Provo Maintenance

State Implementation Plan

Photochemical Model Performance Evaluation

Utah Division of Air Quality

1. Introduction

To assess how accurately the photochemical model predicts observed concentrations and to demonstrate that the model can reliably predict the change in pollution levels in response to changes in emissions, a model performance evaluation was conducted. This model performance evaluation also provides support for the model modifications that were implemented (ammonia injection, ammonia surface resistance adjustment, ozone deposition velocity modification, snow albedo change, vertical diffusion modification, cloud water content adjustment and paved road dust emissions adjustment) to more accurately reproduce winter-time inversion episodes. A detailed explanation of these model modifications was provided earlier.

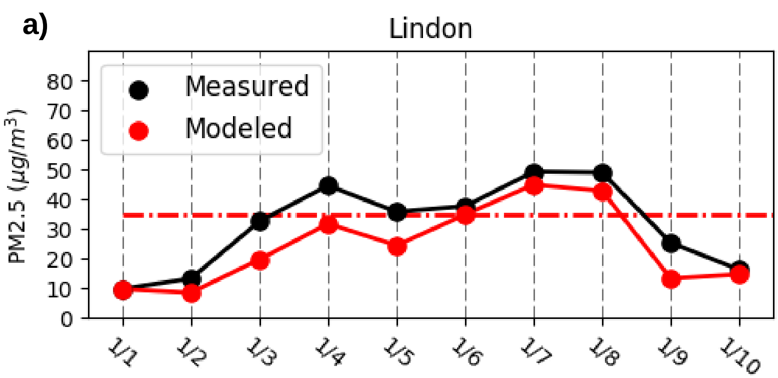
Various statistical metrics and graphical displays were considered for evaluating the model with the objective to determine whether modeled variables are comparable to observations. These included:

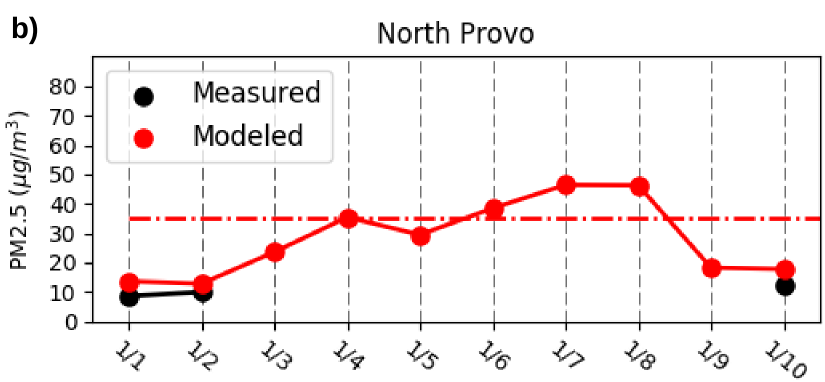
- Time series plots of modeled and observed 24-hr PM2.5 concentrations.
- Scatter plots of modeled and observed 24-hr PM2.5 concentrations.
- Coefficient of determination, R^2, which shows the degree to which modeled and observed 24-hr PM2.5 concentrations are linearly related.
- Pie charts showing modeled and observed PM2.5 chemical species
- Soccer plots with purpose to visualize model performance of both bias and error on a single plot.
- Mean bias, which is a metric that averages the model/observation residual paired in time and space.
- Normalized mean bias, which is a statistic of normalized mean bias to the average observed value.
- Normalized mean error, which is determined by normalizing the mean error by average observation.
- Mean fractional bias, which is determined by normalizing the mean bias by the average of observed and modeled concentrations.
- Mean fractional error, which is determined by normalizing the mean error by the average of observed and modeled concentrations.
- Mean error, which is a performance statistic that averages the absolute value of the model/observation residual paired in time and space.

Available ambient monitoring data were also used for this photochemical model performance evaluation. Data included ozone (O_3), nitrogen oxides (NO, NO2 and NOx where $NOx=NO+NO_2$), carbon monoxide (CO), 24-hr total PM2.5 and 24-hr chemically-speciated PM2.5 measurements collected at monitoring stations in the Provo non-attainment area. Ammonia measurements collected during a special field study carried out in winter of 2017 were also used for this performance evaluation. These measurements were used since measurements of ammonia were not available during 2011. The evaluation was based on the December 31-January 10 2011 episode and the 2011 emissions inventory was used as input data for the model simulations. The evaluation focused on days with PM2.5 concentration exceeding the 24-hr national ambient air quality standard (> 35 µg/m^3). Results for December 31, which is a model spin-up day, are excluded from this evaluation.

2. Daily PM2.5 Concentrations

Figure 1a-c shows 24-hr modeled and observed PM2.5 concentration during January 1-10 2011 at all monitoring stations in the Provo non-attainment area where 24-hr filter PM2.5 data is available. The model overall captures well the temporal variation in PM2.5 at all monitoring stations. The gradual increase in PM2.5 concentration and its transition back to low levels are generally well reproduced by the model. Moreover, with the exception of January 3-5, the bias between measured and modeled $PM_{2.5}$ is overall relatively small, particularly on peak $PM_{2.5}$ exceedance days. The large bias on January 3-5 can be mainly related to the meteorological model performance on these days, when jet wind speeds were overestimated in the WRF model[1].





