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
- Positive model bias in particulate sulfate
- 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 increase increased photolytic chemistry and improved particulate nitrate performance.
- Low-altitude cloud water content over Salt Lake and Utah Counties was reduced by 80 and 95%, respectively. These modifications 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.
- To reduce the model high bias for crustal material, a 93% reduction was applied to paved road dust emissions.

A detailed discussion of these modifications 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.

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

This ammonia shortfall in the model may be explained by:

- 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. Recent observations 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. They also include near-surface ammonia measurements conducted during a special field study in winter 2017 (2017 Utah Winter Fine Particulate Study (UWFPS)[4]).

A table of injected ammonia values per county is provided below:

[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.

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

Table 1. Emissions rates (tons/year) of ammonia injected in different counties, including Utah county in the Provo non-attainment area.

County	Tons/year
Cache	4,511
Box Elder	9,209
Davis	604
Salt Lake	622
Tooele	10,043
Weber	781
Utah	1,427

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.

To assess the model performance for ammonia following the ammonia injection, hourly modeled ammonia (Figure 1) at North Provo was compared to near-surface ammonia measurements (Figure 2) conducted during the 2017 UWFPS[5], 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.

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

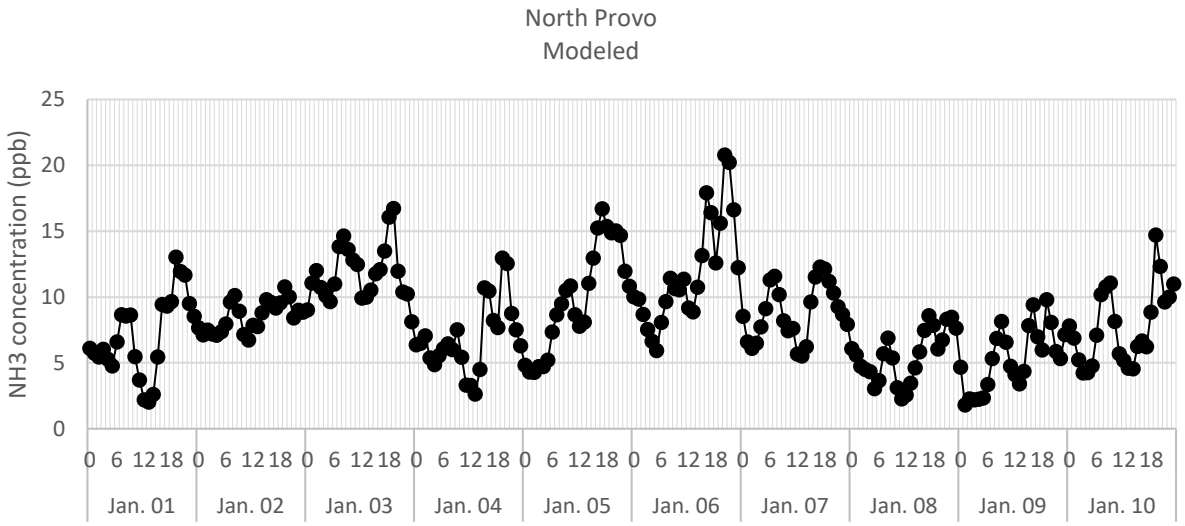

Figure 1. Hourly time series of modeled ammonia (ppb) at North Provo monitoring site during January 1 – 10 2011.

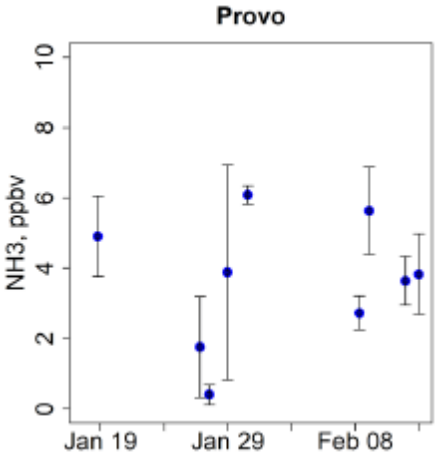

Figure 2. Ammonia mixing ratios during missed approaches at Provo airport in the Utah Valley. Figure retrieved from the 2017 Utah Winter Fine Particulate Study, final report, Figure 3.40 (https://www.esrl.noaa.gov/csd/groups/csd7/measurements/2017uwfps/finalreport.pdf).

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, thin mid-level clouds were observed on January 3-4 in Salt Lake County. These clouds, however, were not simulated in the meteorological model, leading to an increasingly stable low-level boundary layer, particularly at night[6]. This limited the mixing of pollutants on January 3rd in the model, resulting in an over-prediction in PM2.5 on this day (not shown). To reduce this high bias in PM2.5, Utah DAQ applied the KVPATCH utility in CAMx to WRF model output. Applying KVPATCH helped enhance vertical mixing in the lower atmosphere, leading to a better agreement between observed and modeled PM2.5.

