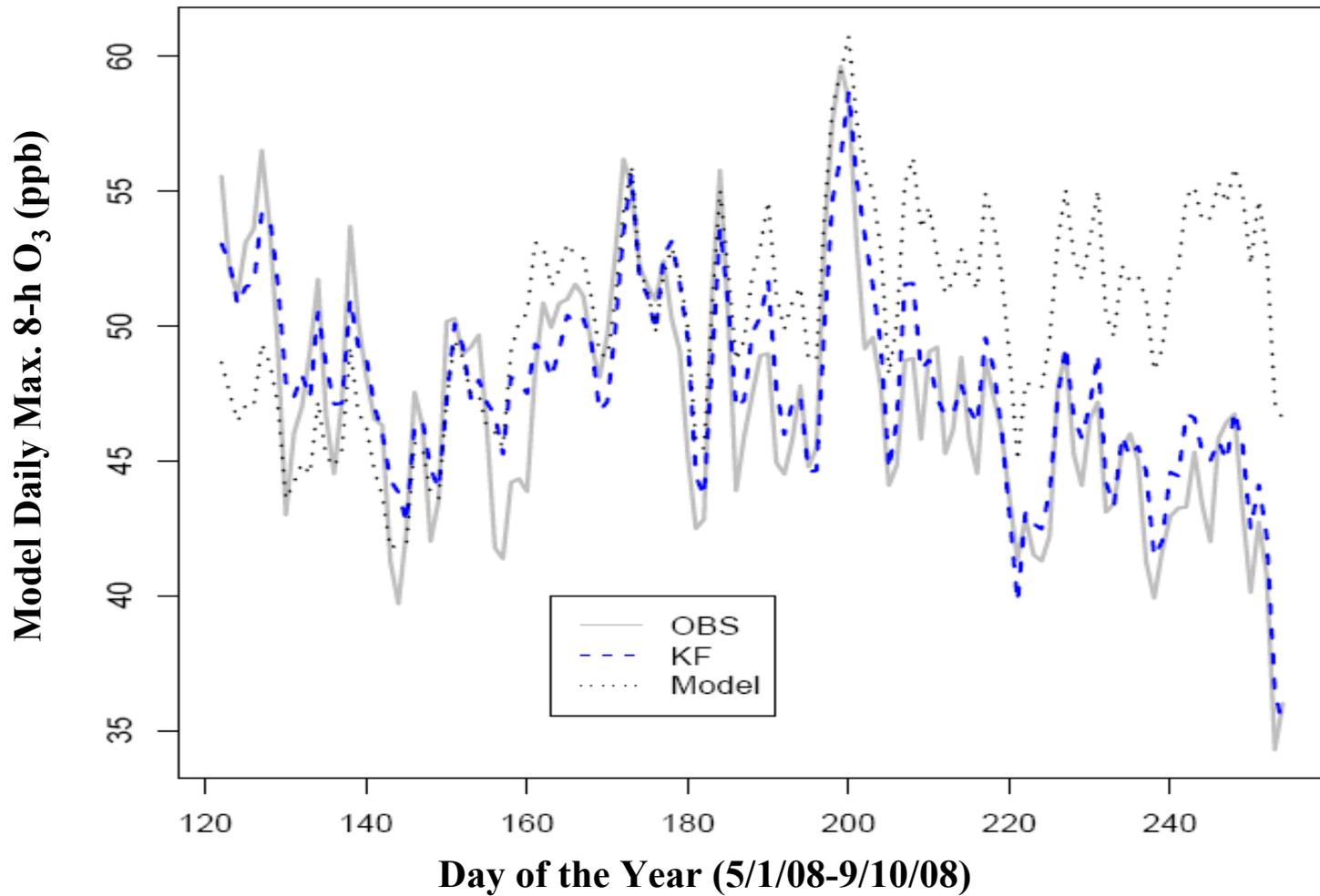


Figure 6. Time series of observed, raw model forecast, and KF bias-adjusted forecast mean daily maximum 8-h O<sub>3</sub> (ppb) over the domain

