Model Modifications

Utah Division of Air Quality

Introduction

Utah DAQ made several key modifications to their CAMx 6.30 modeling. Model modifications improved air quality model performance by reducing three sources of model bias:

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

The modifications are listed below:

- 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 ammonium nitrate performance.
- Vertical diffusion rates were increased to compensate for discrepancies between WRF output and meteorological measurements.
- Changed urban snow surface albedo to 88%. This increase increased photolytic chemistry and improved particulate nitrate performance.
- Low-altitude cloud water over Salt Lake County was reduced by 80%. This modification greatly reduced model bias for particulate sulfate.
- Ozone dry deposition rate was set to nearly zero. This increased the oxidant budget in the Salt Lake Valley airshed and promoted secondary aerosol formation.

These modifications will be discussed in turn.

Ammonia injection

In this document, ammonia injection is defined as artificially adding non-inventoried ammonia emissions to the inventoried emissions input into the air quality model. There are two possible reasons additional ammonia is needed in the Utah DAQ emissions inventory:

1. Ammonia deposition velocity rates are too high in current air quality models[1].
2. Utah's emissions inventory lacks ammonia sources.

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[1] 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.

Ammonia is also a key precursor for ammonium nitrate formation. Ammonium nitrate can make up more than 60% of measured PM2.5 during wintertime persistent cold air pool conditions in the the Wasatch Front. Salt Lake Valley measurements of ambient ammonia concentrations are typically a lot larger than modeled ammonia. This low model bias in ammonia mirrors a profound underprediction of ammonium nitrate during elevated wintertime PM2.5 periods. Utah DAQ took several measures (mentioned later) to lower the discrepancy between measured and modeled ammonium nitrate. However, a negative model bias in ammonium nitrate persisted.

Utah DAQ speculated on the reason for possible missing sources of ammonia in the Utah emissions inventory. For example, mobile ammonia emissions may be underestimated by the MOVES 2014a model used for mobile emissions modeling. It's also possible that some agricultural sources are misrepresented or not captured in Utah's area source inventory. However, the actual reason for any gap in Utah's ammonia inventory is undetermined to date.

For a given county in the Salt Lake nonattainment area, Utah DAQ injected ammonia uniformly across grid-cells that corresponded to low elevation regions (< 6,000 ft ASL). It is reasonable to expect that missing anthropogenic ammonia sources are more likely located along valley floors. Also, there are no reliable ammonia measurements taken in upper elevation areas at this point.

Recent observations of ammonia showed that the discrepancy between measured and modeled ammonia varies among counties. Observations include ammonia measurements, collected using passive samplers by Utah State University (Randy Martin, 2016), at several locations throughout the Salt Lake and Cache Valleys for the period of January 19 - February 23, 2016. These measurements also include hourly ammonia data, using a URG 9000D ambient ion monitor located in the Salt Lake Valley during the winter of 2016.

To address the spatial variability in modeled ammonia bias, Utah DAQ varied the amount of injected ammonia on a county-by-county basis. Below, is an table of injected ammonia values:

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

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

Ammonia injection emissions rates were 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.

Figure 1, below, compares weekly averaged 2016 passive ammonia measurements (bottom panel) to 2011 daily averaged modeled ammonia (with ammonia injection, top panel) at four sites within the Salt Lake nonattainment area. The two panels suggest that CAMx is within range of measured ammonia concentrations after ammonia injection.

