

Salt Lake Maintenance
State Implementation Plan

Photochemical Model Performance
Evaluation

Utah Division of Air Quality

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Photochemical Model Performance Evaluation

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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, ozone deposition velocity, snow albedo, vertical diffusion modifications, cloud water content modification and paved road dust emissions adjustment) to more accurately reproduce winter-time inversion episodes. A detailed explanation of these model modifications was provided earlier.

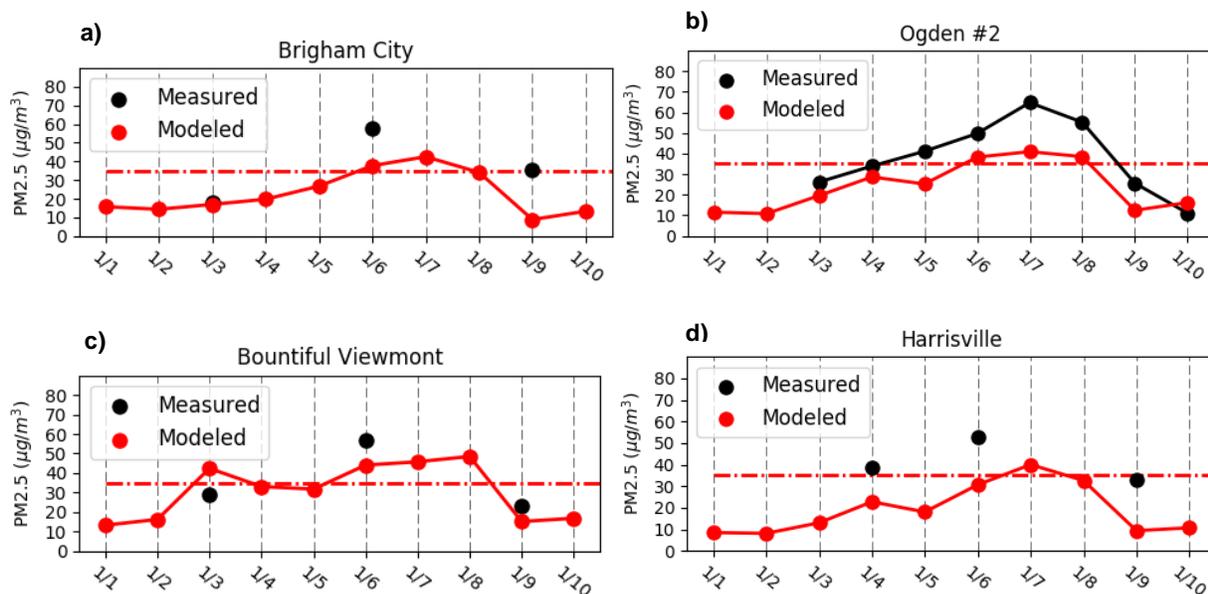
Various statistical metrics and graphical displays were considered for evaluating the model with the objective to determine whether modeled variables are comparable to observations. These included:

- Time series plots of modeled and observed 24-hr PM_{2.5} concentrations.
- Scatter plots of modeled and observed 24-hr PM_{2.5} concentrations.
- Coefficient of determination, R^2 , which shows the degree to which modeled and observed 24-hr PM_{2.5} concentrations are linearly related.
- Pie charts showing modeled and observed PM_{2.5} 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 (O₃), nitrogen oxides (NO, NO₂ and NO_x where NO_x=NO+NO₂), carbon monoxide (CO), 24-hr total PM_{2.5} and 24-hr chemically-specified PM_{2.5} measurements collected at monitoring stations in the Salt Lake non-attainment area. Ammonia, halogens and carbonyls measurements collected during special field studies carried out in winter of 2016 and 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 PM_{2.5} concentration exceeding the 24-hr national ambient air quality standard (> 35 µg/m³). Results for December 31, which is a model spin-up day, are excluded from this evaluation.

2. Daily PM2.5 Concentrations

Figure 1a-h shows 24-hr modeled and observed PM2.5 concentration during January 1-10 2011 at all monitoring stations in the Salt Lake non-attainment area where 24-hr PM2.5 filter 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. The overestimation in PM2.5 that is observed on January 3rd, mainly at Hawthorne, Rose Park and Bountiful Viewmont stations, is related to the meteorological model performance on this day. Thin mid-level clouds, which were observed on January 3-4, were not simulated in the meteorological model, leading to an increasingly stable low-level boundary layer, particularly at night¹. This limited the mixing of pollutants in the photochemical model on January 3rd, resulting in an over-prediction in PM2.5 levels. The underestimation in PM2.5 on January 5 2011 at the Hawthorne station is also related to the meteorological model performance on this day, where the WRF model overestimated the wind shear near the mixing height².



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

²<https://documents.deq.utah.gov/air-quality/planning/technical-analysis/research/model-improvements/3-wintertime-episodes/DAQ-2017-014342.pdf>

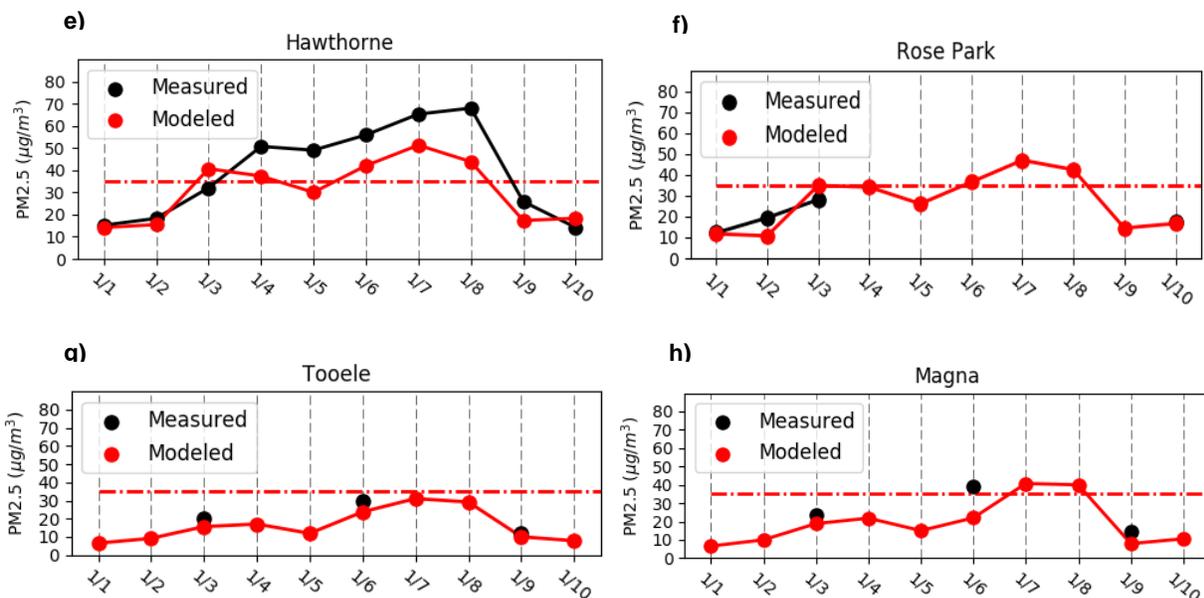


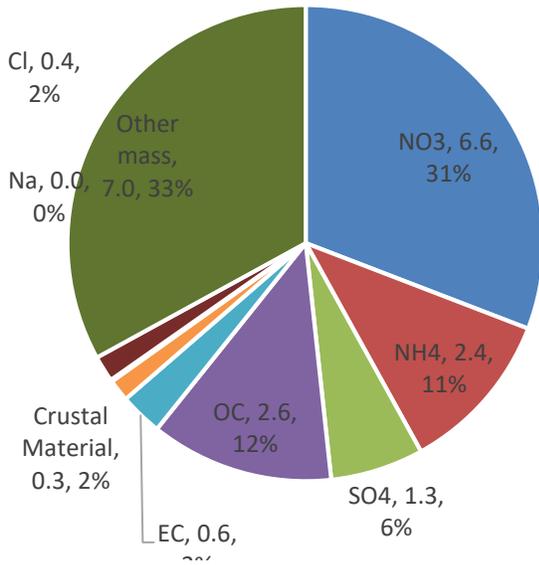
Figure 1a-h. Measured and modeled 24-hr average PM_{2.5} concentration during January 1-10 2011 (MDT) at monitoring stations in the Salt Lake non-attainment area. Dashed line represents 24-hr PM_{2.5} National Ambient Air Quality Standard (NAAQS).