[1] https://documents.deq.utah.gov/air-quality/planning/technical-analysis/research/model-improvements/3-wintertime-episodes/DAQ-2017-014342.pdf

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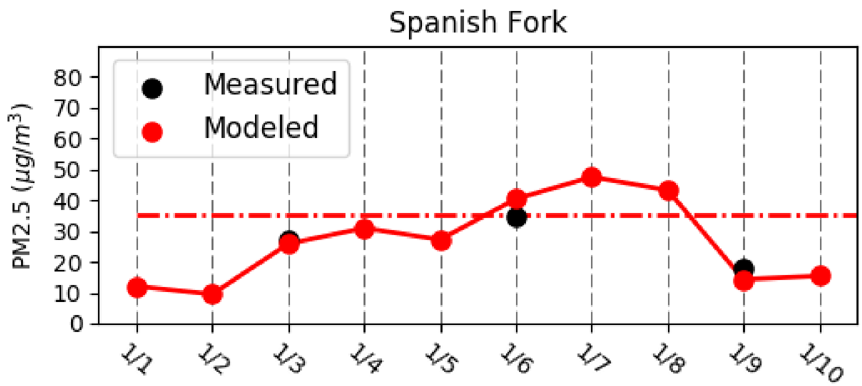

Figure 1a-c. Time series of 24-hr PM2.5 during January 1-10 2011 at Lindon, North Provo and Spanish Fork monitoring sites in the Provo non-attainment area.

3. PM2.5 Chemical Speciation

To further investigate the photochemical model performance, measured and modeled PM2.5 chemical species were compared at Lindon monitoring site, which is part of EPA's Chemical Speciation Network (CSN). Figures 2a-b and 3a-b show a comparison of the bulk chemical composition of measured and modeled PM2.5 at Lindon monitoring station on January 3, 7 and 9 2011, which correspond to days when measurement data are available and both modeled and measured PM2.5 were either above or below 35 ug/m3. Chemical species, including nitrate (NO3), sulfate (SO4), ammonium (NH4), organic carbon (OC), elemental carbon (EC), chloride (Cl), sodium (Na), crustal material (CM) and other species (other mass), were considered in this analysis.

On PM2.5 non-exceedance days (days when PM2.5 measured and modeled were both below 35 ug/m3) (Figures 2a-b), the model underestimated nitrate and ammonium by about 5.1 and 1.8 ug/m3, respectively. On the other hand, the model performance for sulfate and OC was very good. Measured and modeled concentrations of sulfate were in very close agreement, both accounting for about 1 ug/m3 of PM2.5. Measured and modeled OC concentrations were also quite comparable, contributing to 2.2 and 2.3 ug/m3 of PM2.5, respectively. The model also overall overestimated crustal material and EC. This overprediction may be related to an overestimation in source emissions. Chloride, on the other hand, was biased low in the model.

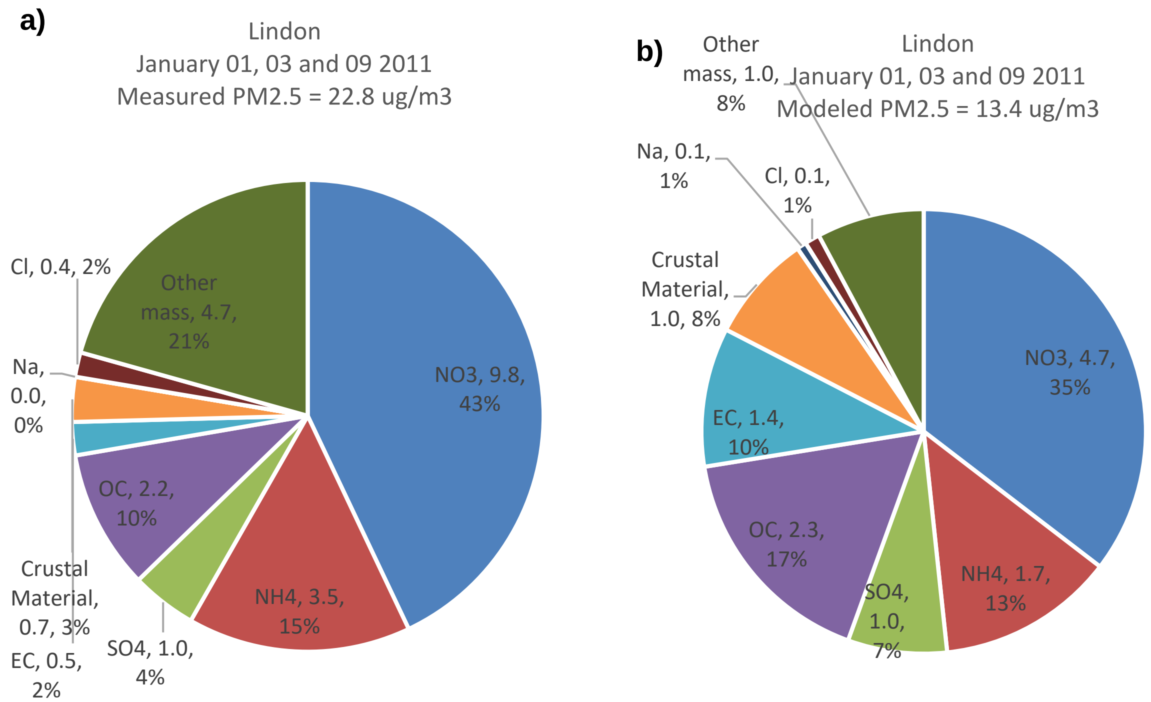

Figure 2a-b. Average a) measured and b) modeled chemical composition of 24-hr PM2.5 in ug/m3 and percent of PM2.5 at Lindon monitoring station over January 1, 3 and 9 2011.

On January 7, which corresponds to a PM2.5 exceedance day, the photochemical model performance was generally better. The model performance for particulate nitrate, which is the major component of PM2.5, was good, with both modeled and measured NO3 accounting for similar contributions to PM2.5 filter mass. Modeled and observed nitrate concentrations were also in close agreement, accounting for 22.6 and 23.5 ug/m3 of PM2.5 mass. The model, on the other hand, was biased low for ammonium by about 41%. The underestimation in modeled ammonium can be related to an underestimation in modeled hydrochloric acid (HCl). Modeled HCl was underestimated in the model, possibly resulting in an underestimation in ammonium chloride in the model. A previous source apportionment analysis showed that ammonium chloride accounts for 10-15% of total PM2.5 mass along the Wasatch Front during high wintertime PM2.5 pollution episodes[2]. Modeled HCl levels were underpredicted in the model. Values as high as 8 ppb were observed over Utah county during the 2017 Utah Winter Fine Particulate Study (UWFPS)[3](Figure 6) while maximum hourly values of about 0.14 and 0.35 ppb were modeled over Utah county (Figures 4 and 5) on modeled non-exceedance and exceedance days.