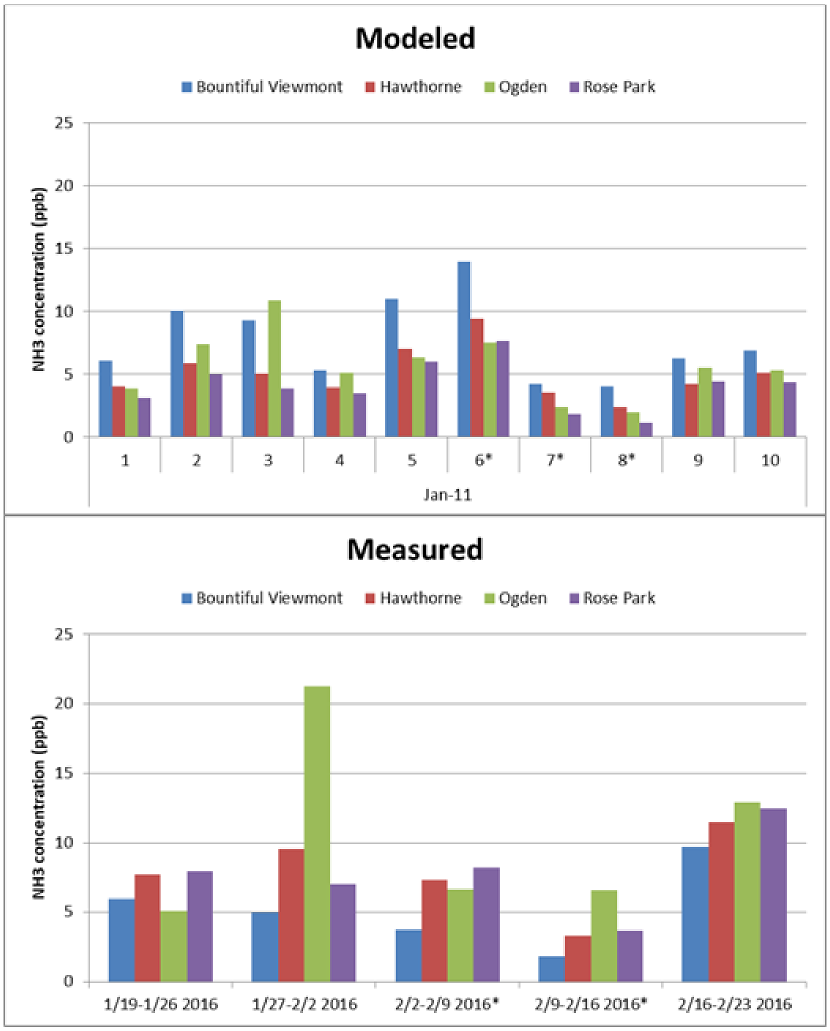

Figure 1: (top) Daily averaged modeled ammonia (top panel) for January 1-10, 2011. Asterisks note days where modeled 24-hour $PM_{2.5}$ was greater than 35 µg/m^3. (bottom) Seven-day averaged measured ammonia for January 19 - February 23, 2016. Asterisks note weeks where measured $PM_{2.5}$ was greater than 35 µg/m^3 for most of that week.

Increased surface resistance to ammonia

Ramboll discovered CAMx underpredicted ammonia because the ammonia dry deposition rate in the model was too high. The ammonia dry deposition rate was too high because there was no surface resistance to ammonia in the model. Utah DAQ modified the CAMx chemistry parameter (Rscale) so that surface resistance to ammonia was maximum. Therefore, the ammonia dry deposition rate was decreased and ammonium nitrate performance improved.

Increased vertical diffusion rates

During the January, 2011 episode, clouds in Salt Lake County trapped heat near the surface and increased the the mixing layer depth. These clouds were not simulated by WRF and modeled 24-hour PM2.5 concentrations were biased quite high during this period (not shown). To reduce the unrealistic bias in PM2.5, Utah DAQ applied the KVPATCH (Ramboll) cloud water adjustment utility to WRF input. Utah DAQ used KVPATCH to increase vertical diffusion rates in the lower atmosphere. Increasing the vertical diffusion rates had the desired effect of depositing particulate compounds quicker and hence, lowering PM2.5 concentrations.

Increased urban snow albedo

The 10 day period of January 1- 10, 2011 saw the Salt Lake Valley covered in snow. Figure 2, below, shows snow covering the Salt Lake City metropolitan area during the first day of our modeled episode period. Due to persistent cold temperatures and high pressure conditions, snow stayed on the surface during the duration of the 10 day episode.