3. PM_{2.5} Chemical Speciation

To further investigate the photochemical model performance, measured and modeled PM_{2.5} chemical species were compared at Hawthorne and Bountiful Viewmont monitoring sites, which are part of EPA's Chemical Speciation Network (CSN). Figures 2a-b, 3a-b and 4a-b show a comparison of the bulk chemical composition of measured and modeled PM_{2.5} at Hawthorne and Bountiful monitoring stations on January 1, 7 and 9 2011, which correspond to days when measurement data are available. 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 PM_{2.5} non-exceedance days (days when PM_{2.5} measured and modeled were both below 35 µg/m³) (Figures 2 and 3a-b), the model underestimated nitrate by about 2.8 µg/m³ at both Hawthorne and Bountiful stations. Ammonium was also underestimated by about 0.79 and 0.67 µg/m³ at Hawthorne and Bountiful, respectively. On the other hand, the model performance for sulfate was reasonably good. Measured and modeled concentrations of sulfate were generally comparable, respectively accounting for 1.3 and 1.2 µg/m³ of PM_{2.5} at Hawthorne and 1.3 and 1.4 µg/m³ of PM_{2.5} at Bountiful. The model also overall overestimated OC and primary PM_{2.5} species, including crustal material and EC. The overprediction in these species, even on days when the mixing height was underestimated, suggests that this overestimation in measured concentrations is potentially related to an overestimation in source emissions.

a) Hawthorne
January 01 and 09 2011
Measured, PM2.5 = 21.3 ug/m3



b) Hawthorne
January 01 and 09 2011
Modeled, PM2.5 = 15.8 ug/m3

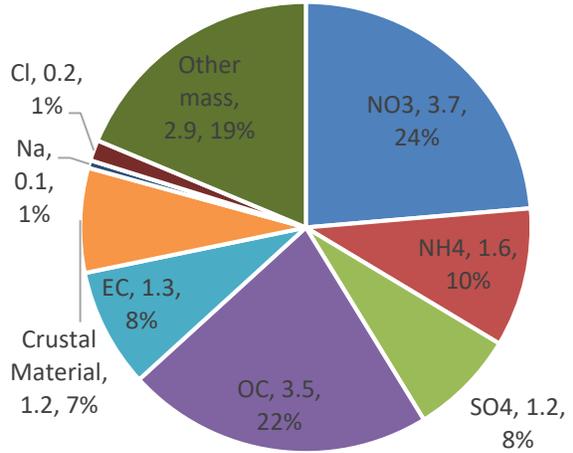
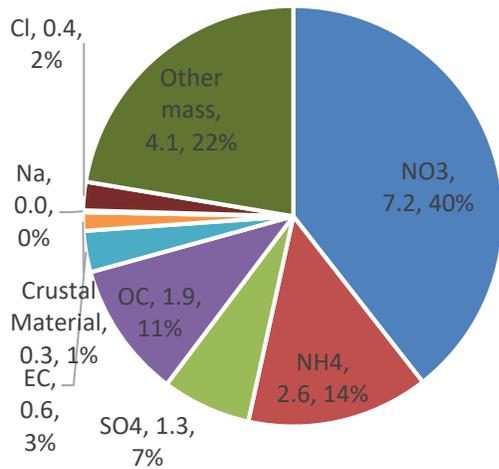


Figure 2a-b. Average measured and b) modeled chemical composition of 24-hr PM2.5 in ug/m3 and percent of PM2.5 at Hawthorne monitoring station over January 1 and 9 2011.

a) Bountiful Viewmont
January 09 2011
Measured, PM2.5 = 18.3 ug/m3



b) Bountiful Viewmont
January 09 2011
Modeled, PM2.5 = 15.12 ug/m3

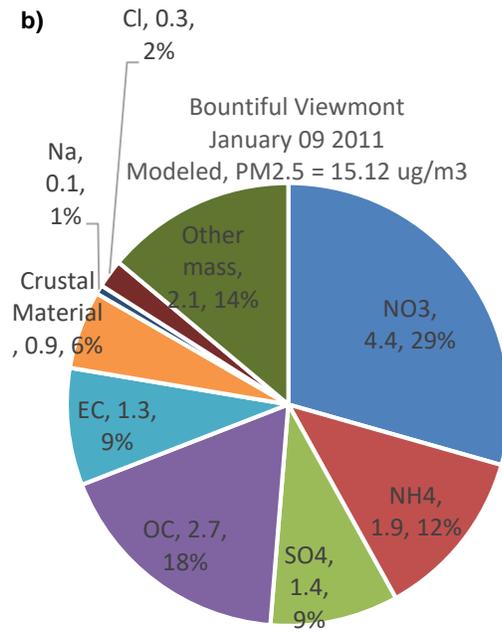


Figure 3a-b. Measured and b) modeled chemical composition of 24-hr PM2.5 in ug/m3 and percent of PM2.5 at Bountiful monitoring station on January 9 2011.

The photochemical model performance on PM_{2.5} exceedance days was overall similar to that on PM_{2.5} non-exceedance days. Figure 4a-b shows a comparison of the bulk chemical composition of measured and modeled PM_{2.5} at Hawthorne on January 7 2011, which corresponds to a peak PM_{2.5} exceedance day with available measurement data.

The model performance for particulate nitrate, which is the major component of PM_{2.5}, was good, with both modeled and measured NO₃ accounting for similar contributions to PM_{2.5} filter mass. Modeled and observed nitrate concentrations were also comparable, with modeled concentration being biased low by about 15%. Similarly to its performance for nitrate, the model was also biased low for ammonium by about 34%. The underestimation in modeled nitrate and ammonium can be related to an underestimation in modeled nitryl chloride (ClNO₂) and hydrochloric acid (HCl). Modeled ClNO₂ respectively reached a peak concentration of about 0.3 ppbv and 0.2 ppb at Hawthorne monitoring station on January 7 and 5 (Figures 5 and 6), which correspond to PM_{2.5} exceedance and non-exceedance days, while mixing ratios exceeding 0.8 ppbv were observed over Salt Lake City during a special field study (2017 Utah Winter Fine Particulate Study (UWFPS)³, Figure 7). Similarly, modeled HCl was underestimated in the model, possibly resulting in an underestimation in ammonium chloride (NH₄Cl) in the model. A previous source apportionment analysis showed that ammonium chloride accounts for 10-15% of total PM_{2.5} mass at Hawthorne during high wintertime PM_{2.5} pollution episodes⁴. Modeled HCl emissions, particularly from US Magnesium plant, a large source of HCl emissions on the west side of the Great Salt Lake, were underpredicted in the model. Values as high as 100 ppb were observed in the afternoon in the vicinity of US Magnesium during the 2017 UWFPS⁵ (Figure 9) while maximum hourly values of about 12 and 35 ppb were modeled near US Magnesium (Figures 8a-b) on typical exceedance and non-exceedance days.