[2] Kerry E. Kelly, Robert Kotchenruther, Roman Kuprov & Geoffrey D. Silcox (2013) Receptor model source attributions for Utah's Salt Lake City airshed and the impacts of wintertime secondary ammonium nitrate and ammonium chloride aerosol, Journal of the Air & Waste Management Association, 63:5, 575-590.

[3] https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf.

The model performance for particulate sulfate was good, with sulfate being biased low in the model by about 20%. The model performance for organic carbon was also reasonably good for January 7, with modeled and observed concentrations contributing to 4.3 and 5.6 ug/m3 of PM2.5 mass. The model, on the other hand, was biased high for EC and CM by about 21 and 72%, respectively.

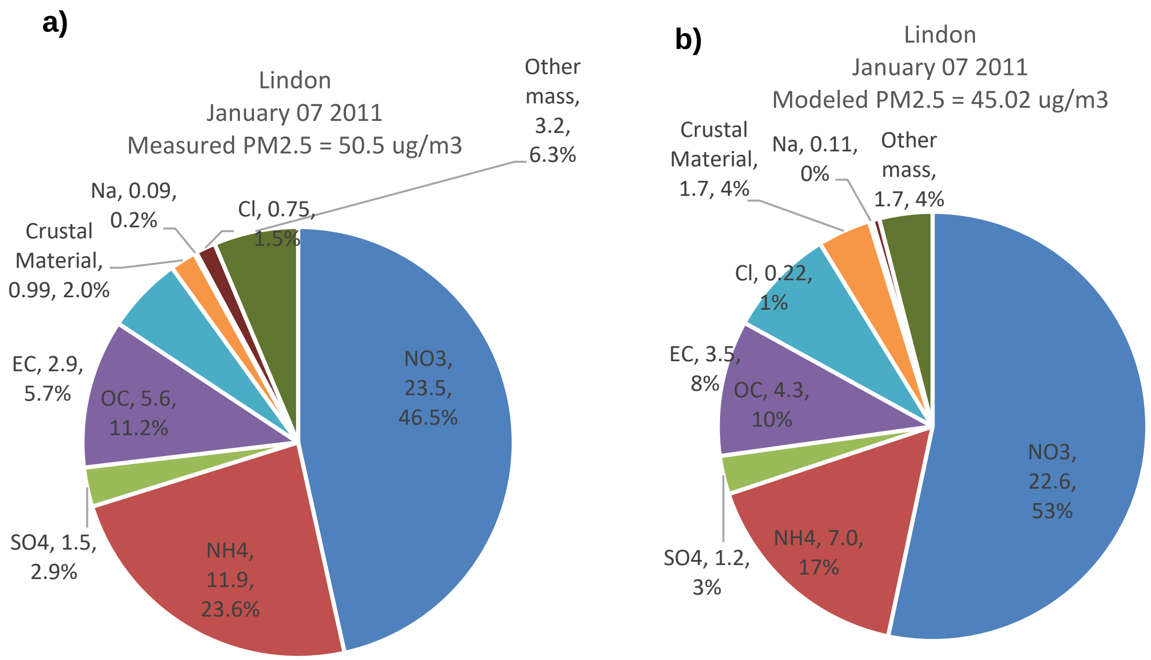

Figure 3a-b. a) Measured and b) modeled chemical composition of 24-hr PM2.5 in ug/m3 and percent of PM2.5 at Lindon monitoring station on January 7 2011.

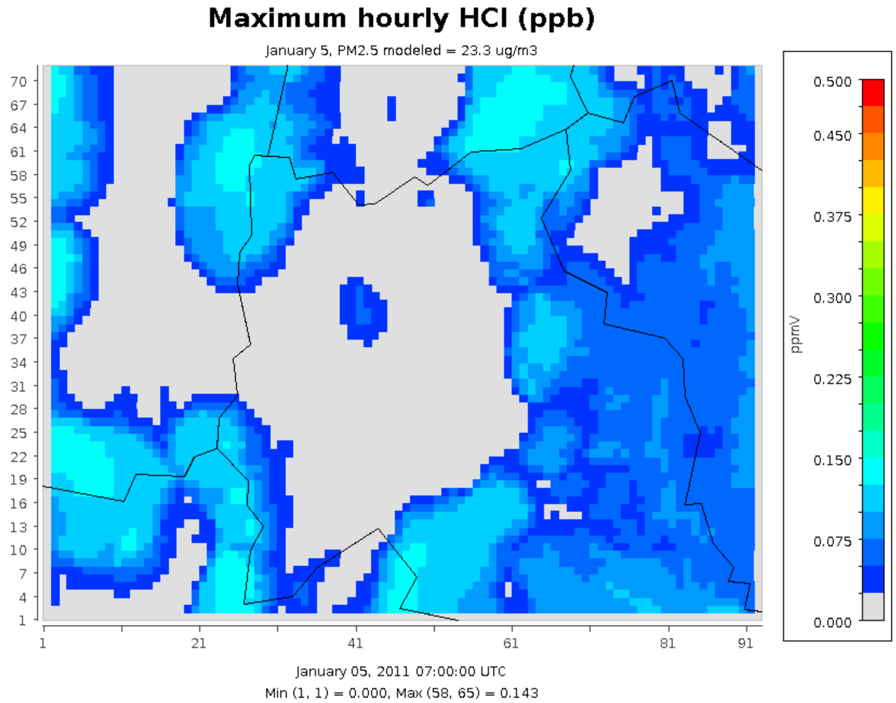

Figure 4. Spatial distribution of maximum hourly HCl concentrations (in ppb) over Utah county on January 7 2011. The latter represents a typical exceedance day.