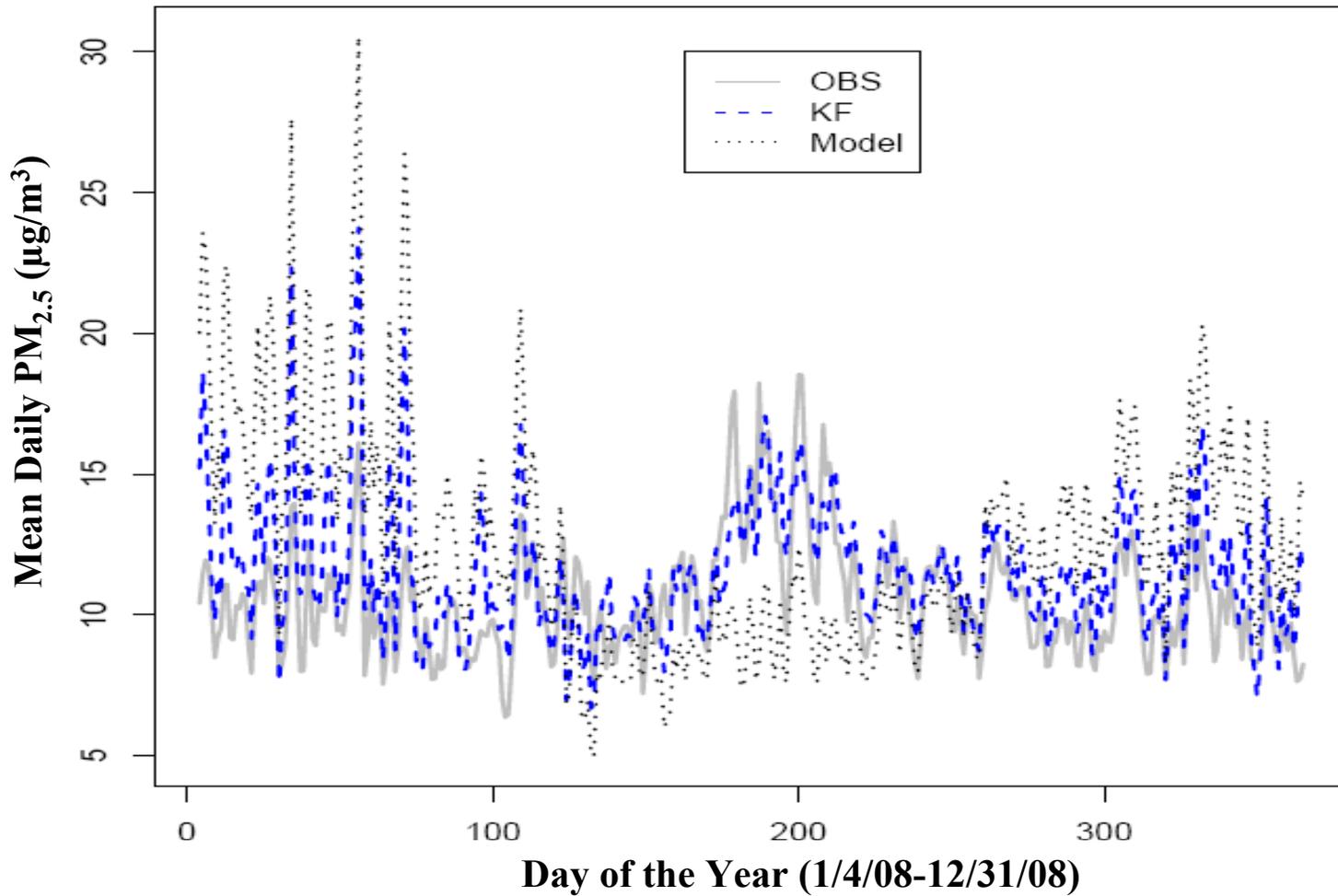


Figure 7. Time series of observed, raw model forecast, and KF bias-adjusted forecast mean daily PM<sub>2.5</sub> ( $\mu\text{g}/\text{m}^3$ ) over the domain