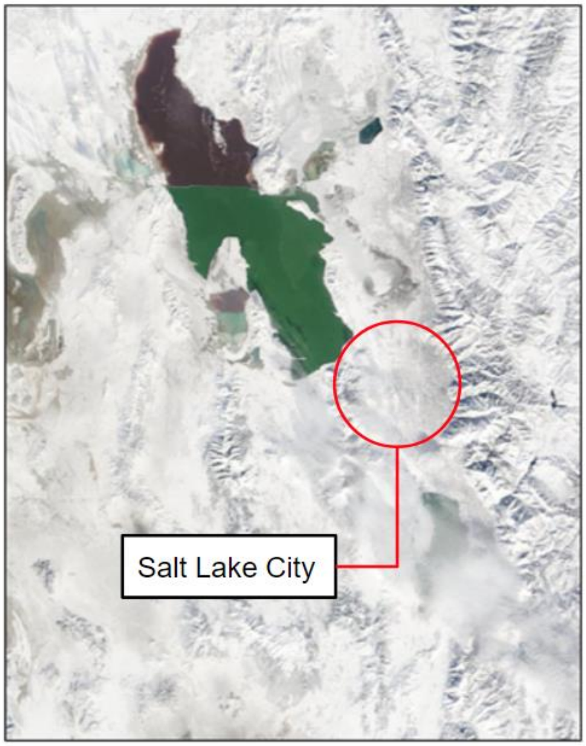

Figure 2: January 1, 2011 MODIS satellite imagery from the Terra platform centered over the GSL and SLV. Red Circle indicates Salt Lake City metropolitan area.

The Persistent Cold Air Pool Study (PCAPS) field campaign conducted by the University of Utah suggests that surface albedo during early January, 2011 period was significantly higher than what CAMx initially simulated over urban areas in Salt Lake Valley. Albedo measurements were derived from radiation measurements at 7 stations (figure 3, left panel) located throughout the Salt Lake Valley.

Because radiation depends on solar angle, only radiation measurements taken around when solar angle was near maximum was used for albedo calculations. Three monitoring stations were located in urban areas, where the local landscape is dominated by man-made structures and roads. Figure 3 (right panel), below, shows a comparison between CAMx (prior and post-modification) to January 1-8, 2011 observations.