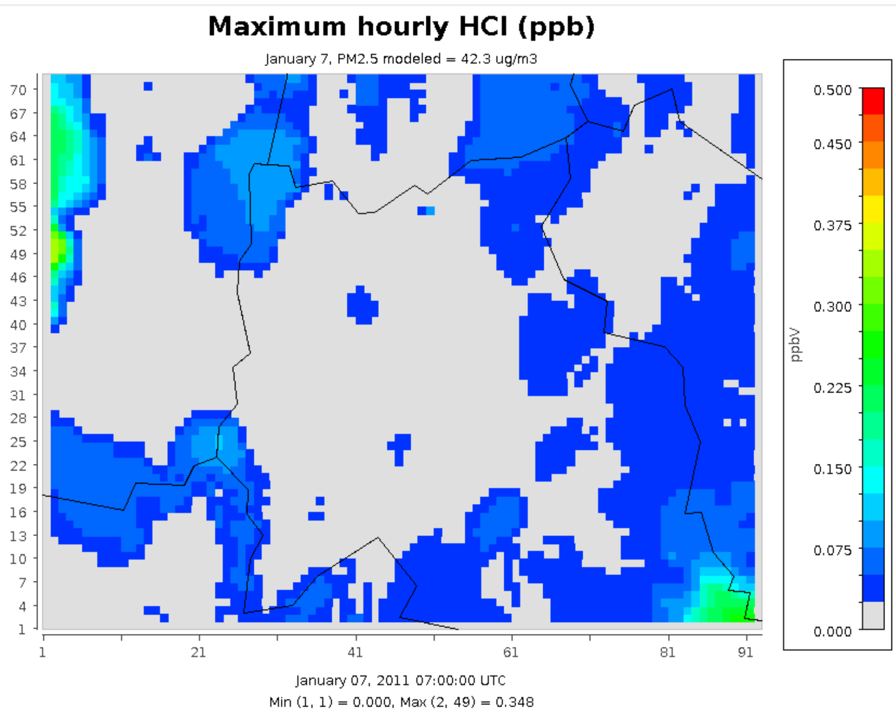

Figure 5. Spatial distribution of maximum hourly HCl concentrations (in ppb) over Utah county on January 7 2011. The latter represents a typical exceedance day.

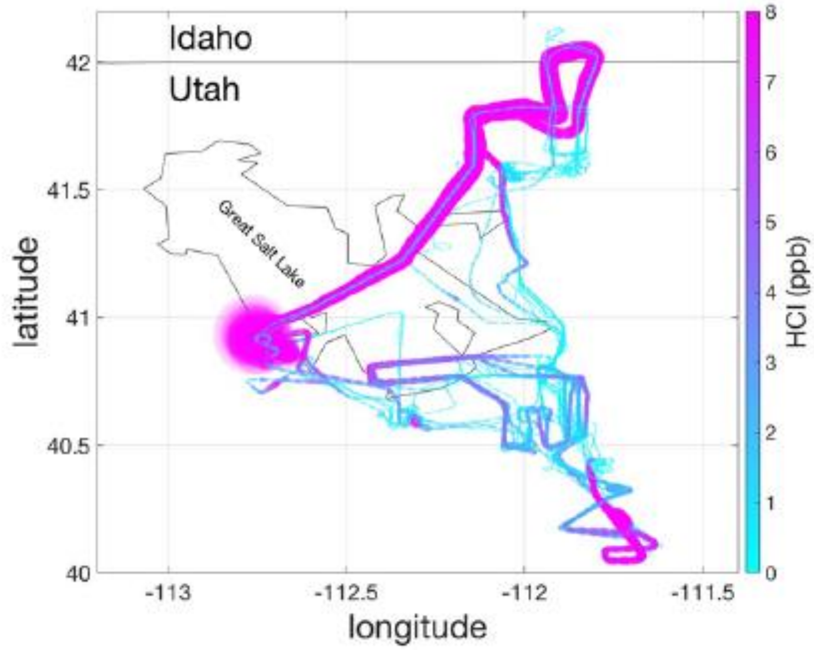

Figure 6. Spatial distribution of HCl during the 2017 Utah Winter Fine Particulate Study. Figure retrieved from the 2017 Utah Winter Fine Particulate Study, final report, Figure 3.44 (https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf).

4. Hourly Ambient Gaseous Compounds

The model performance was also evaluated for gaseous compounds, particularly precursor species to PM2.5 formation. Gaseous compounds considered in this analysis include carbon monoxide (CO), nitrogen oxides (NO, NO2, and NOx defined as NO+NO2)), ozone (O3) and ammonia (NH3). Model outputs were compared to measurements collected at North Provo station during January 1-10 2011. 2011 measurements are not available for the Lindon monitoring station.

The model performance was evaluated for CO by comparing modeled and measured hourly CO concentrations during January 1-10 2011 (Figure 7). Modeled CO was overall underestimated during nighttime hours (12 am – 6 am), particularly during January 4-10 2011, which may be related to overmixing vertically.

A comparison of modeled and measured nitrogen oxides (NO, NO2 and NOx, Figures 8-10) and ozone (Figure 11) shows that modeled NO, NO2 and NOx are overall underestimated and ozone is overestimated during overnight hours (12 am – 6 am). The overprediction in ozone is likely a result of reduced ozone titration due to a lack of nightly modeled NOx, which may be related to overmixing vertically and/or underestimation of nighttime NOx emissions. During daytime hours, ozone and NOx concentrations were generally better reproduced.