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 in the Salt Lake Valley 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 Utah Valley were not available. However, while measurements for the Salt Lake Valley cannot be directly compared to those for the Utah 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 the Utah Valley[7]. 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 show in Figure 4 (right panel). Simulated CAMx albedo over PM2.5 non-attainment areas before and after the model modification is also shown in Figure 5. This increased urban albedo improved modeled nitrate performance.

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

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

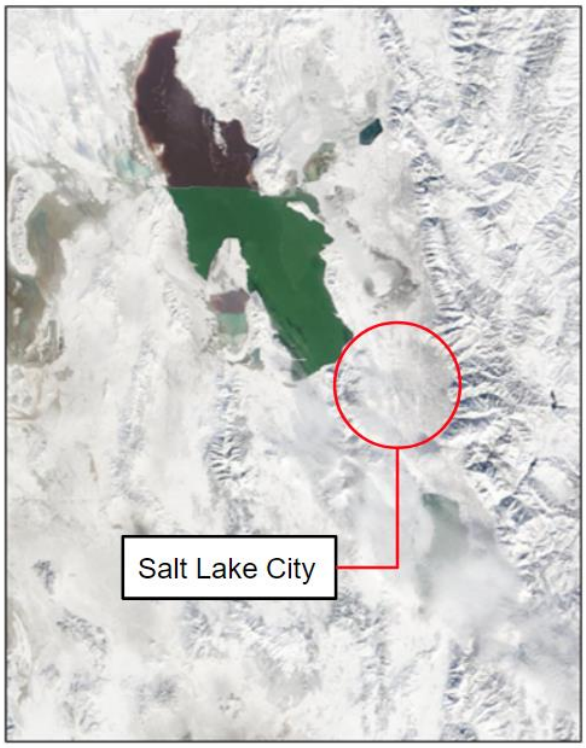

Figure 3. January 1, 2011 MODIS satellite imagery from the Terra platform centered over the GSL and SLV. Red Circle indicates Salt Lake City metropolitan area.

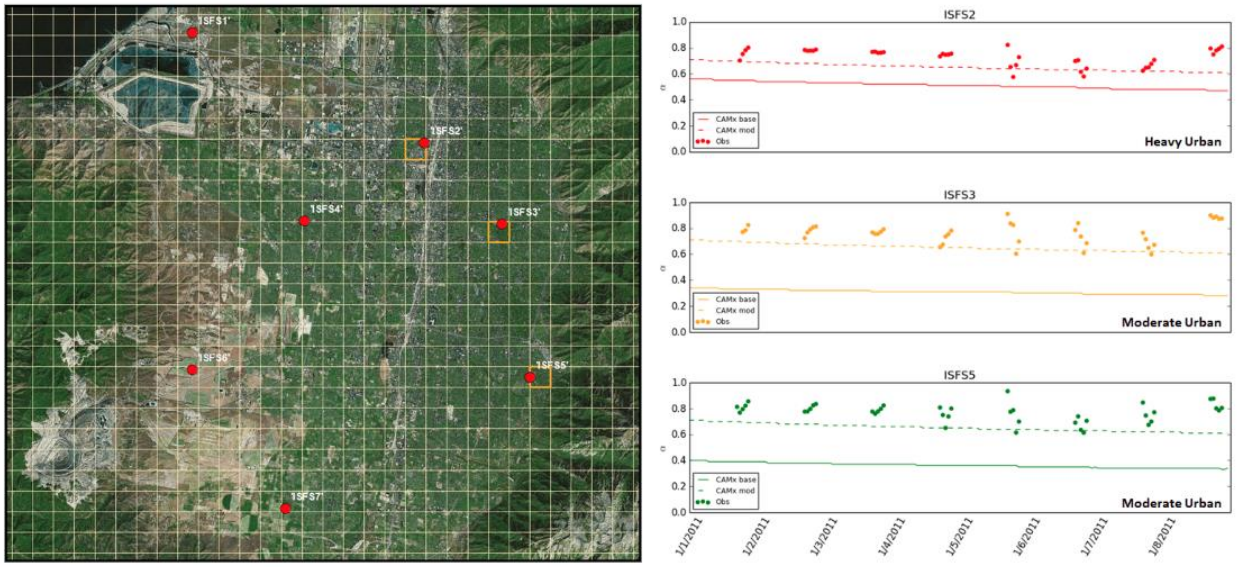

Figure 4. Left) Map of University of Utah surface radiation monitoring stations during January 2011 field monitoring study. Red dots show 7 monitor locations. Orange squares highlight model domain 1.33 km grid-cells collocated with 3 urban monitors. Right) For each of 3 urban monitors, dots show albedo 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.