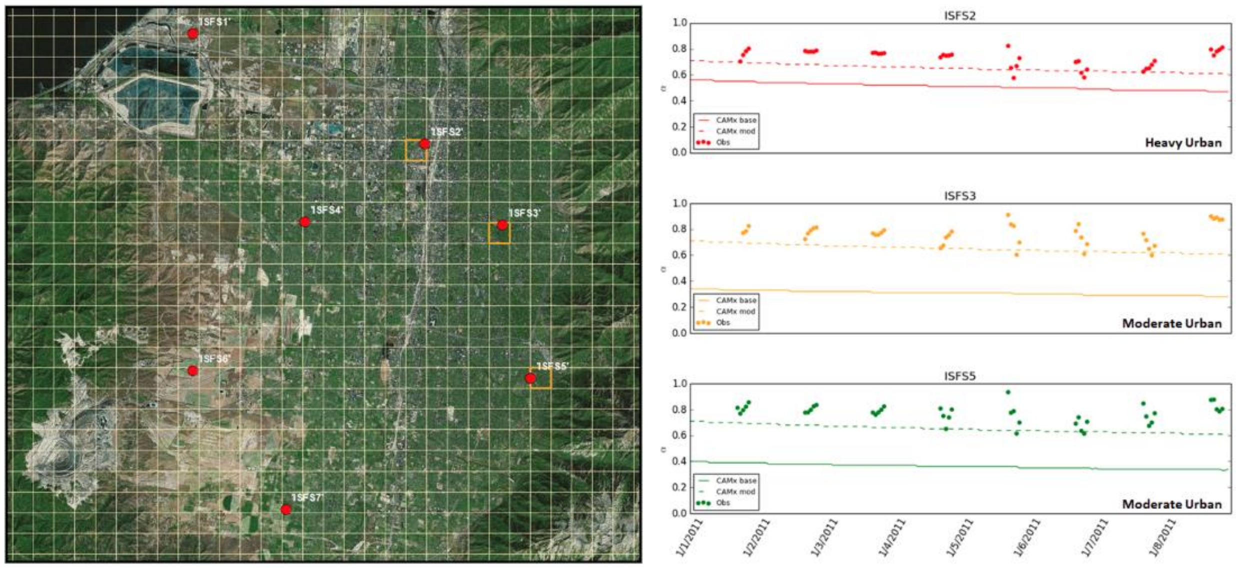

Figure 3: (left) Map of Univ. of Utah surface radiation monitoring stations during 2011 study. Red dots show 7 montor locations. Orange squares highlight model domain 1.33 km grid-cells collocated with 3 urban monitors. (right) For each of 3 urban monitors, dots show albedo measurements derived from observed radiation flux for January 1-8, 2011. Solid lines shows default CAMx albedo at grid-cells collocated with each of 3 urban monitors. Dashed lines show CAMx albedo after model modification.

Low surface albedo inhibits photolytic chemistry and therefore, limits the production of secondary aerosol. Utah DAQ modified the CAMx source code to change the urban albedo from ~33% to 88%. Figure 4, below, shows simulated CAMx albedo in North Utah before and after the model modification. This increased urban albedo improved modeled nitrate performance at Salt Lake Valley monitors.

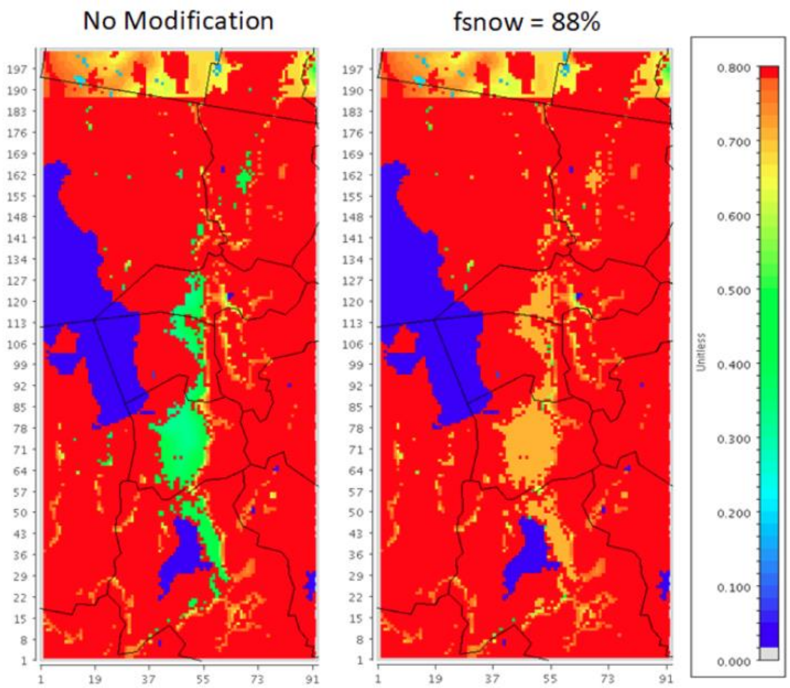

Figure 4: CAMx albedo for January 1, 2011 in North Utah. (left) Default CAMx albedo. (right) CAMx albedo after modification to urban land use albedo. After the CAMx modification, surface albedo in urban areas was closer to observations during this period in the Salt Lake Valley.

Reduced cloud water

Utah DAQ modified cloud water concentrations to improve the model performance of particulate sulfate. Initial model runs showed that the CAMx model produced a high modeled bias for sulfate during January 6 - 8. During this time, near-surface clouds were observed over the Salt Lake Valley (figure 5, below). This high model bias was related to the effect of ammonia on the gas-to-particle partitioning of sulfate in clouds. The presence of ammonia increased the in-cloud neutralization of sulfuric acid on these days, which resulted in the increased conversion of gaseous sulfur dioxides to particulate sulfate.