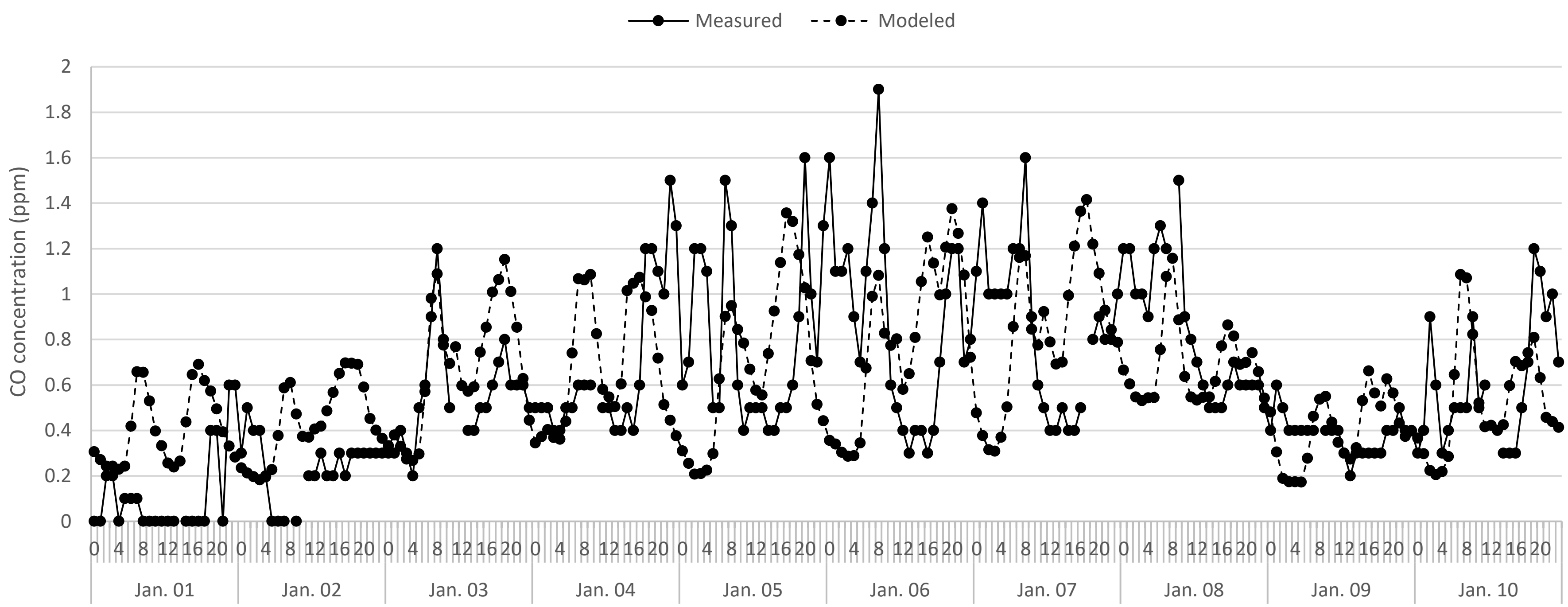

Figure 7. Modeled and measured CO concentration during January 1-10 2011 at North Provo monitoring station in the Provo NAA.

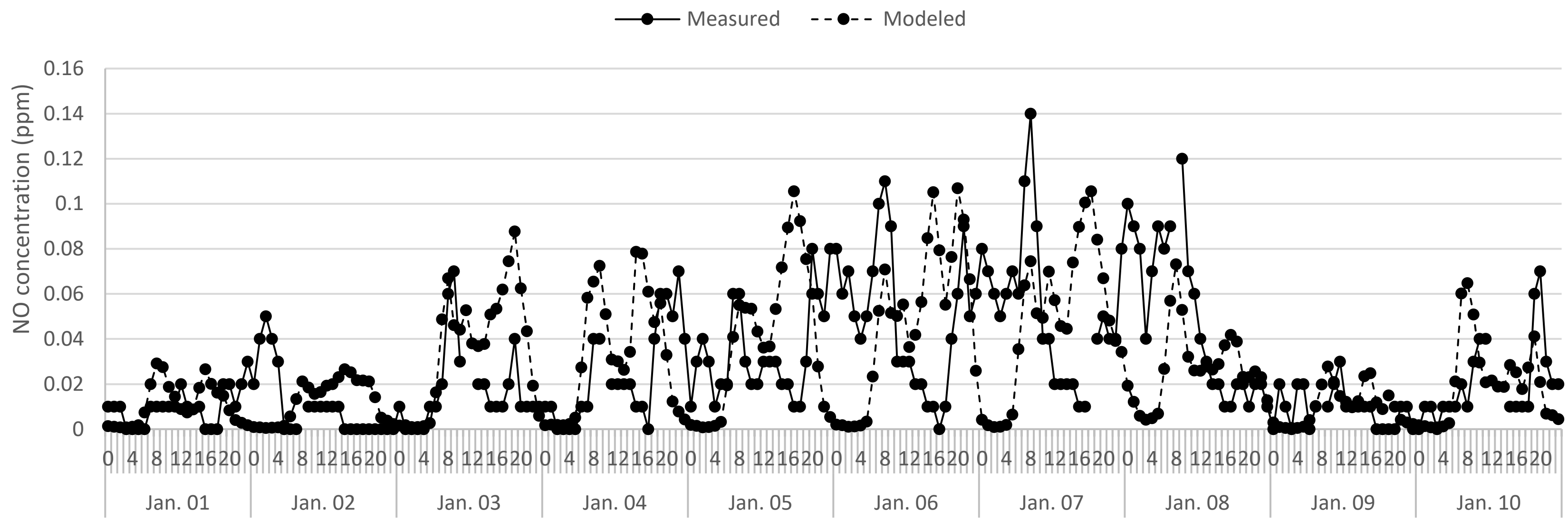

Figure 8. Time series of NO concentration during January 1-10 2011 at North Provo monitoring station in the Provo NAA.

