Model Modifications and Settings

Utah Division of Air Quality

Introduction

To improve the photochemical model performance, Utah DAQ made several key modifications to the modeling system. Model modifications improved the model performance for PM2.5 by reducing three main model biases:

- Positive model bias in primary aerosol
- Negative model bias in particulate nitrate

The model modifications and settings include:

- Ammonia injection: non-inventoried ammonia was added to the model domain in order to compensate for low ammonium nitrate performance.
- Surface resistance to ammonia was maximized. This modification effectively lowered the ammonia dry deposition rate and increased the model performance for ammonium nitrate.
- Vertical diffusion rates were increased to compensate for discrepancies between WRF output and meteorological measurements.
- Changed urban snow surface albedo to 88%. This change increased photolytic chemistry and improved particulate nitrate performance.
- Ozone dry deposition rate was set to nearly zero. This increased the oxidant budget and promoted secondary aerosol formation.
- To reduce the model high bias for crustal material, a 93% reduction was applied to paved road dust emissions.

A detailed discussion of these applications is provided below.

Ammonia Injection

Preliminary model performance evaluation results showed an underprediction in ammonium nitrate, which accounts for over 50% of PM2.5 mass during winter-time inversion episodes along Utah's Wasatch Front and Cache Valley[1]. This low model bias for ammonium nitrate was likely related to an underprediction in ammonia, which is an important precursor to the formation of ammonium nitrate. Recent measurements of ammonia conducted during a special air monitoring field study showed that modeled ammonia concentrations are significantly lower than those measured.

This ammonia shortfall in the model may be explained by:

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

- High ammonia deposition velocity rates in current air quality models[2].
- Lack of ammonia sources in Utah's emissions inventory. It is possible that mobile ammonia emissions are underestimated by the MOVES 2014a model used for mobile emissions modeling[3]. Some agricultural sources may also be misrepresented or not captured in Utah's area source emissions inventory. The actual reason for any gap in Utah's ammonia inventory is undetermined to date.

To reduce the model's low bias for ammonium nitrate, ammonia emissions were increased by injecting additional ammonia, above the reported inventory, into the emissions. Throughout this document, ammonia injection is defined as artificially adding non-inventoried ammonia emissions to the inventoried emissions input into the air quality model.

For a given county in the non-attainment area, ammonia was injected uniformly across grid-cells that correspond to low elevation regions (< 6,000 ft ASL). Low elevation areas were considered since it is reasonable to expect that missing anthropogenic ammonia sources are more likely located along valley floors. Moreover, there are no reliable ammonia measurements taken in upper elevation areas at this point.

The amount of injected ammonia was also varied on a county-by-county basis since modeled ammonia bias varied spatially. A table of injected ammonia values per county is provided below:

Table 1. Emissions rates (tons/year) of ammonia injected in the five counties comprising the Salt Lake non-attainment area.

County	Tons/year
Box Elder	9,209
Davis	604
Salt Lake	622
Tooele	10,043
Weber	781

Ammonia injection emissions rates were also held constant over time. The quantity of ammonia injected into a particular county was not only a function of measurements (if available), but also the geographical size of low-elevated terrain in the county.

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[2] Rodriguez M.A., Barna M.G., Gebhart K.A., Hand J.L., Adelman Z. E., Schichtel B.A., Collett Jr. J.L., and Malm W.C., 2011. Modeling the fate of atmospheric reduced nitrogen during the Rocky Mountain Atmospheric Nitrogen and Sulfur Study (RoMANS): Performance evaluation and diagnosis using integrated processes rate analysis. Atmospheric Environment 45, 223-234.
[3] Sun, K., L. Tao, D.J. Miller, M.A. Khan, M.A. Zondlo, 2014. On-Road Ammonia Emissions Characterized by Mobile, Open-Path Measurements. Environ. Sci. Technol., 48, 3943−3950.