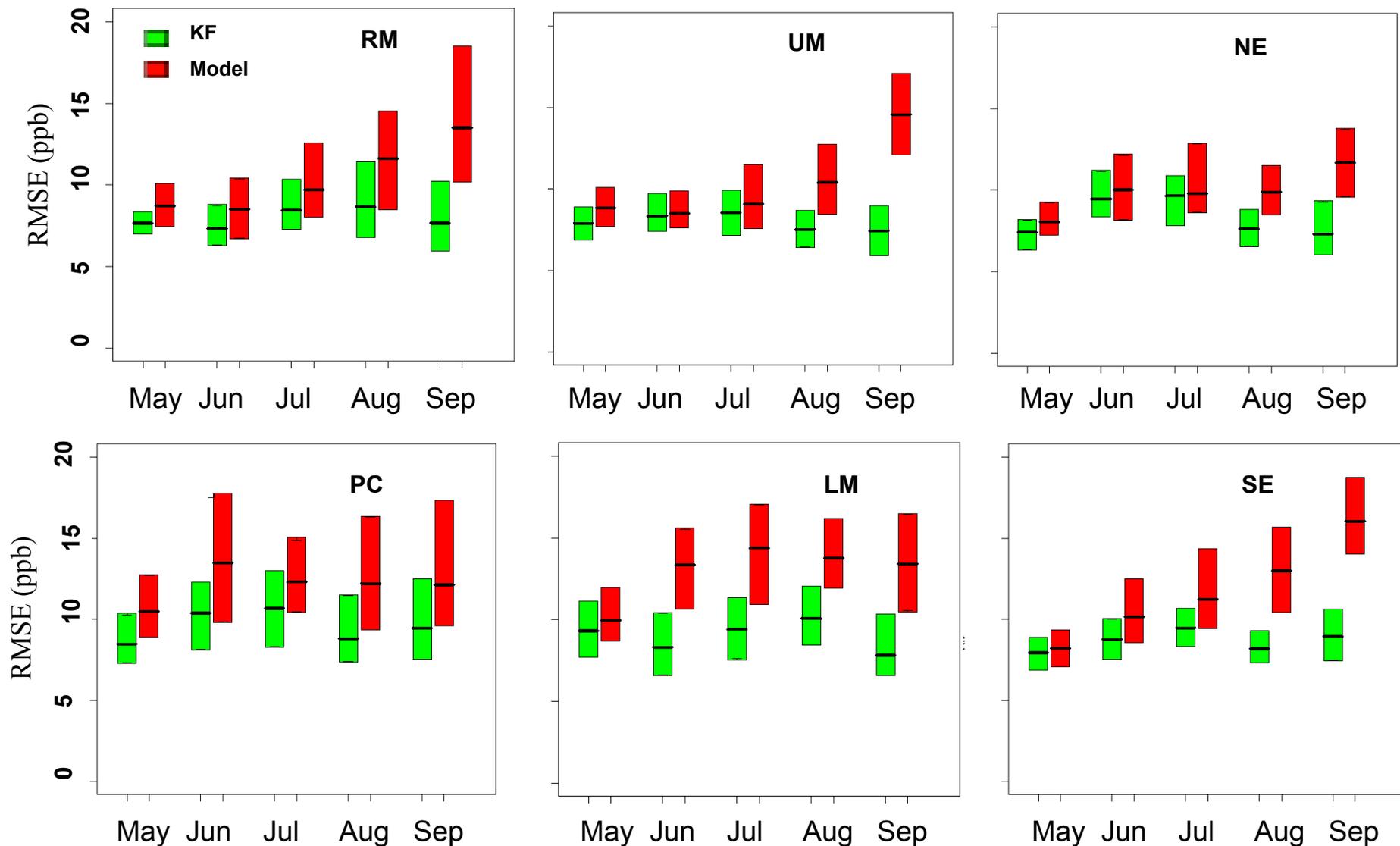


Figure 8. Monthly box plots (only 25<sup>th</sup> and 75<sup>th</sup> percentiles and median values are shown) of RMSE values of the daily maximum 8-h O<sub>3</sub> (ppb) for the raw model and KF bias-adjusted forecasts for all sub-regions

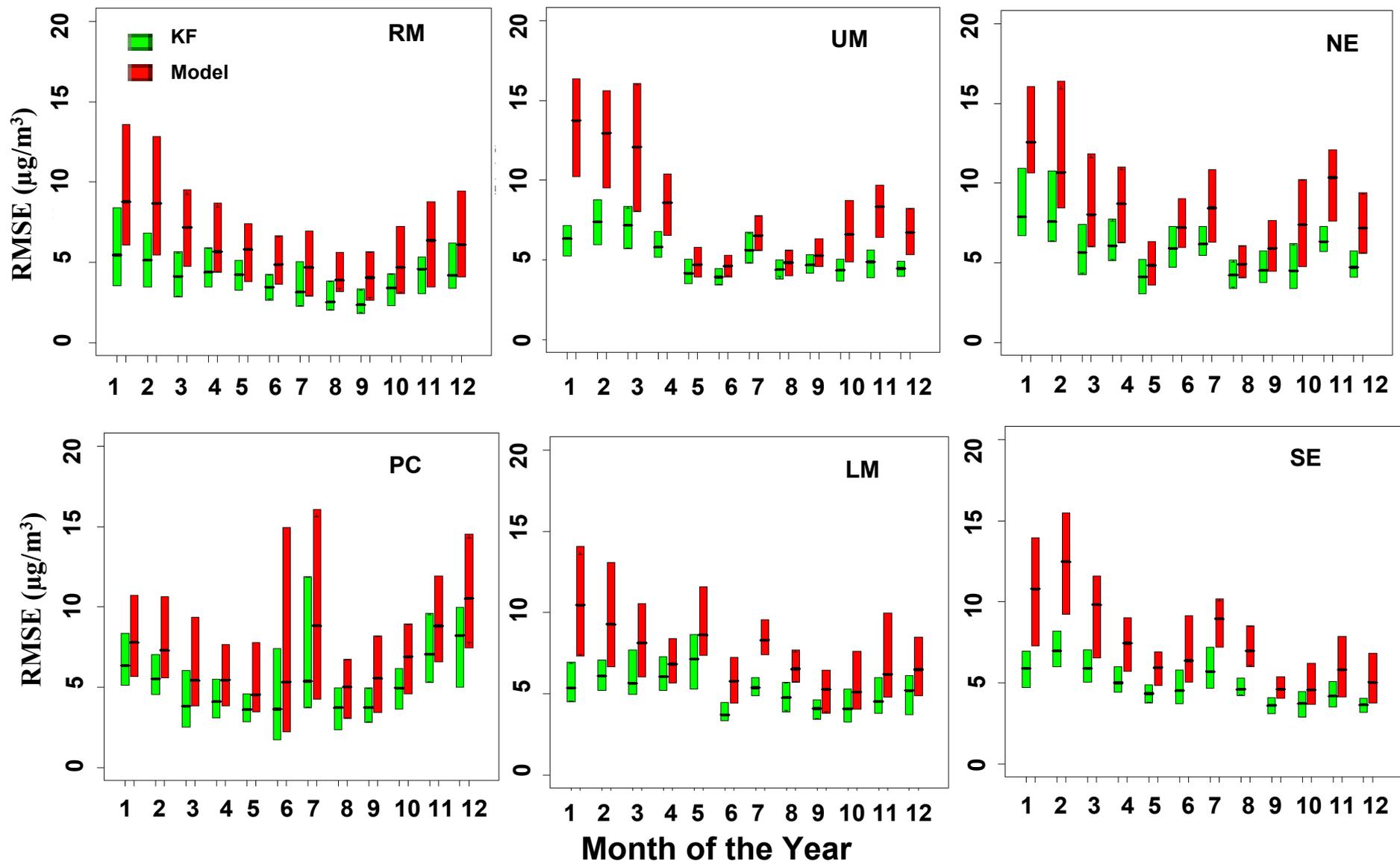


Figure 9. Monthly box plots (only 25<sup>th</sup> and 75<sup>th</sup> percentiles and median values are shown) of RMSE values of the daily mean PM<sub>2.5</sub> ( $\mu\text{g}/\text{m}^3$ ) for the raw model and KF bias-adjusted forecasts for all sub-regions