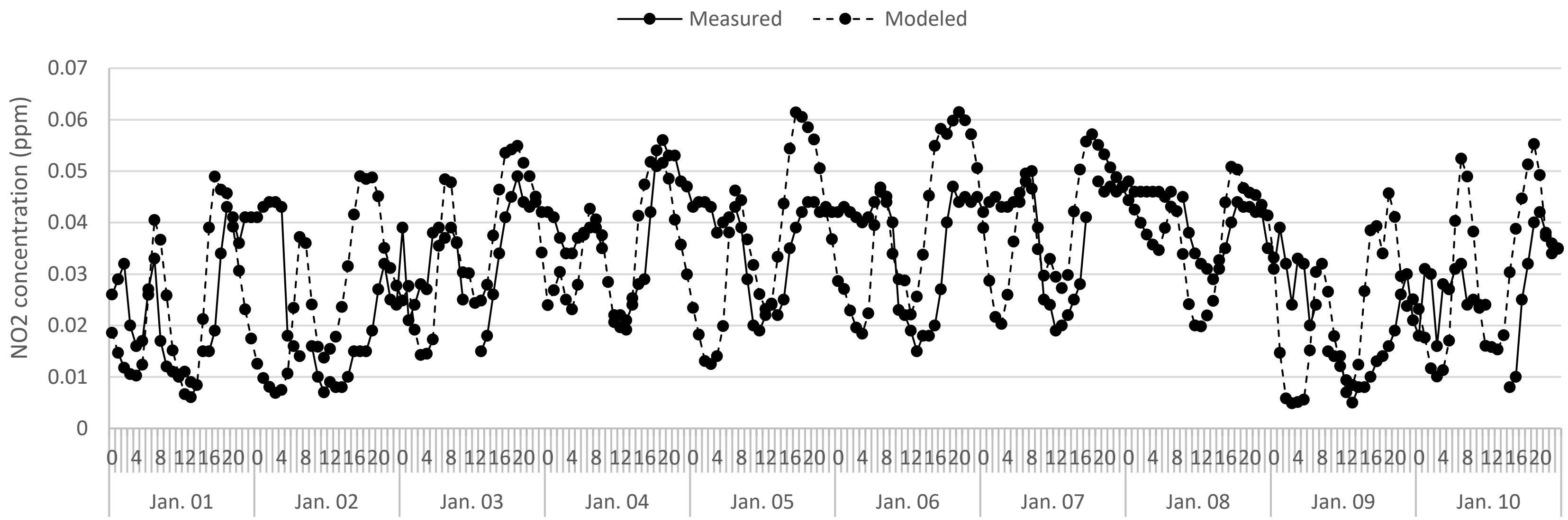

Figure 9. Time series of NO2 concentration during January 1-10 2011 at North Provo monitoring station in the Provo NAA.

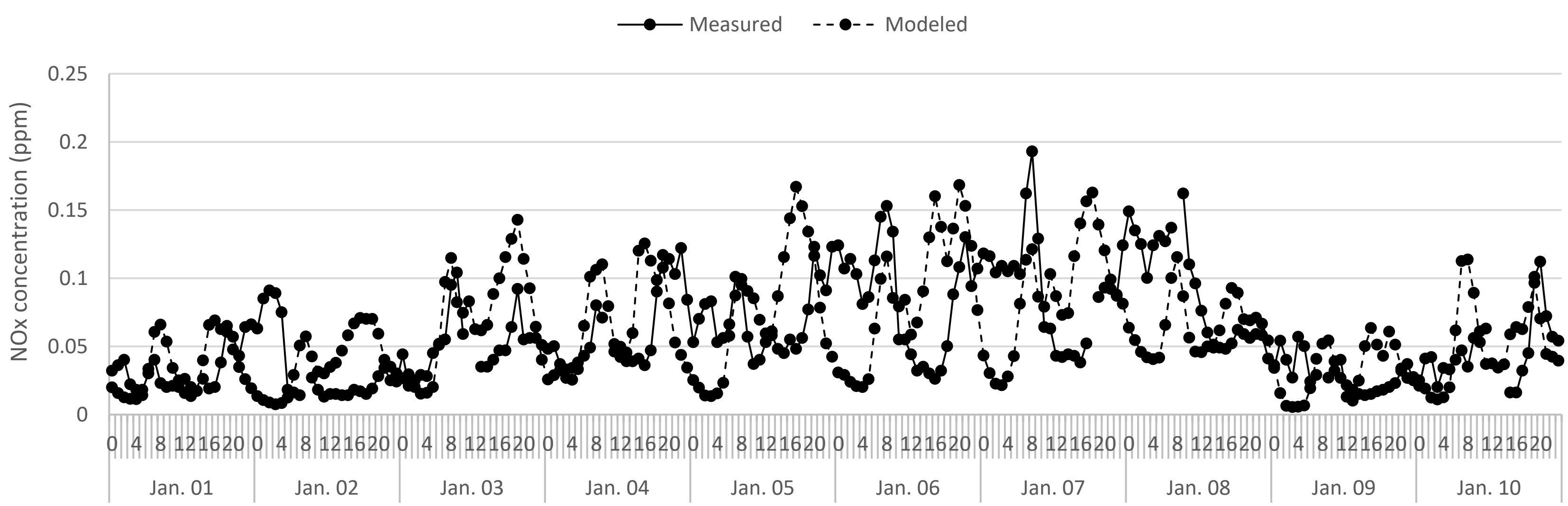

Figure 10. Time series of NOx concentration during January 1-10 2011 at North Provo monitoring station in the Provo NAA.