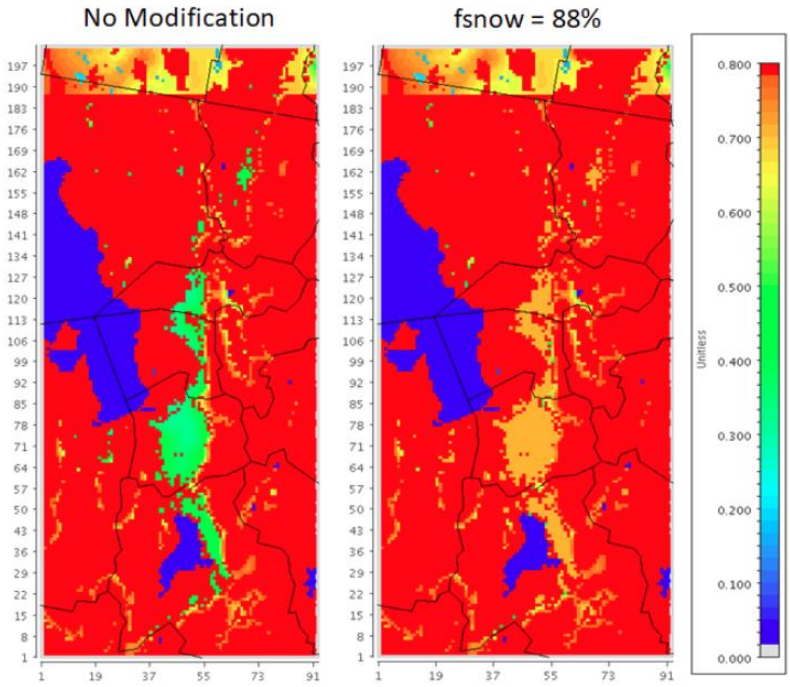

Figure 5. CAMx albedo for January 1 2011 over PM2.5 non-attainment areas. Left) Default CAMx albedo. Right) CAMx albedo after modification to urban land use albedo.

Reduced Cloud Water Content

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 2011, when near-surface clouds were observed over the Salt Lake and Utah Valleys (Figure 6, below). This high model bias was related to the impact of increasing ammonia on the conversion of SO2 to sulfate in clouds. The presence of ammonia increased the in-cloud neutralization of sulfuric acid on these days, which resulted in increased conversion of SO2 to particulate sulfate.

To reduce the high model bias in particulate sulfate at Hawthorne and Lindon air monitoring stations, Utah DAQ applied a utility, developed by Ramboll, that reduced the cloud water content in WRF model output. A cloud water reduction factor of 80 and 95% was applied to the cloud cover extending over the first 17 atmospheric layers over the Salt Lake and Utah Counties, respectively.

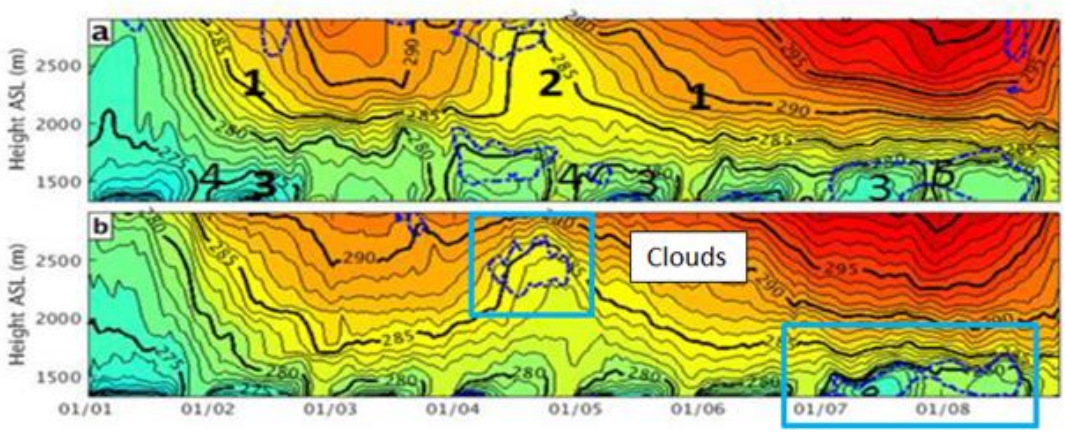

Figure 6. a) Observed potential temperature (K) and RH (90% threshold, dashed blue line) b) Modeled potential temperature (K) and cloud water mixing ratio (0.1 g kg-1 threshold, dashed blue line) in Salt Lake Valley. Courtesy of Erik Crosman, University of Utah.