The model performance for particulate sulfate was reasonably good, with sulfate being biased low in the model by about 27%. The model performance for organic carbon was also good for January 7, with modeled and observed concentrations being quite comparable. The model, on the other hand, overestimated EC and CM. The overprediction in these species on days when the simulated atmospheric mixing was particularly strong, suggests that this overestimation is potentially related to an overestimation in their source emissions.

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

⁴ 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, DOI: 10.1080/10962247.2013.774819

⁵ <https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf>

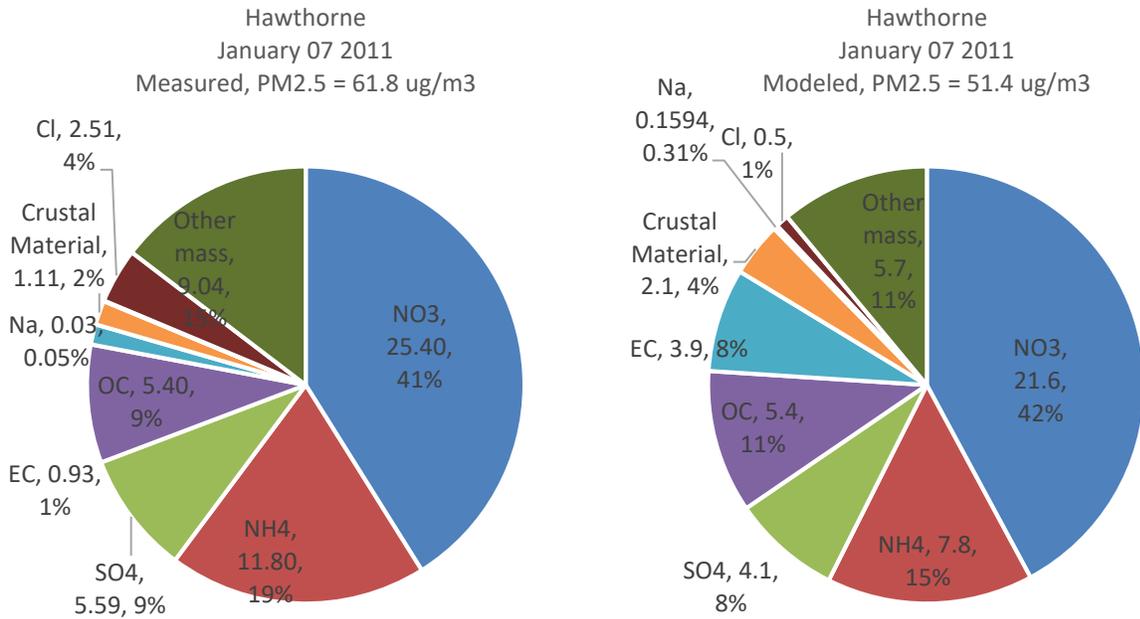


Figure 4. Measured and b) modeled chemical composition of 24-hr PM2.5 in ug/m3 and percent of PM2.5 at Hawthorne monitoring station on January 7 2011.

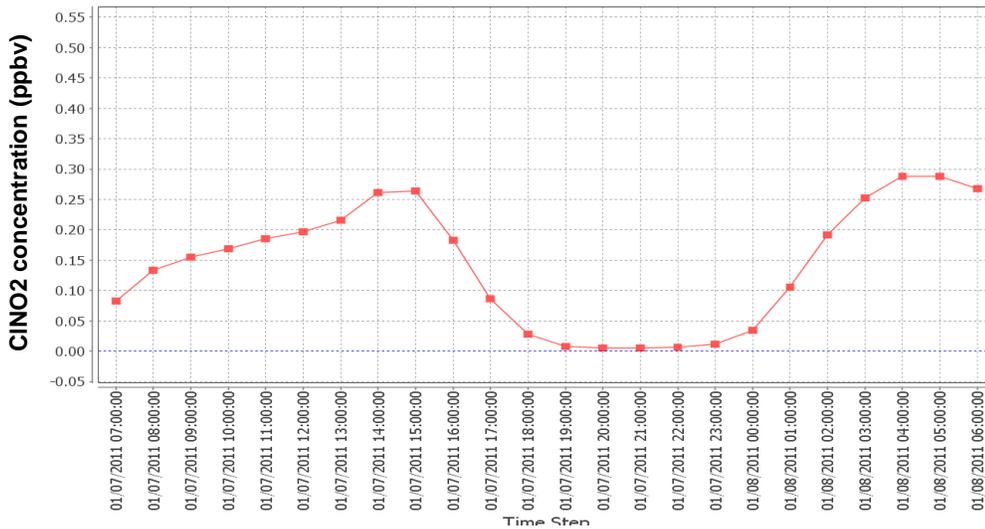


Figure 5. Hourly time series (UTC) of CINO2 concentration in ppbv at Hawthorne monitoring station on January 7 2011.

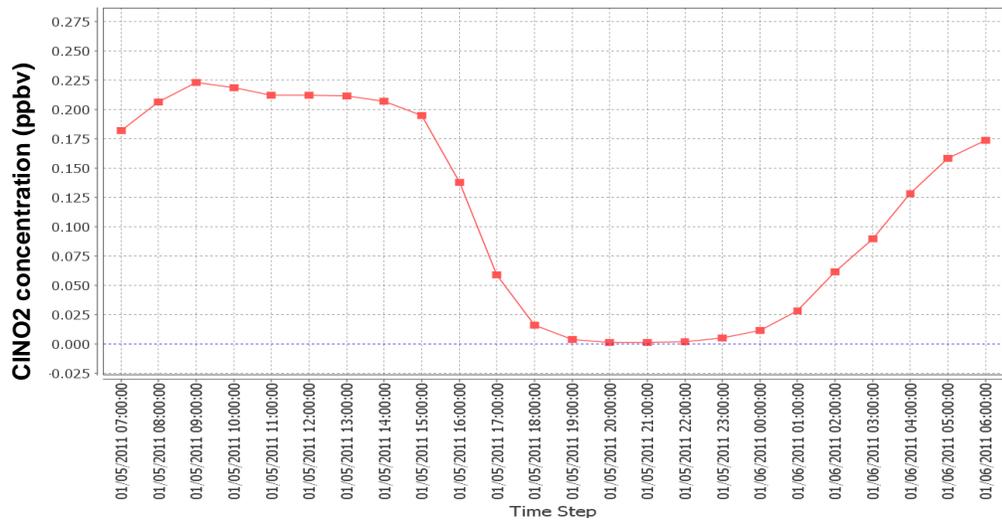


Figure 6. Hourly time series (UTC) of CINO₂ concentration in ppbv at Hawthorne monitoring station on January 5 2011.