To assess the model performance for ammonia following the ammonia injection, hourly modeled ammonia (Figure 1) was compared to hourly ammonia measurements (Figure 2) conducted at the Logan air monitoring station during a special field study in winter 2017. 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 Logan site is well within the range observed in 2017.

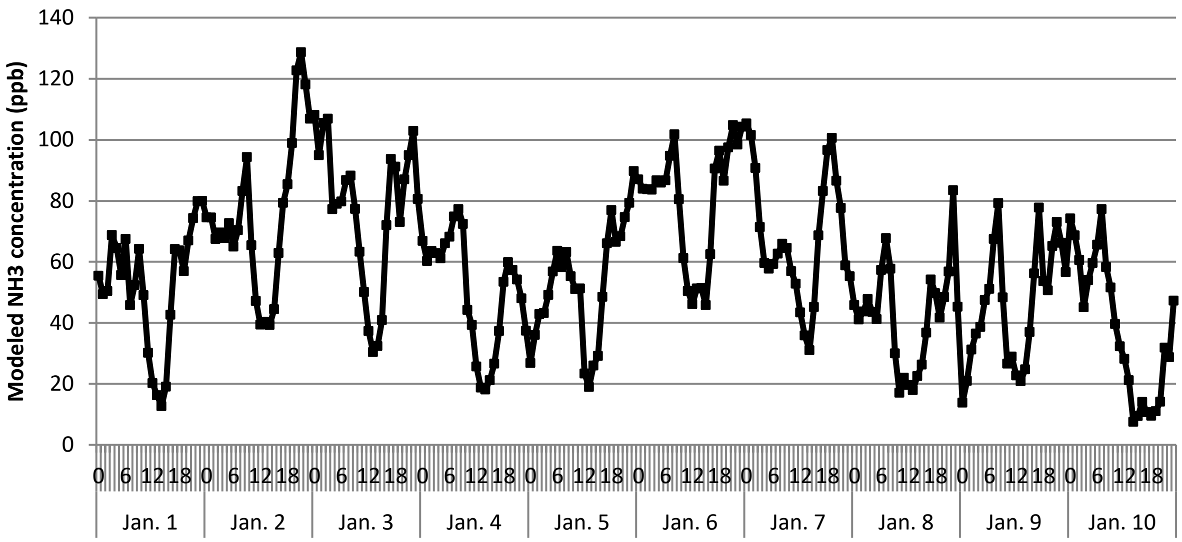

Figure 1. Modeled hourly ammonia concentration (ppb) at Logan monitoring site during January 1-10 2011.

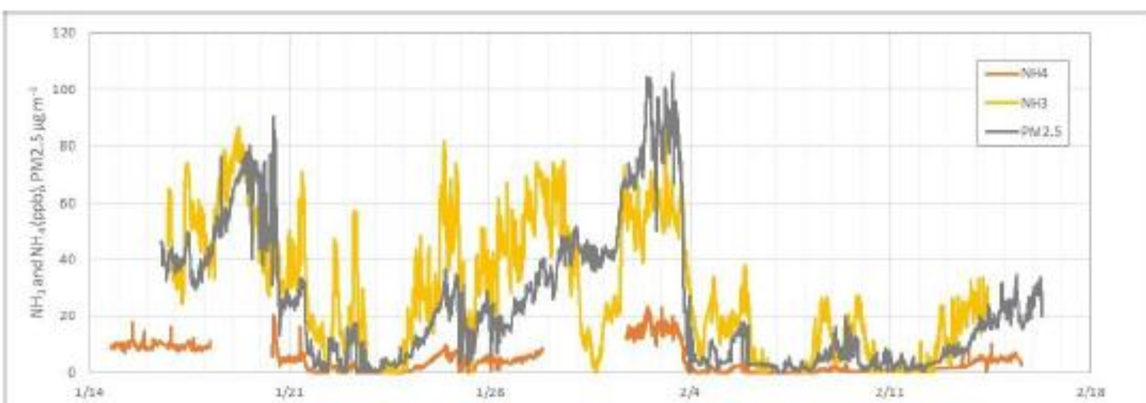

Figure 2. Measured ammonia, ammonium and PM2.5 at Logan monitoring site during the 2017 Utah Winter Fine Particulate Study. Figure retrieved from the 2017 Utah Winter Fine Particulate Study, final report, Figure 3.33 (https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf).