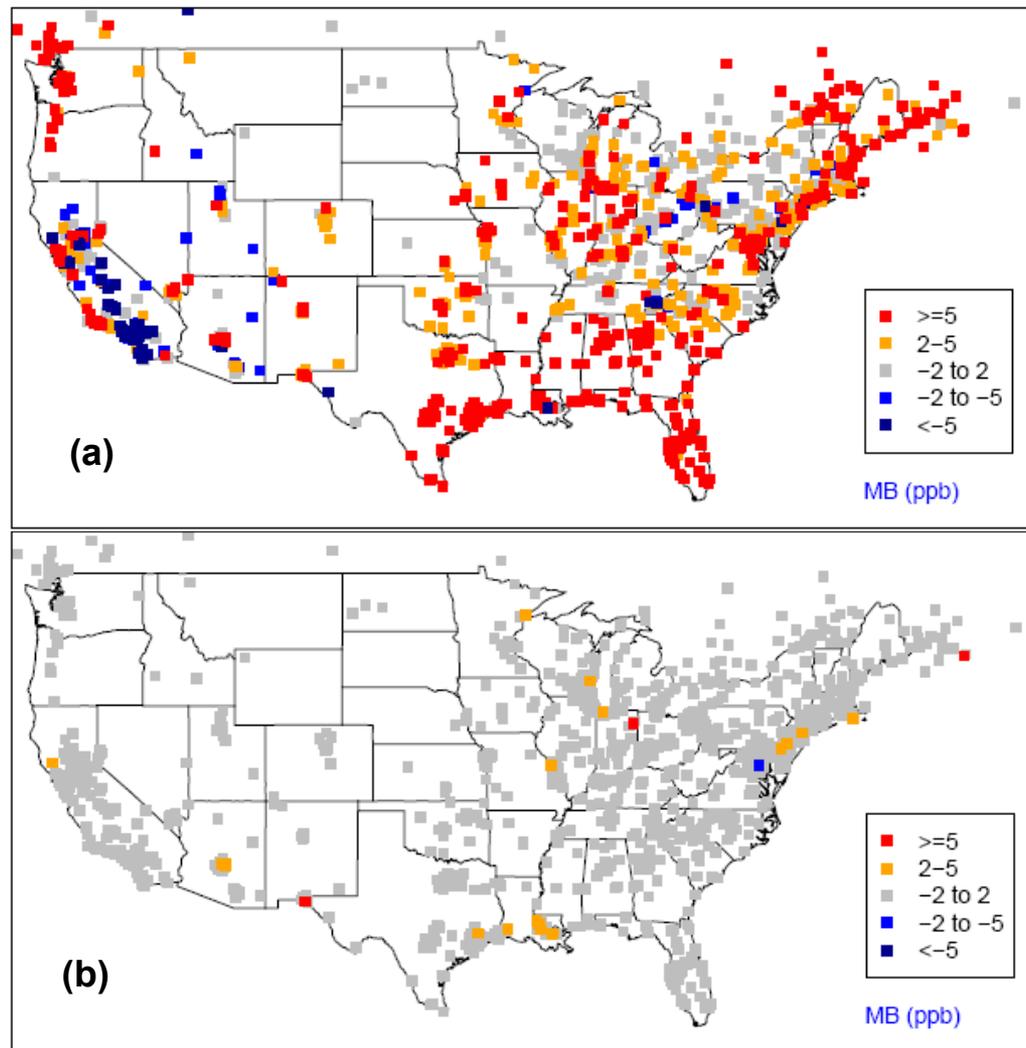


Figure 10. Mean Bias (MB, ppb) for daily maximum 8-h O<sub>3</sub> forecasts at each location within the continental U.S. domain: (a) raw model, (b) KF bias-adjustment