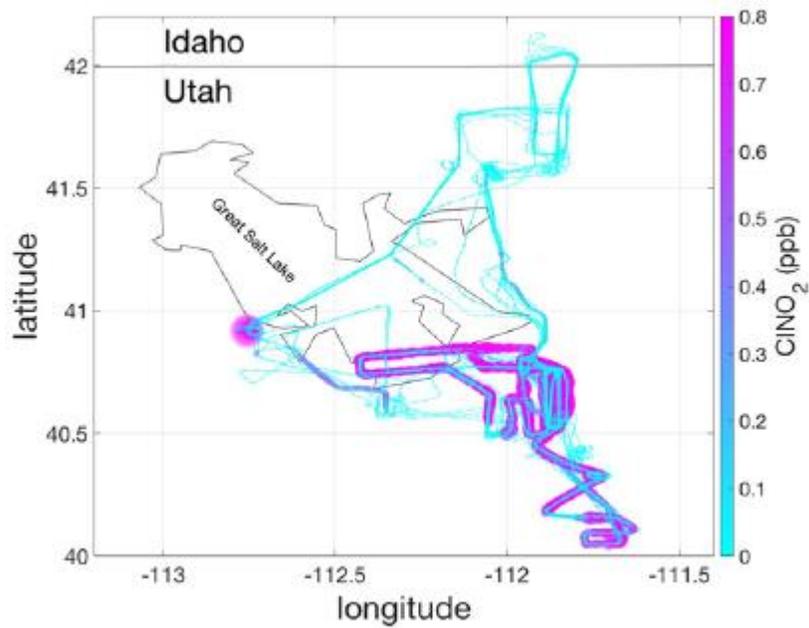


Figure 7. Spatial distribution of CINO₂ during the 2017 Utah Winter Fine Particulate Study. Figure retrieved from the 2017 Utah Winter Fine Particulate Study, final report, Figure 3.49 (<https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf>).

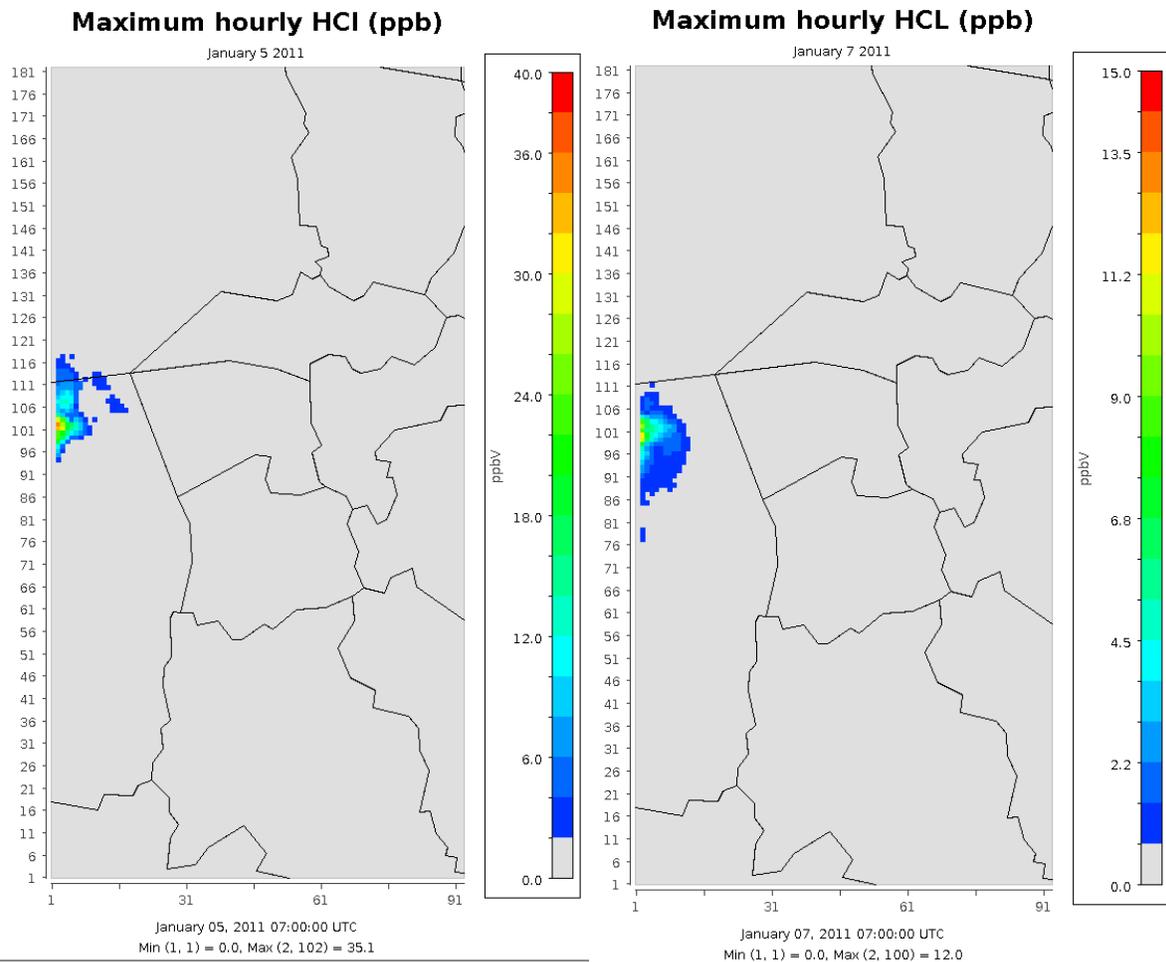


Figure 8. Spatial distribution of maximum hourly HCl concentrations (in ppb) on January 5 and 7 2011. The latter represents a typical exceedance day.

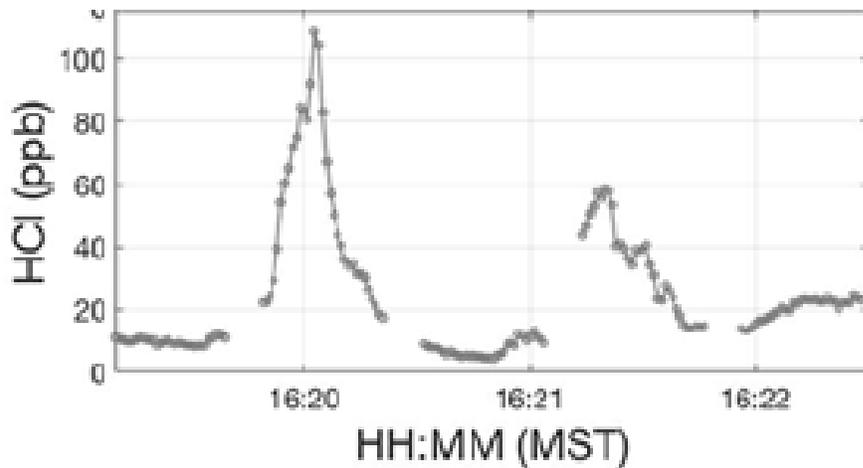
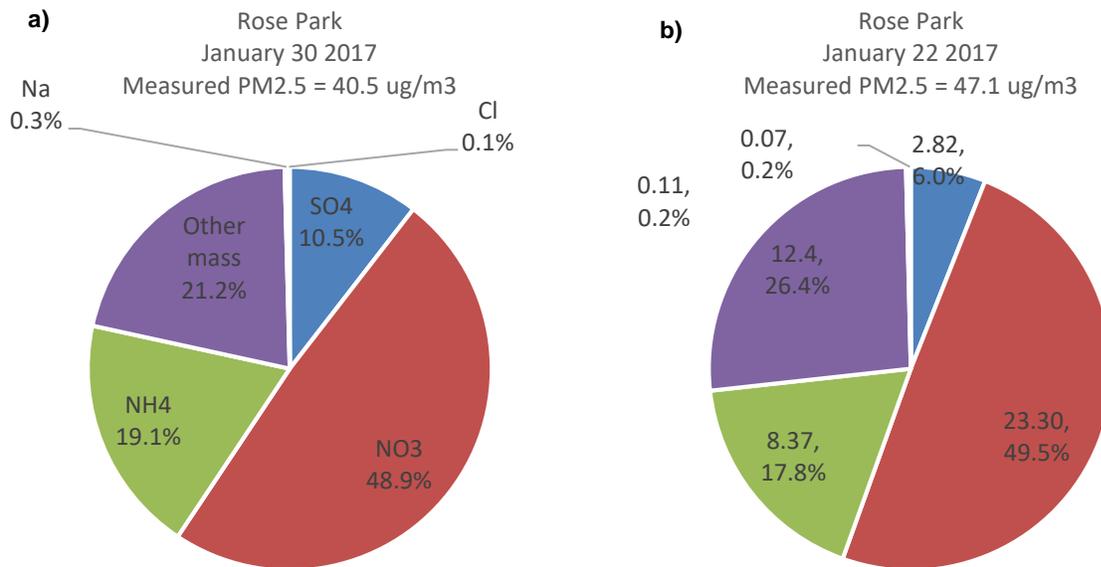