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 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[8]). Measurements showed that mean ozone deposition velocity was near zero during the inversion episode (Figure 7).

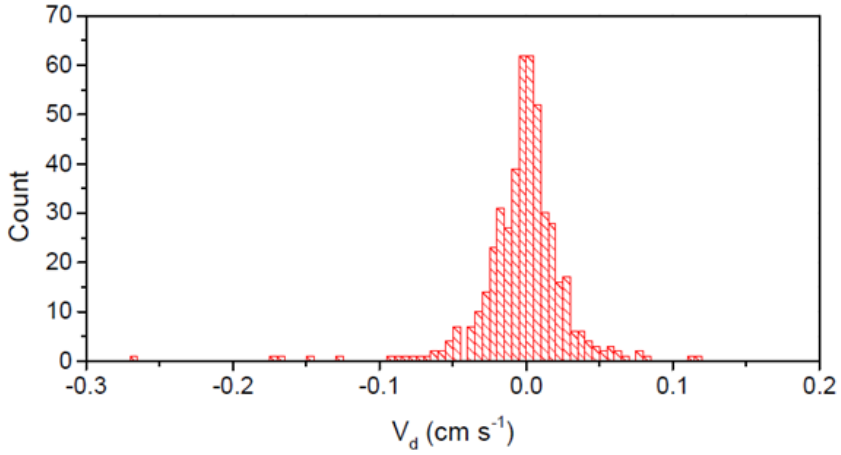

Figure 7. Histogram of ozone deposition velocity calculations for the snow-covered period (early February, 2013) inclusive of both nighttime and daytime data. Mean and median ozone deposition velocity were -0.002 and 0 cm s-1, respectively.

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

Paved Road Dust Emissions Adjustment

Initial CAMx simulations indicated a high model bias for crustal material. This overprediction in crustal material on days when the simulated atmospheric mixing was stronger than observed suggests that this overestimation is related to an overprediction in source emissions. 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).

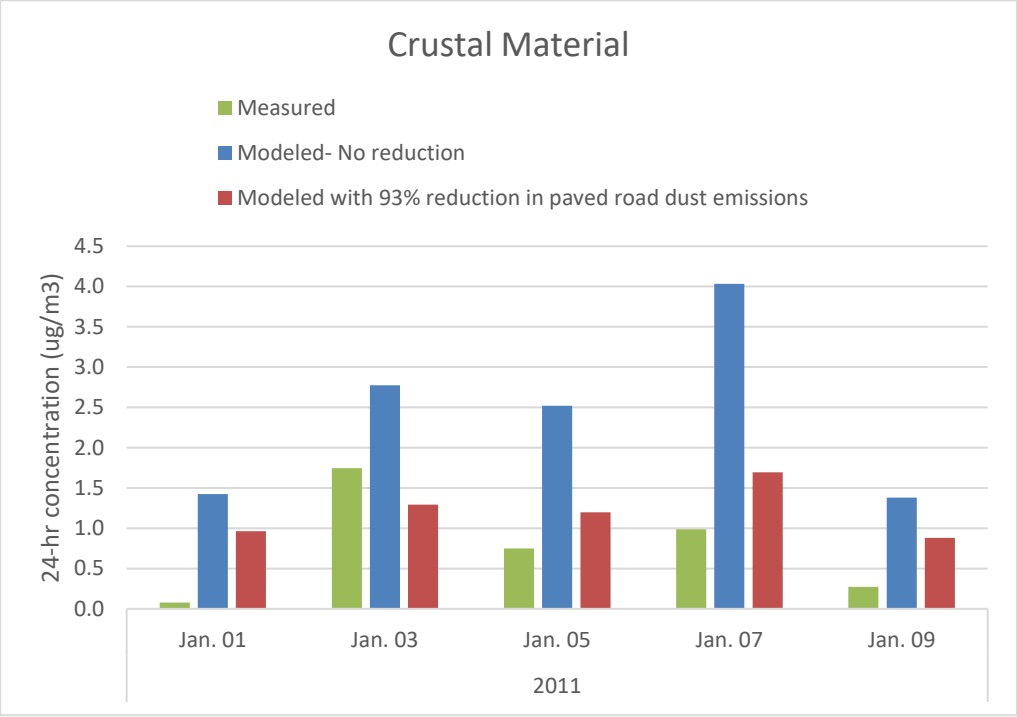

Figure 8. Measured and modeled crustal material concentration at Lindon monitoring station following the application of a 93% reduction factor to paved road dust emissions.