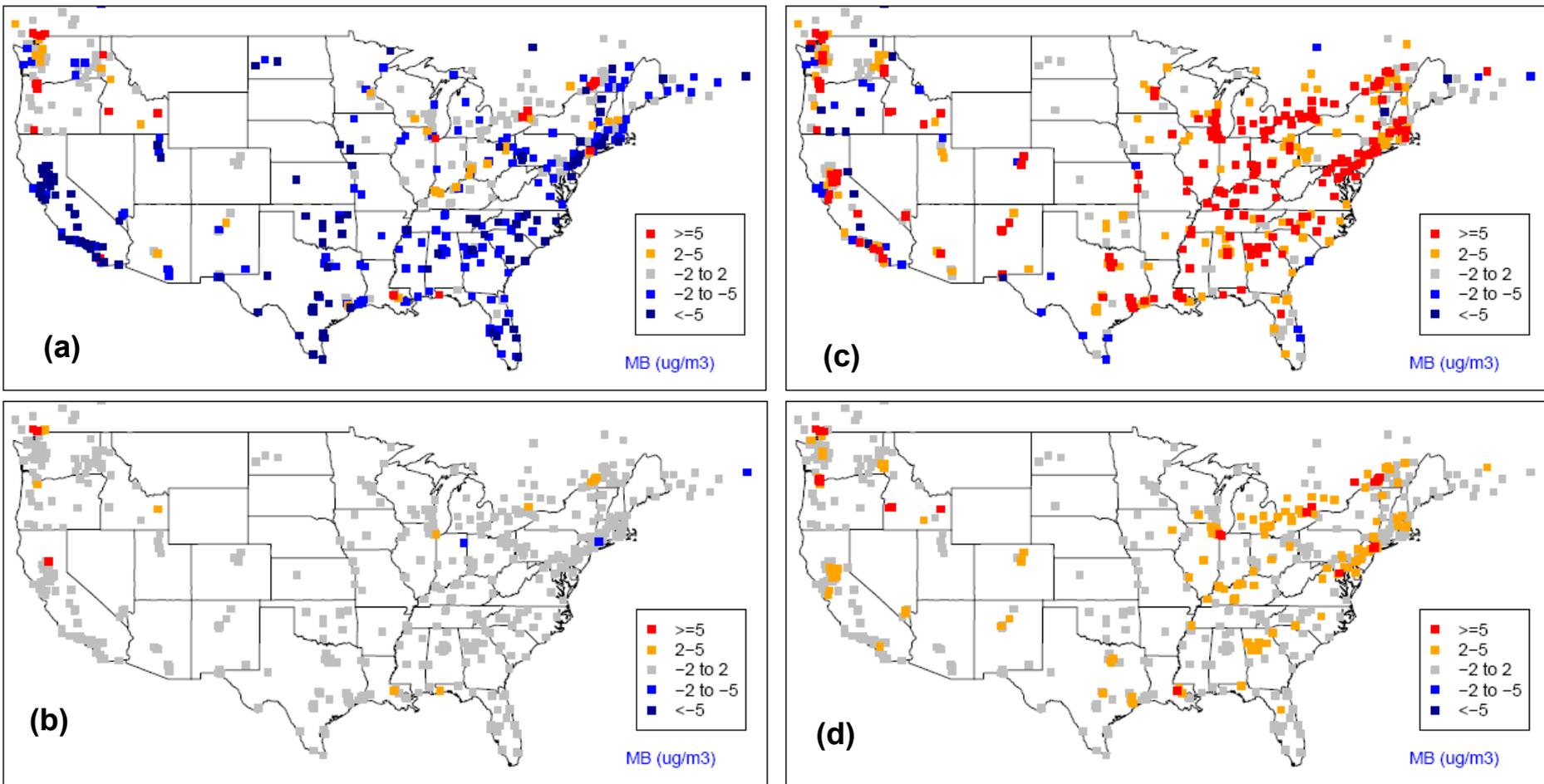


Figure 11. Mean Bias (MB,  $\mu\text{g}/\text{m}^3$ ) for daily mean  $PM_{2.5}$  forecasts at each location within the continental U.S. domain: (a) raw model during warm season, (b) KF bias-adjustment during warm season, (c) raw model during cold season, (d) KF bias-adjustment during cold season

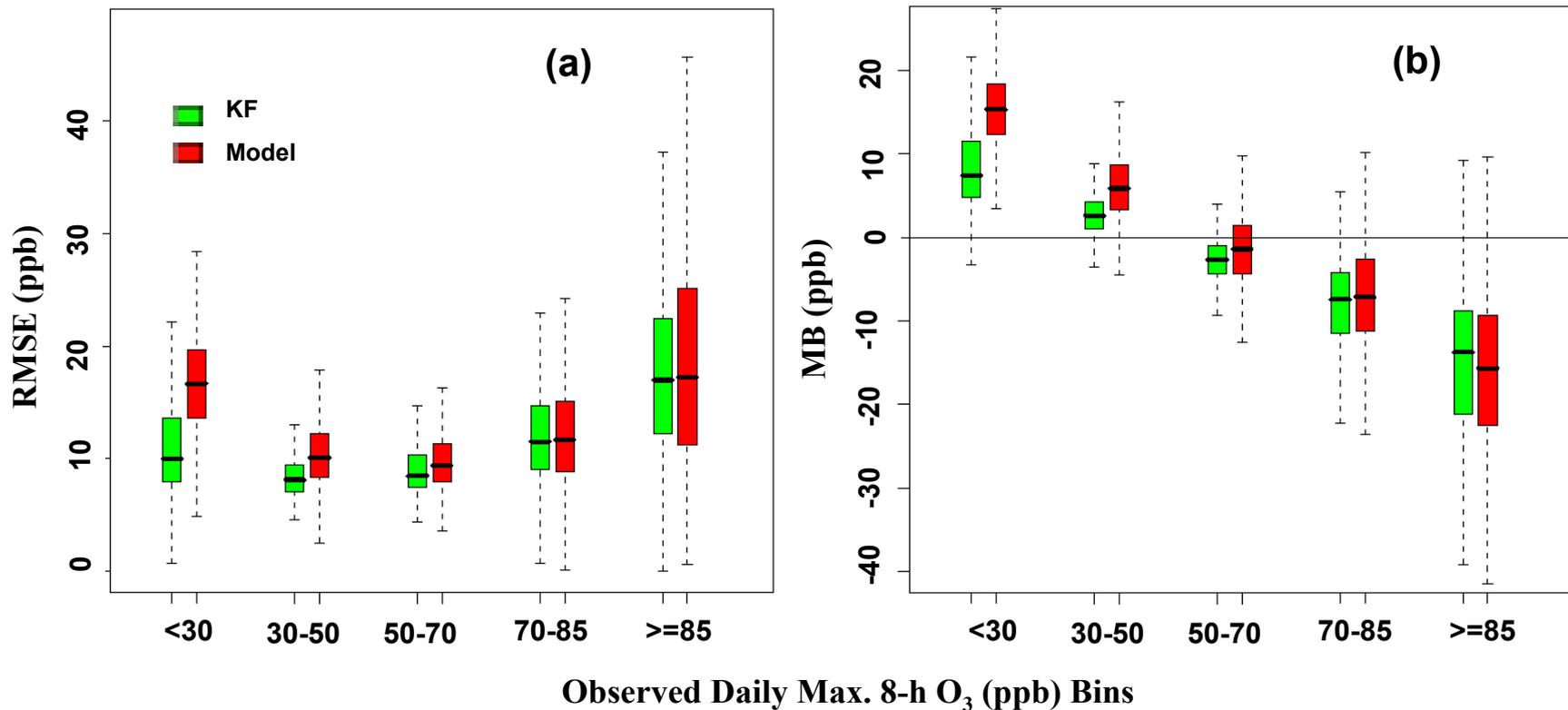


Figure 12. RMSE and MB values over observed daily maximum 8-h O<sub>3</sub> mixing ratio bins for the raw model forecasts and Kalman filter bias-adjusted forecasts over the domain: (a) RMSE and (b) MB