Figure 9. Time series of HCl during an afternoon intercept of the plume from US Magnesium during the 2017 Utah Winter Fine Particulate Study. Figure retrieved from the 2017 Utah Winter Fine Particulate Study, final report, Figure 3.43 (<https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf>).

The model performance was also assessed at Rose Park monitoring station in Salt Lake Valley (Figure 10a-c). Given that measurements of PM_{2.5} chemical species were not available during 2011, this analysis is based on a comparison of the fraction of individual PM_{2.5} chemical species in total PM_{2.5} mass between model outputs and measurements. The latter correspond to FRM filter speciation data collected at Rose Park during an inversion event in 2017. While the 2017 filter measurements cannot be directly compared to day-specific 2011 model simulations, the measurements are useful to assess if the model predicts similar PM_{2.5} chemical composition during strong inversion conditions. Although the concentration of individual PM_{2.5} chemical species may vary between inversion events, their relative contribution to total PM_{2.5} mass is expected to remain the same during typical inversion events. As can be seen, the chemical composition of modeled PM_{2.5} is similar to that of measured PM_{2.5}. Modeled nitrate accounts for about 50% of PM_{2.5}, in agreement with the contribution of measured nitrate to PM_{2.5} mass (about 49 and 50%). Measured and modeled sulfate and ammonium also have similar fractional contributions to PM_{2.5} mass.



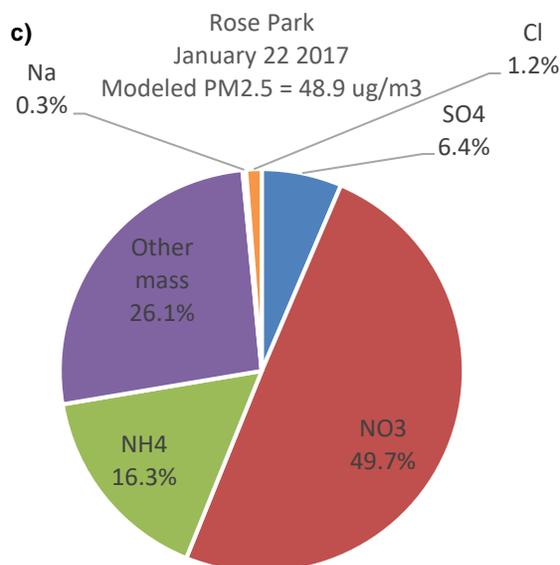


Figure 10a-c. a and b) Measured and c) modeled chemical composition of 24-hr PM2.5 in percent of PM2.5 at Rose Park monitoring station during typical inversion days.

4. Hourly Ambient Gaseous Compounds

The model performance was also evaluated for gaseous compounds. Gaseous compounds considered in this analysis include carbon monoxide (CO), nitrogen oxides (NO, NO₂, and NO_x defined as NO+NO₂), ozone (O₃), ammonia (NH₃), formaldehyde and acetaldehyde. Model outputs were compared to measurements collected at the Hawthorne monitoring station during January 1-10 2011.

A comparison of modeled and measured hourly CO concentrations (Figure 11) showed that modeled CO was overestimated during January 3-4, which is likely related to the meteorological model performance on this day. Thin mid-level clouds, which were observed on these days, were not simulated in the meteorological model, leading to an increasingly stable low-level boundary layer. On the other hand, modeled CO was overall underestimated during nighttime hours (12 am – 6 am) on January 5-6 2011, which may be related to overmixing vertically, where the WRF model overestimated the wind shear near the mixing height⁶. The bias between modeled and measured CO was overall smaller on January 7-8, which correspond to peak PM_{2.5} exceedance days.

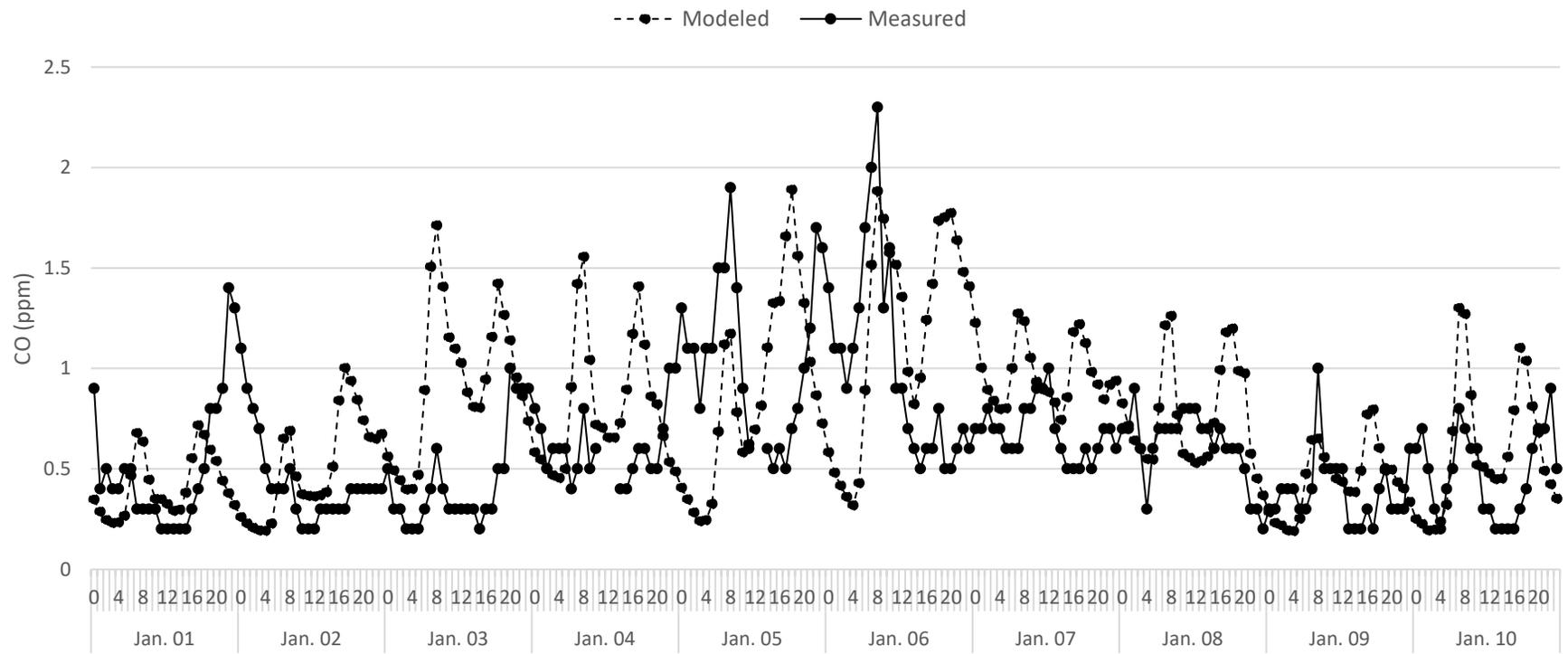


Figure 11. Modeled and measured hourly time series (in MDT) of CO (ppm) at Hawthorne monitoring site during January 1-10 2011.