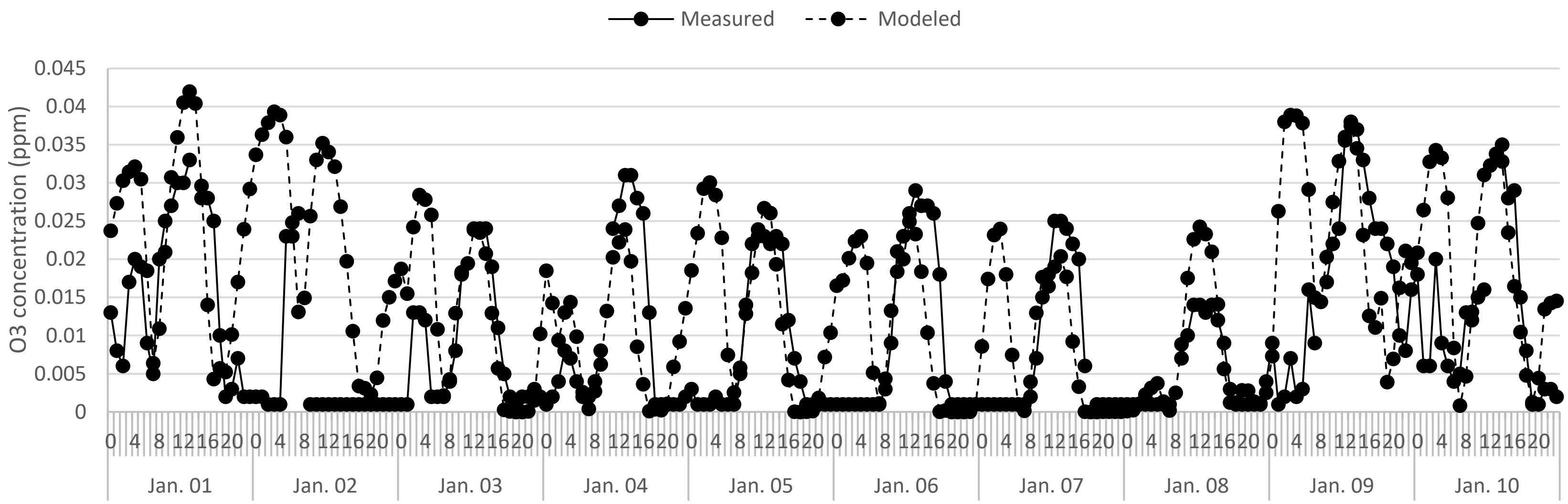

Figure 11. Time series of O3 concentration during January 1-10 2011 at North Provo monitoring station in the Provo NAA.

The model performance was also evaluated for ammonia (NH_3), which is an important precursor to the formation of ammonium nitrate, ammonium sulfate and ammonium chloride, all of which are important $PM_{2.5}$ species accounting for over 50% of the $PM_{2.5}$ mass during winter-time inversion events.

Hourly modeled ammonia (Figure 12) at North Provo was compared to near-surface ammonia measurements (Figure 13) conducted during a special field study in winter 2017 (2017 Utah Winter Fine Particulate Study (UWFPS)[4]), where ammonia near the surface was measured during missed approaches at an airport in Provo. Measurements from 2017 were considered since measurements of ammonia were not available during 2011. However, while these 2017 field study measurements cannot be directly compared to day-specific 2011 model simulations, the measurements are qualitatively useful to assess if the model predicts similar levels of ammonia during strong inversion conditions. A comparison of measured and modeled ammonia shows that modeled ammonia at the Provo site is well within the range observed in 2017. Modeled NH3 concentrations were mostly in the range of 3 to 12 ppb during peak PM2.5 exceedance days (January 7-8 2011), which is similar to the measured NH3 concentrations during the inversion episode of January 28-30 2017.

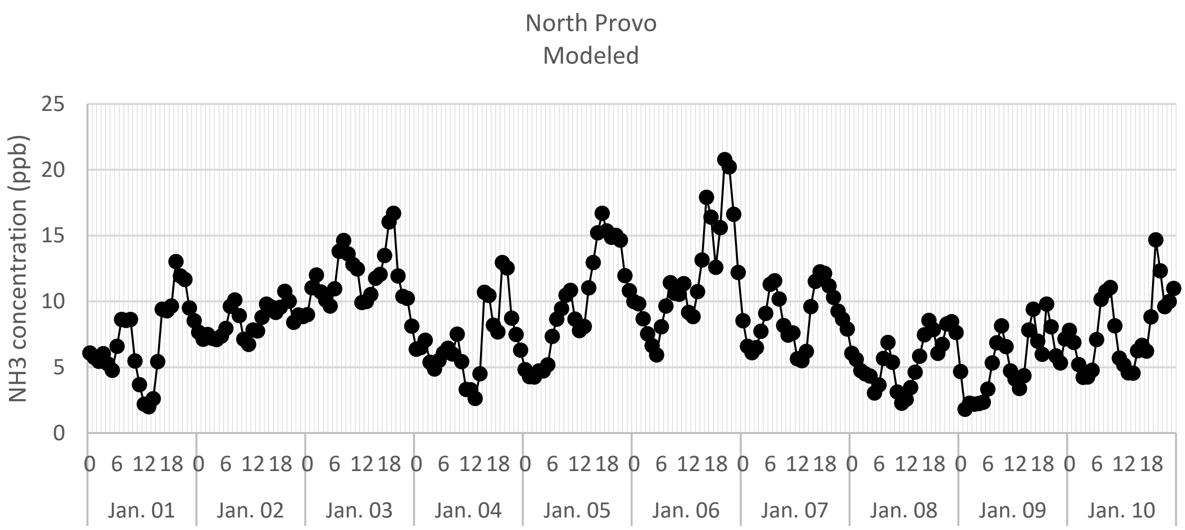

Figure 12. Hourly time series of modeled ammonia (ppb) at North Provo monitoring site during January 1 – 10 2011.

[4] https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf.

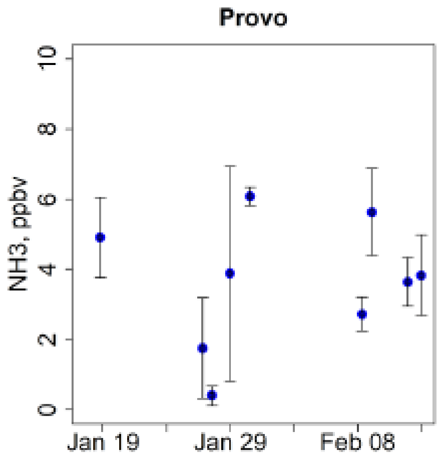

Figure 13. Ammonia mixing ratios during missed approaches at Provo airport in the Utah Valley.Figure retrieved from the 2017 Utah Winter Fine Particulate Study, final report, Figure 3.40 (https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf).