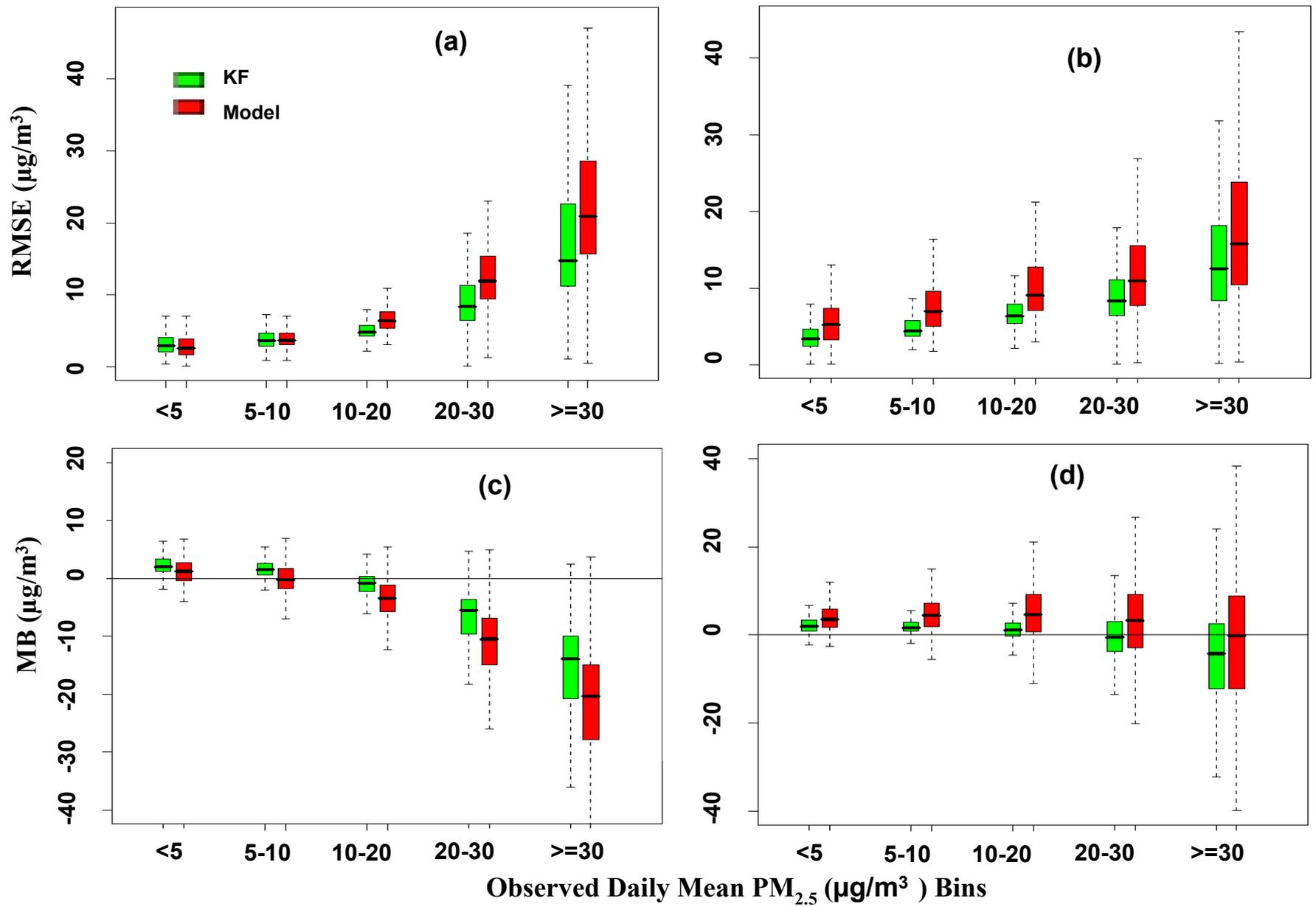


Figure 13. RMSE and MB values over observed daily mean PM<sub>2.5</sub> concentration bins for the raw model forecasts and Kalman filter bias-adjusted forecasts over the domain: (a) RMSE during warm season, (b) RMSE during cool season, (c) MB during warm season, and (d) MB during cool season