A comparison of modeled and measured nitrogen oxides (NO, NO₂ and NO_x, Figures 12-14) and ozone (Figure 15) shows that modeled NO, NO₂ and NO_x are overall underestimated and ozone is overestimated during overnight hours (12 am – 6 am) on January 5-6. The overprediction in ozone is likely a result of reduced ozone titration due to a lack of nightly modeled NO_x, which may be related to overmixing vertically. The model performance was better on January 7, which corresponds to a peak PM_{2.5} exceedance day, particularly for ozone, with modeled ozone concentration being comparable to that measured.

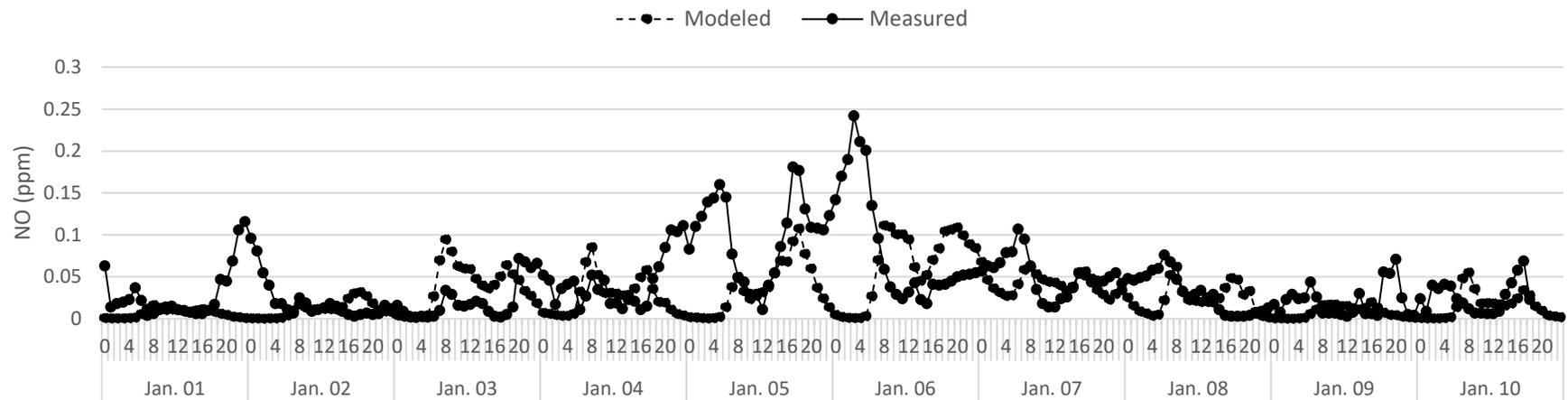


Figure 12. Modeled and measured hourly time series (in MDT) of NO (ppm) at Hawthorne monitoring site during January 1-10 2011.

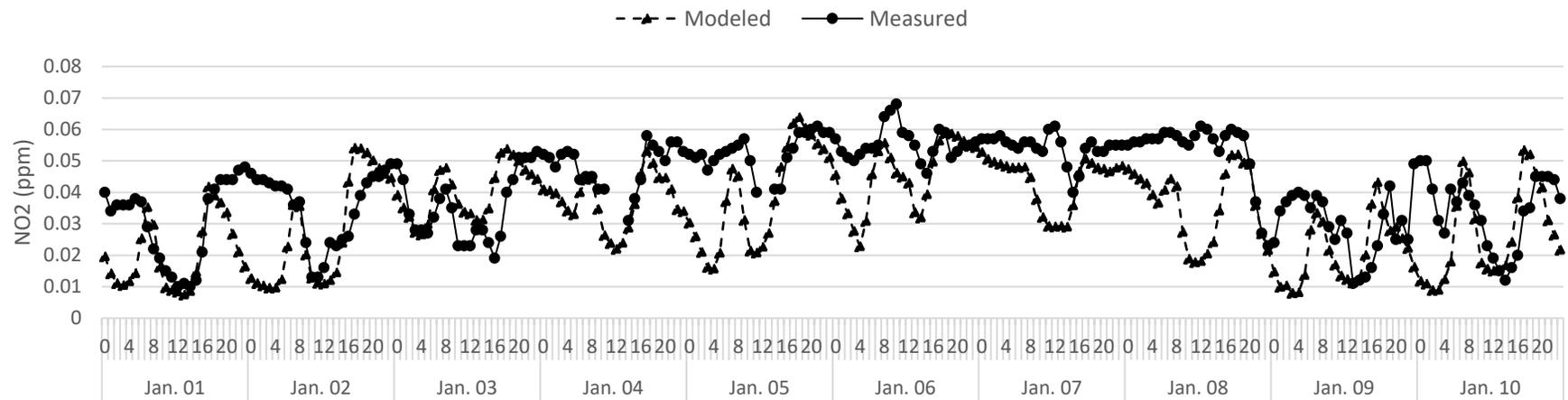


Figure 13. Modeled and measured hourly time series (in MDT) of NO₂ (ppm) at Hawthorne monitoring site during January 1-10 2011.

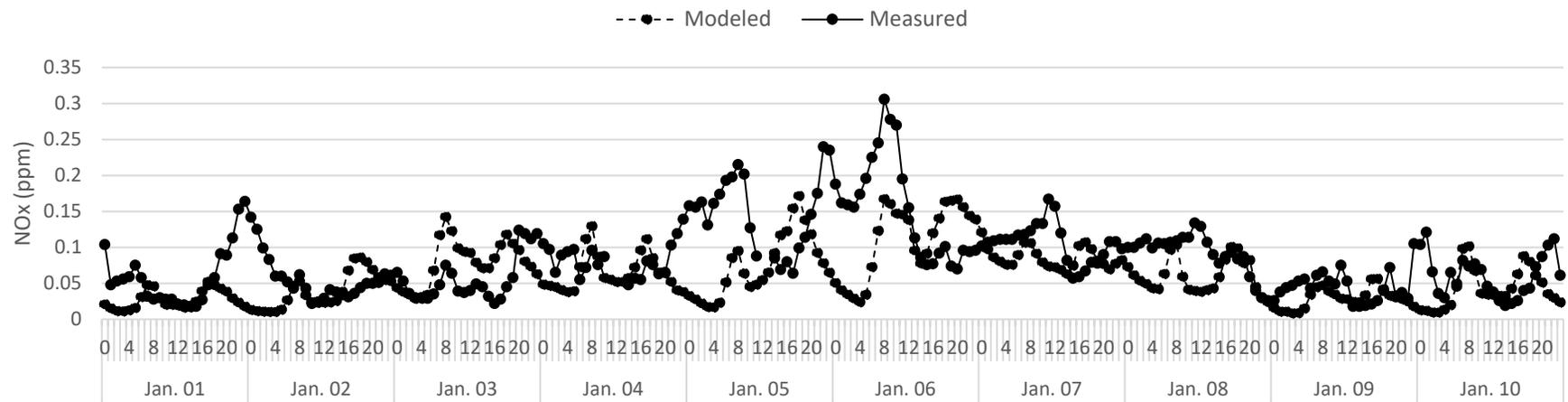


Figure 14. Modeled and measured hourly time series (in MDT) of NOx (NO+NO2 in ppm) at Hawthorne monitoring site during January 1-10 2011.