5. Model Performance Evaluation Metrics

The model performance was further evaluated by examining various bias and error metrics. These were developed according to Boylan et al. 2008[5] and are discussed in "Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze" (EPA, April 2007). Chemical speciation data collected at the Lindon monitoring station on January 1, 3, 5, 7 and 9 2011 was considered for this analysis. Speciation data for other days is not available.

Soccer plots were first considered for the model performance evaluation, where two thresholds of +/-30% and +/-60% were considered for the normalized mean bias and fractional mean bias evaluation (Figure 14). As can be seen, the model performance was generally good for nitrate and sulfate and weaker for the other species, particularly crustal material and OC.

[5] James W. Boylan, Armistead G. Russell (2006) PM and light extinction model performance metrics, goals, and criteria for three-dimensional air quality models, Atmospheric Environment 40 (2006) 4946–4959, doi:10.1016/j.atmosenv.2005.09.087

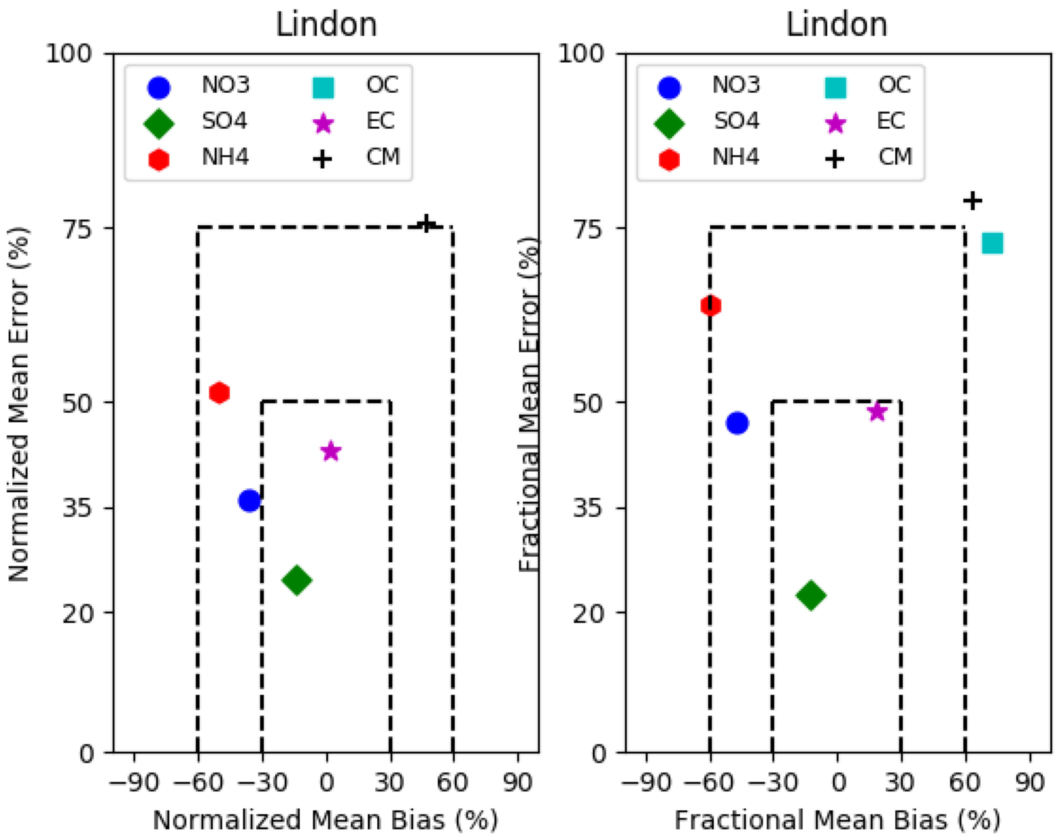

Figure 14. Soccer plot depicting modeled PM2.5 species performance for four days during the modeling episode when speciated PM2.5 filter data was available at Lindon monitoring site.

Model performance was further evaluated by examining various model performance metrics for PM2.5 species at the Lindon monitoring site during the January 2011 modeling episode (Table 1). As can be seen, the model was biased low for secondary nitrate and ammonium while it was biased high for OC. Model bias for crustal material (FCRS) and sulfate was low.

Table 1. Model performance statistics for two days during the modeling episode when speciated PM2.5 filter data was available at Lindon monitoring site.

PM2.5 Species	Mean (obs) ug/m3	Mean (modeled) ug/m3	Mean Bias ug/m3	Mean Error ug/m3	Normalized Mean Bias	Normalized Mean Error	Mean Fractional Bias	Mean Fractional Error
FCRS	0.766	1.125	0.359	0.579	46.908	75.664	63.904	78.885
OC	2.328	5.138	2.81	2.81	120.689	120.689	72.789	72.789
PEC	1.308	1.329	0.022	0.563	1.649	43.055	18.75	48.793
PNH4	6.012	2.962	-3.05	3.089	-50.726	51.384	-59.274	63.936
PNO3	14.053	9.006	-5.048	5.048	-35.918	35.918	-47.121	47.121
PSO4	1.134	0.98	-0.153	0.279	-13.539	24.591	-12.601	22.512

6. Summary of Model Performance

The model performance was overall good. The model captures well the temporal variation in $PM_{2.5}$. The gradual increase in $PM_{2.5}$ concentration and its transition back to low levels are generally well reproduced by the model. The model also predicts well $PM_{2.5}$ concentration on peak days. It also overall replicates well the composition of $PM_{2.5}$ on exceedance days, with good model performance for secondary nitrate and ammonium which account for over 50% of $PM_{2.5}$ mass. Simulated ammonia concentrations are also within the range of those observed, further indicating that the model overall performs well.