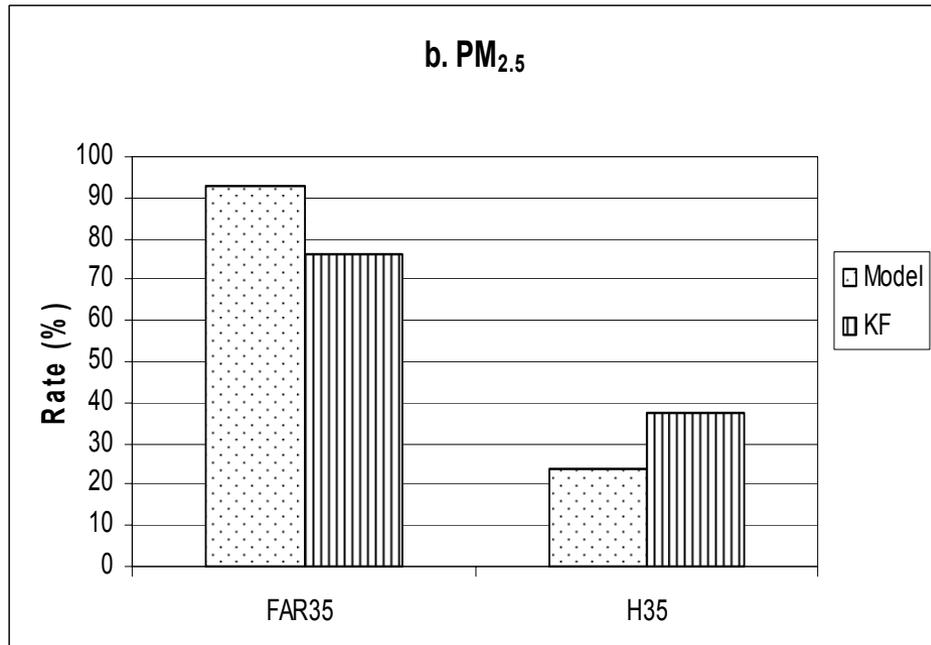
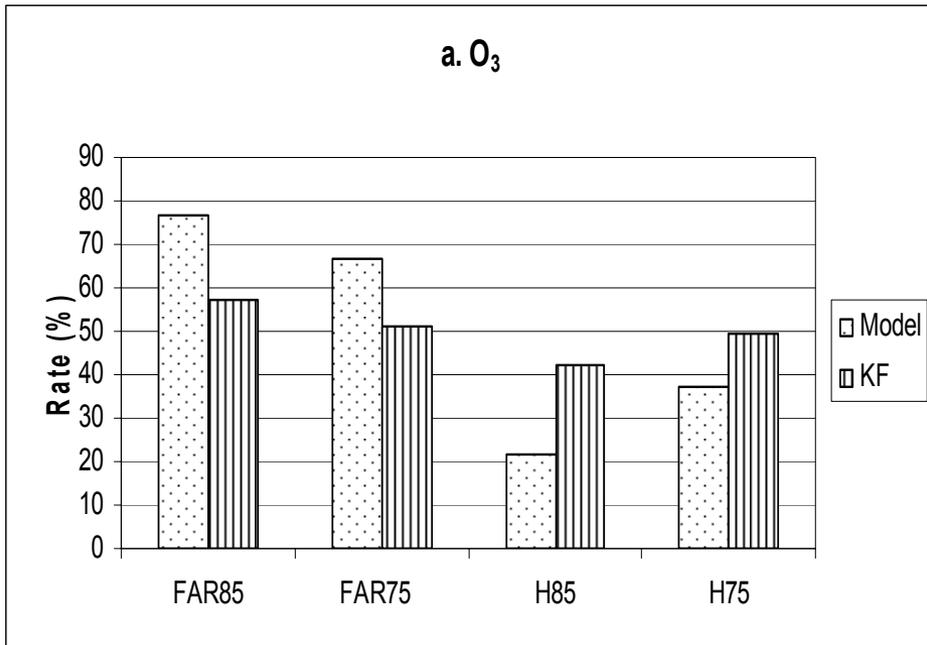


Figure 14. FAR and H values for both raw model and KF forecasts: a. daily maximum 8-h O<sub>3</sub> (ppb), and b. daily mean PM<sub>2.5</sub> (μg/m<sup>3</sup>)