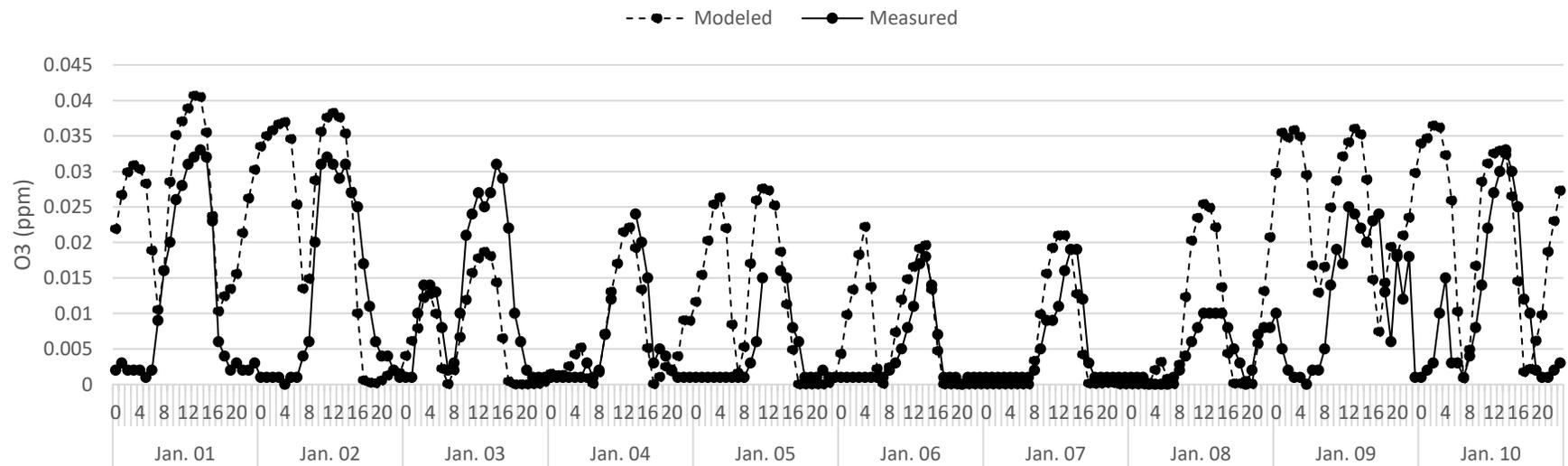


Figure 15. Modeled and measured hourly time series of ozone (ppm) at Hawthorne monitoring site during January 1-10 2011.

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 $\text{PM}_{2.5}$ species accounting for over 50% of the $\text{PM}_{2.5}$ mass during winter-time inversion events.

Hourly modeled ammonia (Figure 16) was compared to hourly ammonia measurements (Figure 17) conducted at Neil Armstrong Academy during a special field study in winter 2016. Measurements from 2016 were considered since measurements of ammonia were not available during 2011. Hourly measurements were also only available at Neil Armstrong Academy, located in West Valley City in the Salt Lake NAA. However, while these 2016 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.

Modeled ammonia at Hawthorne and Neil Armstrong Academy is well within the range observed in 2016. It also displays a similar behavior to measured NH_3 , with ammonia concentration dropping during peak $\text{PM}_{2.5}$ events. For example, during the inversion episode from February 7-14 2016, Figure 17 shows that measured NH_3 concentrations were mostly in the range of 2 to 5 ppb, which is similar to the modeled NH_3 concentrations during the January 2011 inversion episode shown in Figure 16.

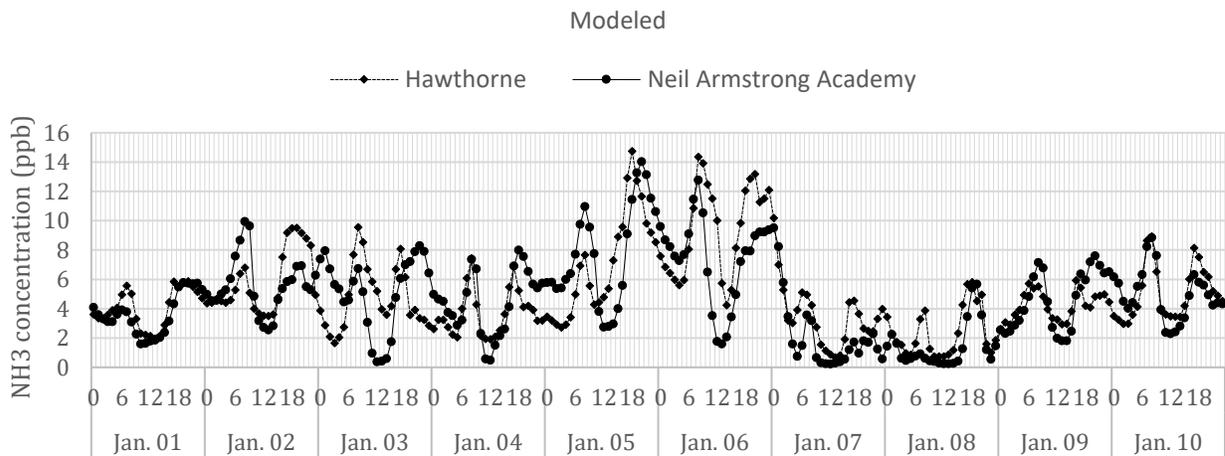


Figure 16. Hourly time series of modeled ammonia (ppb) at Hawthorne and Neil Armstrong Academy during January 1 – 10 2011

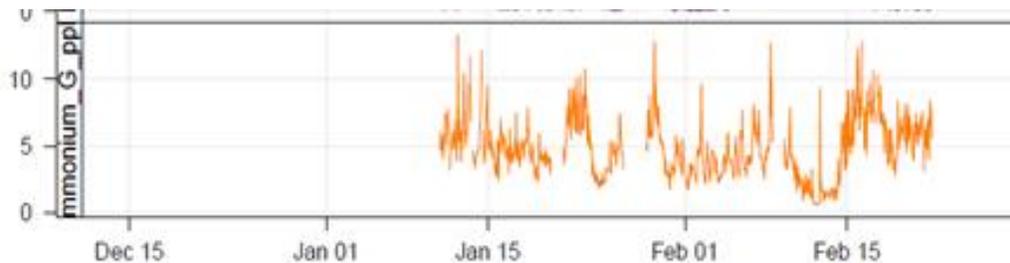


Figure 17. Hourly measured ammonia on y-axis (ppb) at Neil Armstrong Academy in the SLC NAA during January – February 2016. Note that ammonia drops during the PCAP of Feb. 7-14 2016.

The model performance was also evaluated for carbonyls, which can act as radical sources important for the photochemical production of PM_{2.5} during wintertime inversion episodes in the Salt Lake Valley⁷. Given that measurements of carbonyls were not available during 2011, the modeling results were compared to observations conducted in winter 2017 at the University of Utah (2017 Utah Winter Fine Particulate Study (UWFPS)). While these field study measurements from 2017 cannot be directly compared to day-specific 2011 model simulations, they're qualitatively useful to assess if the model predicts similar levels of VOCs during strong inversion conditions.