Increased Surface Resistance to Ammonia

To more appropriately estimate NH3 dry deposition rate, the dry deposition parameter for ammonia, "Rscale", was changed from “0” to “1” in the CAMx chemistry parameter file. This was implemented following the technical advice of Ramboll, developer of CAMx. By setting Rscale to 1, the surface resistance to ammonia was increased and its dry deposition rate was decreased, leading to an improvement in the model's performance for ammonium nitrate. CAMx latest version now includes this change in Rscale value for ammonia. At the time CAMx was compiled to conduct the simulations for this maintenance plan, this change was not included.

Increased Vertical Diffusion Rates

During the January 2011 episode, the mixing height was underestimated by about 100 m in the meteorological model on December 31-January 2, leading to an increasingly stable low-level boundary layer[4], which limited the mixing of pollutants in the photochemical model on these days and resulted in an over-prediction in PM2.5 levels (not shown). To reduce this high bias in PM2.5, Utah DAQ applied the KVPATCH utility in CAMx to WRF model output for December 31-January 2. Applying KVPATCH helped enhance vertical mixing in the lower atmosphere, leading to a better agreement between observed and modeled PM2.5 on these days.

Increased Urban Snow Albedo

The January 1- 10 2011 modeling episode was characterized by a complete snow cover. Figure 3 shows snow covering the Salt Lake City metropolitan area during the first day of the modeling episode. Due to persistent cold temperatures and high-pressure conditions, snow remained on the surface for the duration of the 10-day episode. Initial CAMx simulations indicated that surface albedo over urban areas was significantly lower than measured surface albedo, where measurements were acquired from a field campaign conducted by the University of Utah (Persistent Cold Air Pool Study (PCAPS)) during the January 1-10 2011 period. The albedo measurements were derived from radiation measurements taken at 7 stations (Figure 4, left panel) located throughout the Salt Lake Valley, with three of the monitoring stations being located in urban areas. Because radiation depends on solar angle, only radiation measurements taken around when solar angle was near maximum were used for albedo calculations. Measurements specific to the Cache Valley were not available. However, while measurements for the Salt Lake Valley cannot be directly compared to those for the Cache Valley, the measurements are qualitatively useful to assess if the model predicts similar albedo values over urban areas. Low surface albedo inhibits photolytic chemistry and therefore limits the production of secondary aerosol, which accounts over 50% of PM2.5 mass during winter-time inversions in Utah's PM2.5 non-attainment areas[5]. To enhance the model performance for secondary inorganic ionic species, Utah DAQ modified the CAMx source code to change the urban albedo from ~33% to 88%. A comparison between modeled (prior and post-modification) and measured albedo during January 1-8 2011 is shown in Figure 4 (right panel). Simulated CAMx albedo over PM2.5 non-attainment areas before

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[4]PM2.5 State Implementation Plan Meteorological Modeling, available at https://documents.deq.utah.gov/air-quality/planning/technical-analysis/research/model-improvements/3-wintertime-episodes/DAQ-2017-014342.pdf

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

and after the model modification is also shown in Figure 5. This increased urban albedo improved modeled nitrate performance.