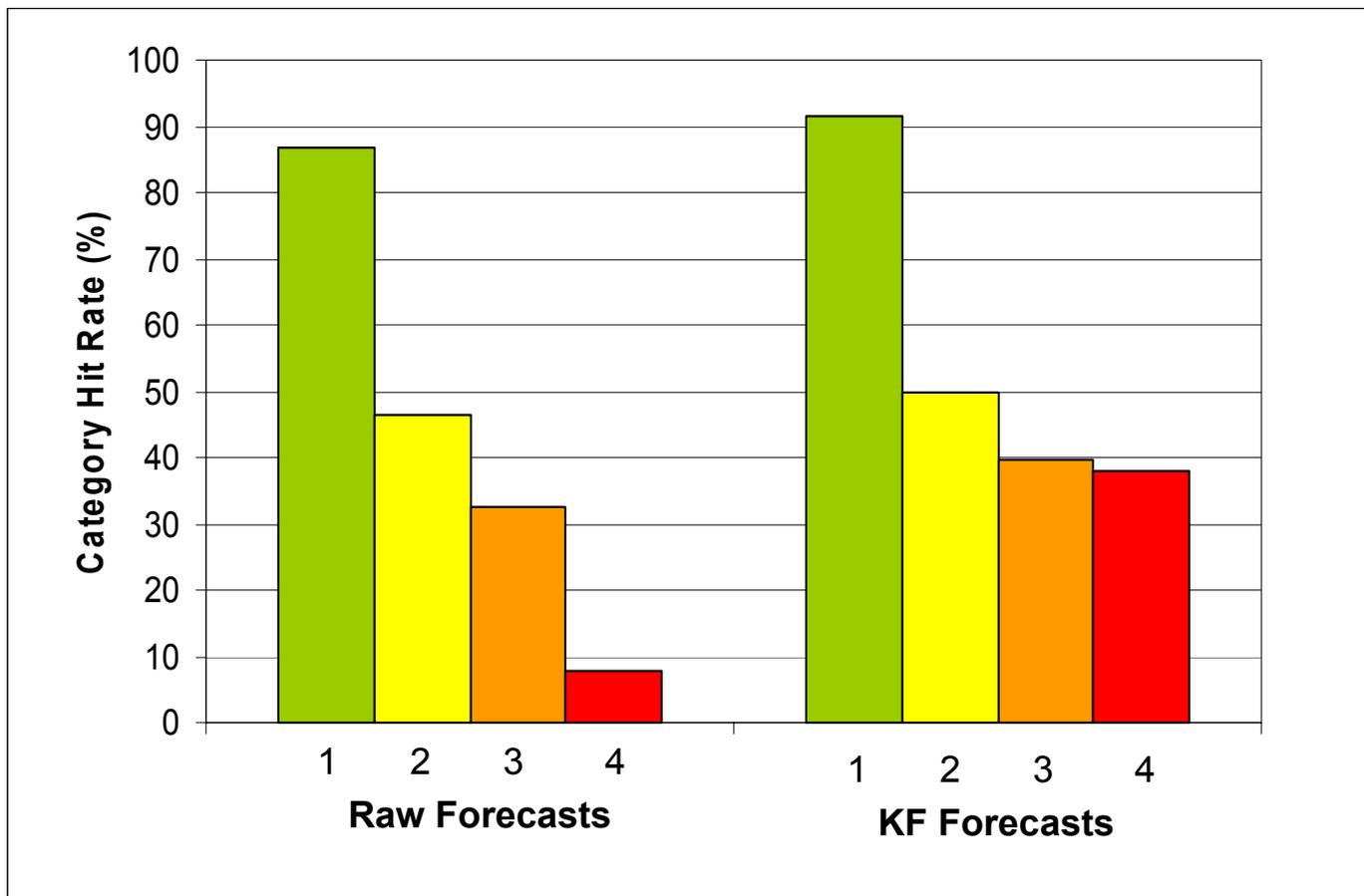


Figure 15. Categorical Hit Rates for each AQI Category for daily maximum 8-hr O<sub>3</sub>

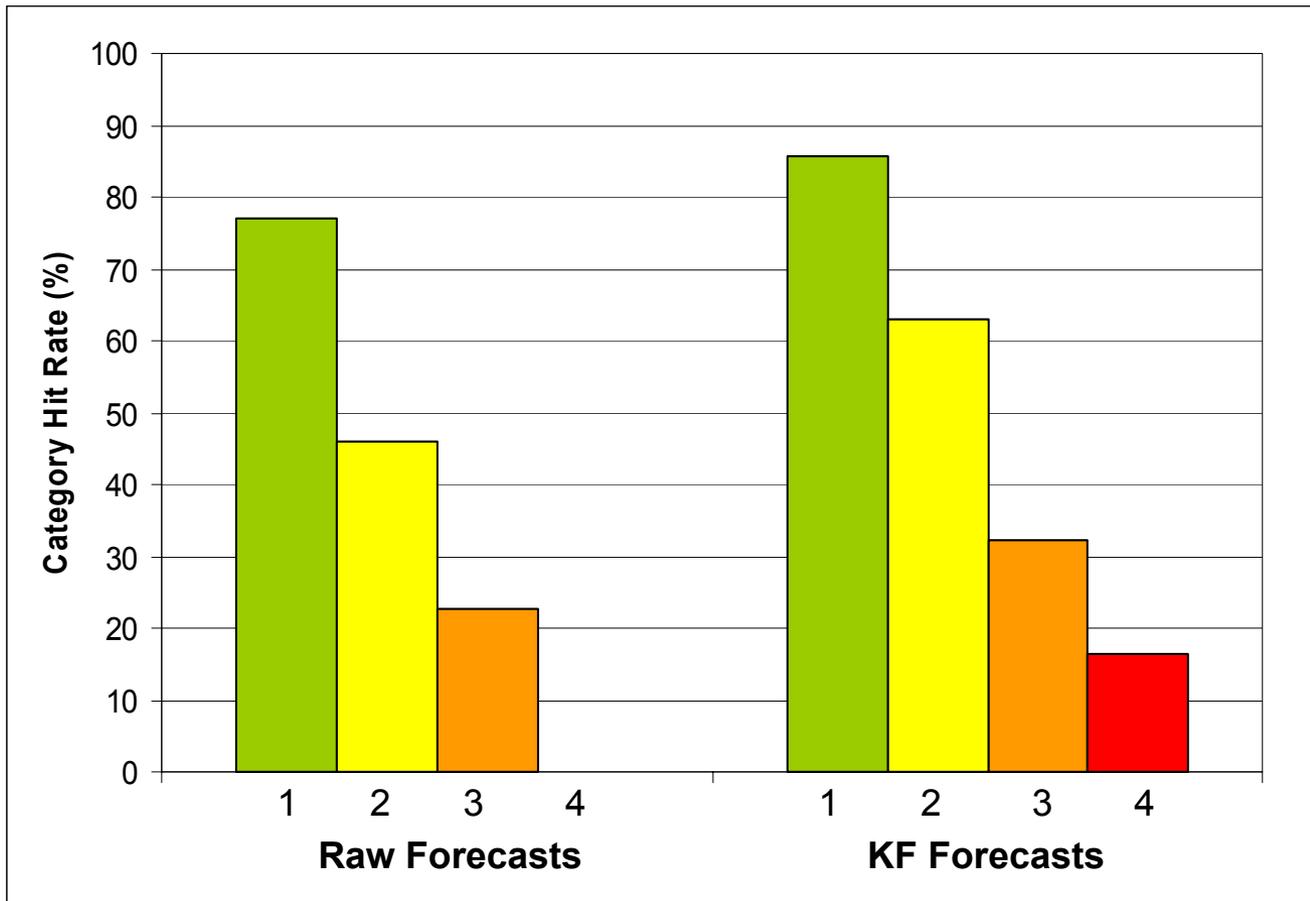


Figure 16. Categorical Hit Rates for each AQI Category for daily mean  $PM_{2.5}$