A comparison of the modeling results and measurements showed that formaldehyde may be underrepresented in the model during mid-day hours. On average during peak PM_{2.5} exceedance days, measured formaldehyde peaked at about 3 ppb around 11 am (Figure 19) while modeled formaldehyde peaked at 6 pm and displayed a concentration of 1.8 ppb at 11 am (figure 18). Modeled formaldehyde also displayed a temporal trend different from that of measured formaldehyde, with observations indicating direct emission as well as secondary production of formaldehyde. Similarly, modeled acetaldehyde exhibited a temporal trend different from that measured on peak PM_{2.5} days. This comparison suggests that acetaldehyde and formaldehyde, an important source of radicals, may be underestimated in the model during mid-day hours.

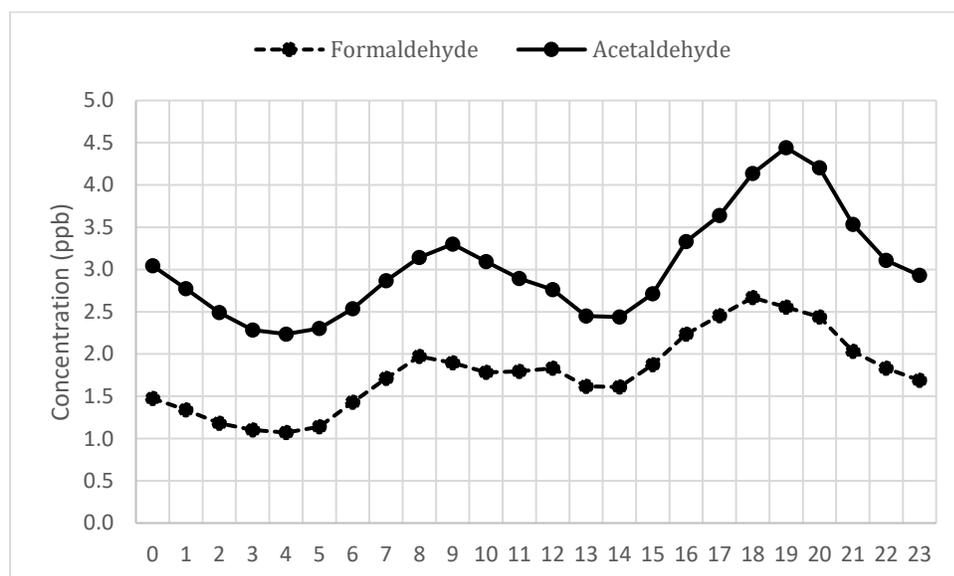


Figure 18. Hourly time series of average modeled formaldehyde and acetaldehyde during January 6-8 2011 at the University of Utah.

⁷ <https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf>. Chapter 3.

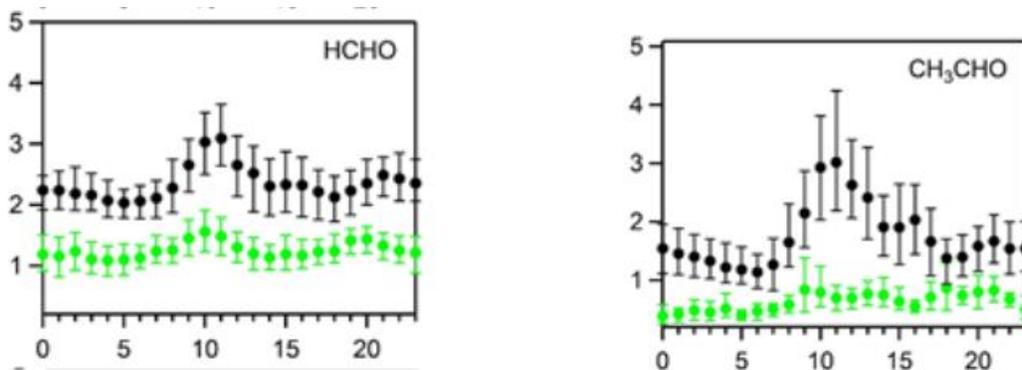


Figure 19. Diurnal trend of hourly averaged formaldehyde (HCHO) and acetaldehyde (CH₃CHO) measured at the University of Utah during polluted (black lines) and clean (green lines) conditions in winter 2017. Figure retrieved from the 2017 Utah Winter Fine Particulate Study, final report, Figure 3.59 (<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. 2008⁸ and are discussed in “Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM_{2.5}, and Regional Haze” (EPA, April 2007). Chemical speciation data collected at the Hawthorne monitoring station on January 1, 5, 7 and 9 2011 was considered for this analysis.

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 20). As can be seen, the model performance for OC and primary species CM and EC was weak while that for secondary inorganic ionic species, including SO₄, nitrate and ammonium which account for over 50% of PM_{2.5} mass on wintertime inversion days, was better.

⁸ 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

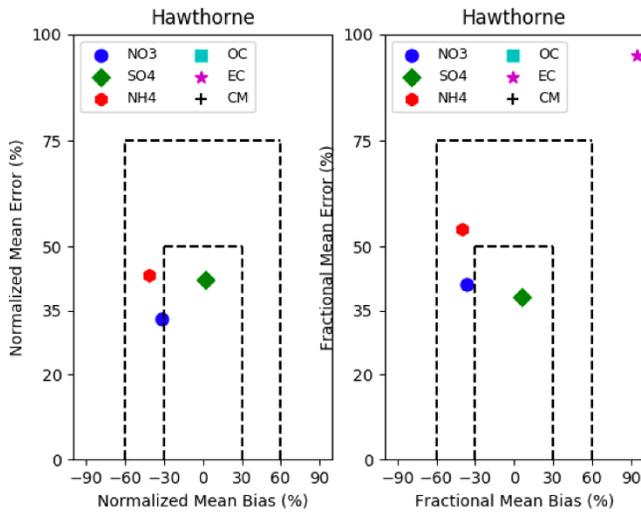


Figure 20. Soccer plot depicting modeled PM_{2.5} species performance for days during the modeling episode when speciated PM_{2.5} filter data was available at Hawthorne monitoring site.

Model performance was further evaluated by examining various model performance metrics for PM_{2.5} species at the Hawthorne monitoring site during the January 2011 modeling episode (Table 1). As can be seen, the model was biased low for secondary nitrate and ammonium species while it was biased high for crustal material, EC and OC.

Table 1. Model performance statistics for four days during the modeling episode when speciated PM_{2.5} filter data was available at Hawthorne monitoring site.

PM _{2.5} Species	Mean (obs) ug/m ³	Mean (modeled) ug/m ³	Mean Bias ug/m ³	Mean Error ug/m ³	Normalized Mean Bias	Normalized Mean Error	Mean Fractional Bias	Mean Fractional Error
CM	0.629	1.913	1.284	1.284	204.306	204.306	107.458	107.458
OC	3.651	11.188	7.537	7.537	206.461	206.461	101.851	101.851
PEC	0.888	2.706	1.818	1.818	204.786	204.786	95.053	95.053
PNH ₄	6.276	3.691	-2.585	2.716	-41.189	43.274	-40.403	54.213
PNO ₃	14.391	9.77	-4.621	4.75	-32.113	33.009	-36.472	41.127
PSO ₄	2.218	2.27	0.052	0.936	2.336	42.201	5.67	38.288

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 reasonably 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.