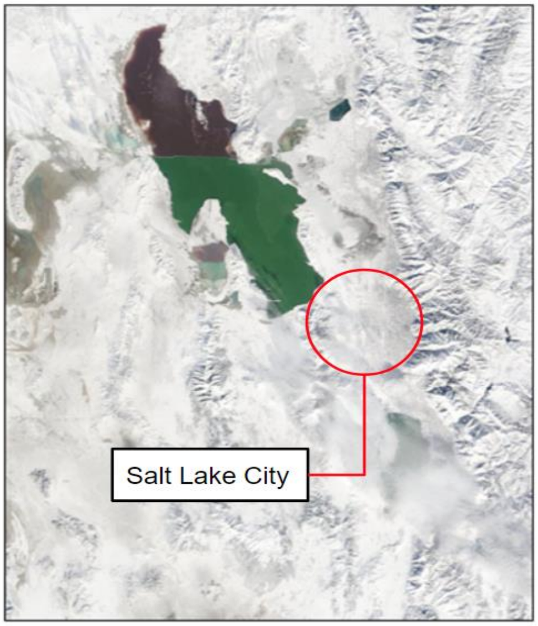

Figure 3. January 1, 2011 MODIS satellite imagery from the Terra platform centered over the GSL and SLV. Red Circle indicates Salt Lake City metropolitan area.

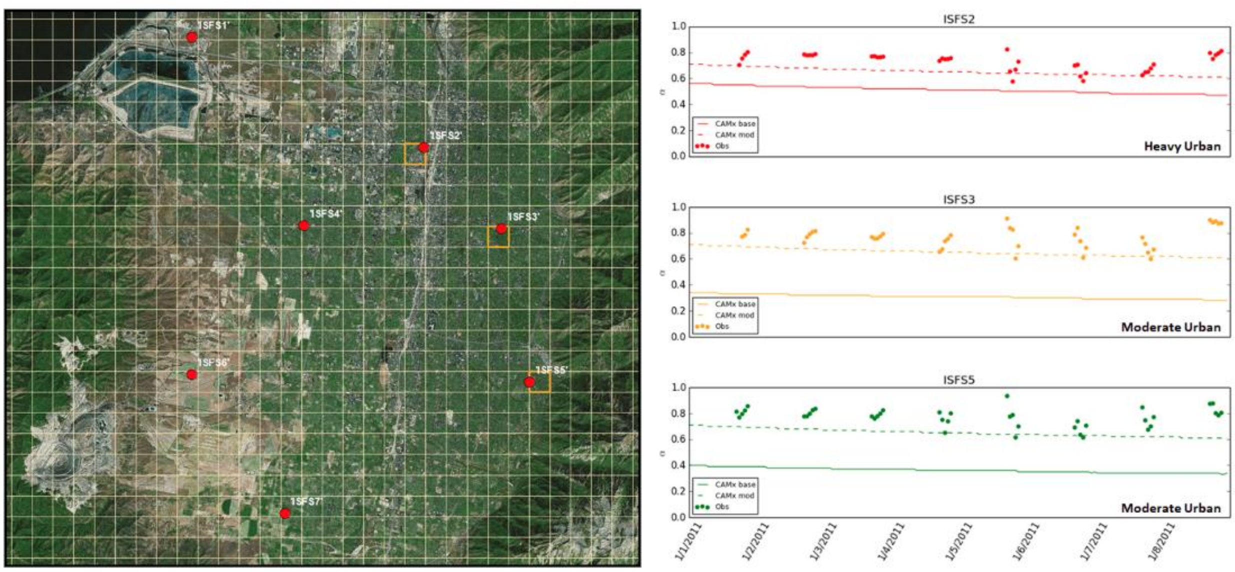

Figure 4. Left) Map of University of Utah surface radiation monitoring stations during January 2011 field monitoring study. Red dots show 7 monitor locations. Orange squares highlight model domain 1.33 km grid-cells collocated with 3 urban monitors. Right) For each of 3 urban monitors, dots show albedo measurements derived from observed radiation flux for January 1-8, 2011. Solid lines show default CAMx albedo at grid-cells collocated with each of the 3 urban monitors. Dashed lines show CAMx albedo after model modification.