To reduce the high model bias in particulate sulfate at Hawthorne, Utah DAQ applied a utility (Ramboll) that reduced the cloud water content in WRF input. A cloud water reduction factor of 80% was applied to the cloud cover extending over Salt Lake County and the first 17 atmospheric layers.

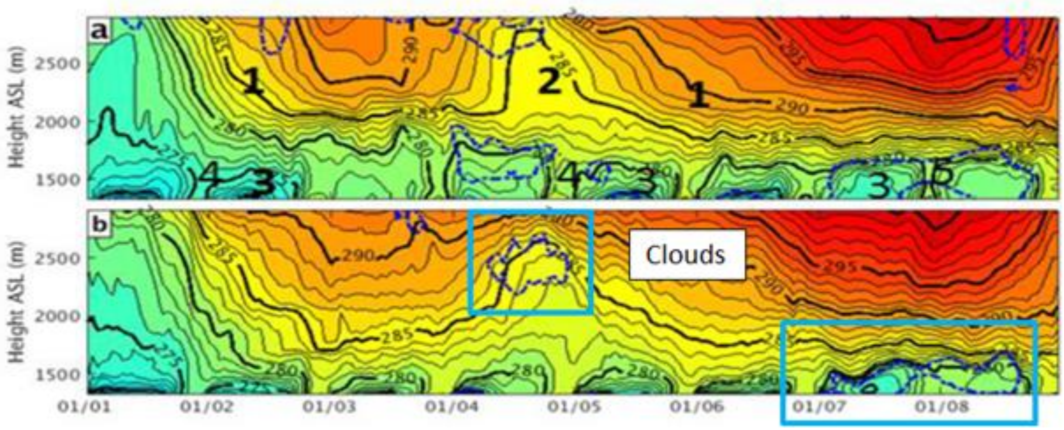

Figure 5: a) Observed potential temperature (K) and RH (90% threshold, dashed blue line) b) Modeled potential temperature (K) and cloud water mixing ratio (0.1 g kg-1 threshold, dashed blue line) in Salt Lake Valley. Courtesy of Erik Crosman, University of Utah.

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 modified to be near 0. Utah DAQ justified this model adjustment based on measurements collected from the 2013 Uintah Basin Ozone Study[2] (UBOS). Figure 6, below, shows that February, 2013 mean ozone deposition measurements in Utah's Uintah Basin region were near zero during wintertime conditions similar to the modeled January, 2011 Salt Lake Valley episode.

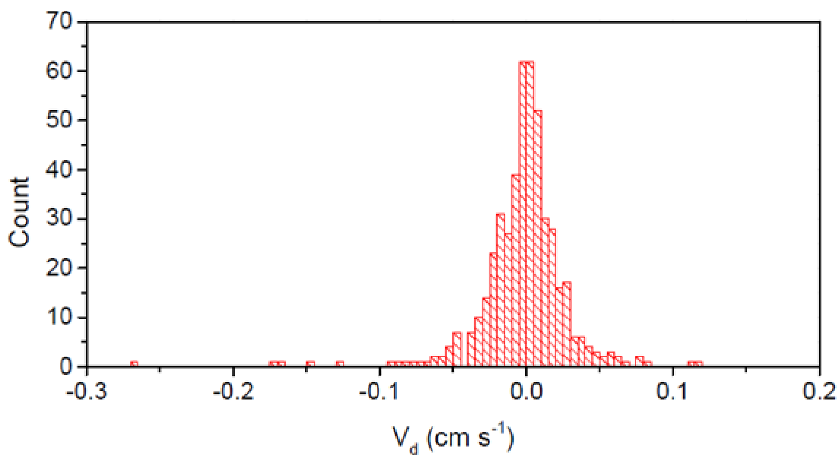

Figure 6: Histogram of ozone deposition velocity calculations for the snow-covered period (early February, 2013) inclusive of both nighttime and daytime data. Mean and median ozone deposition velocity were -0.002 and 0 cm s-1, respectively.

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