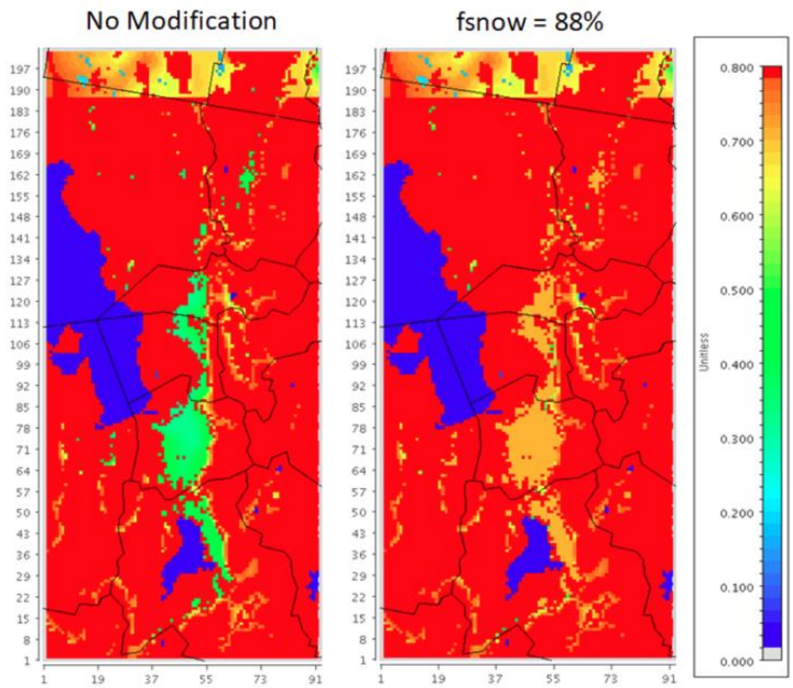

Figure 5. CAMx albedo for January 1 2011 over PM2.5 non-attainment areas. Left) Default CAMx albedo. Right) CAMx albedo after modification to urban land use albedo.

Minimized Ozone Deposition

Utah DAQ also enhanced particulate nitrate performance by reducing the amount of ozone lost to atmospheric chemistry via deposition. In CAMx 6.30, the dry deposition velocities for ozone and sulfur dioxides are explicitly assigned. The ozone dry deposition velocity in CAMx was changed to 0. Utah DAQ justified this model adjustment based on measurements collected in the Uinta Basin in 2013 during a typical winter-time inversion episode (2013 Uinta Basin Ozone Study[6]). Measurements showed that mean ozone deposition velocity was near zero during the inversion episode (Figure 6).

[6] https://documents.deq.utah.gov/air-quality/technical-analysis/DAQ-2017-009834.pdf

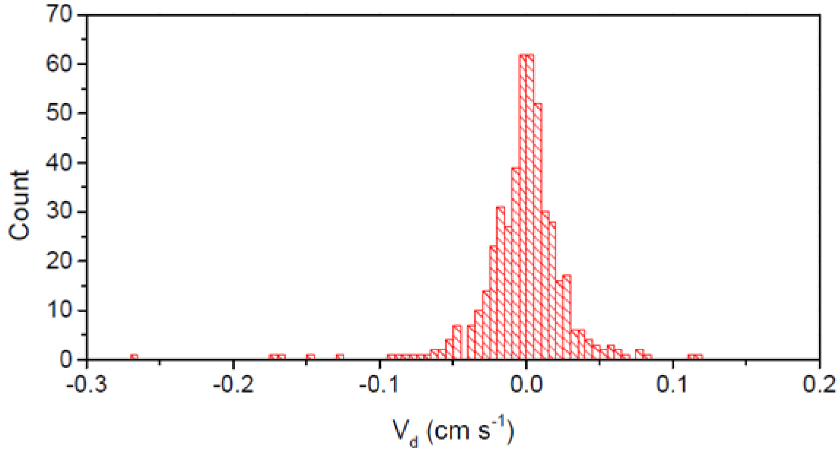

Figure 6. Histogram of ozone deposition velocity calculations for the snow-covered period (early February, 2013) inclusive of both nighttime and daytime data. Mean and median ozone deposition velocity were -0.002 and 0 cm s-1, respectively.

Paved Road Dust Emissions Adjustment

Initial CAMx simulations indicated a high model bias for crustal material. This overprediction in crustal material was attributed to an overestimation in the emissions since applying KVPATCH, which results in enhanced vertical mixing, did not have an impact on modeled crustal material (Figure 7). Considering that paved road dust emissions account for 88% of crustal material emissions, the high model bias was specifically attributed to an overestimation in the emission factor used for estimating paved road dust emissions. To enhance the model performance for crustal material, Utah DAQ reduced paved road dust emissions by 93%. A comparison between measured and modeled PM2.5 species at Logan monitoring station shows better agreement for crustal material following the application of the 93% reduction factor in paved road dust emissions (Figure 8).

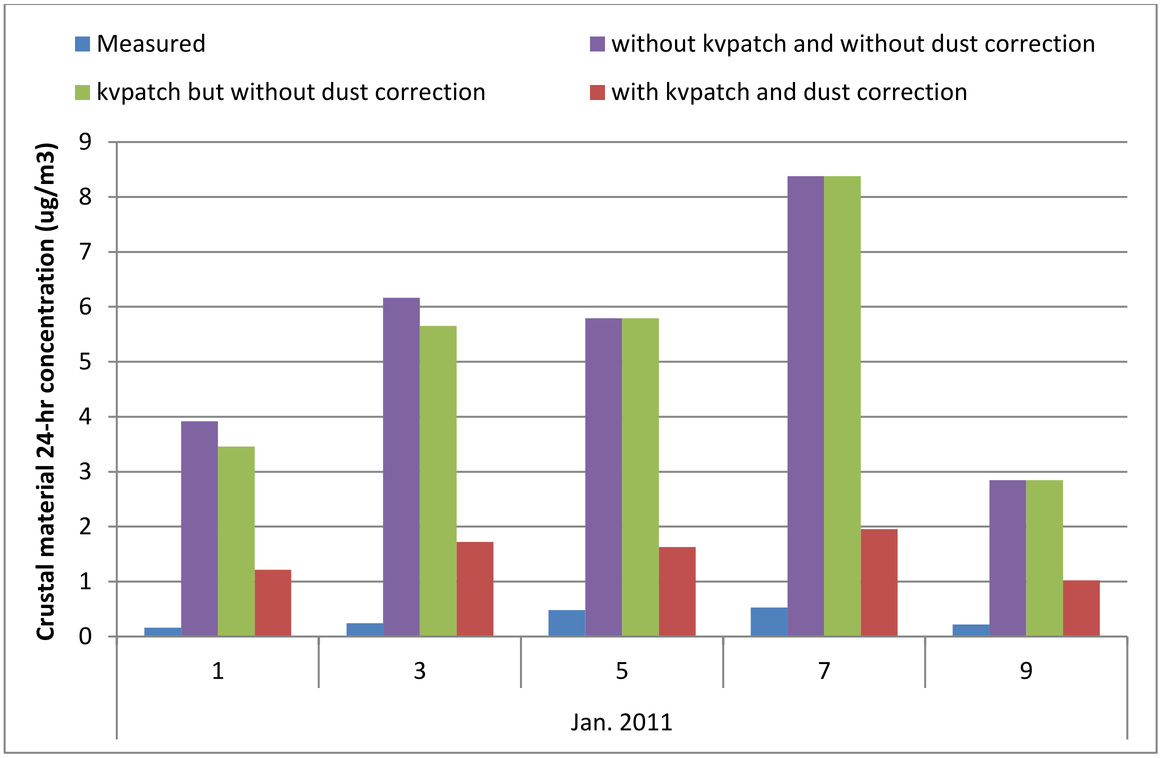

Figure 7. Measured and modeled crustal material concentration on January 1, 3, 5, 7 and 9 2011 following the application of KVPATCH and correction to paved road dust emissions.