Investigating Sources of Ammonia Uncertainty in Modeling the Salt Lake City PM_{2.5} Nonattainment Area

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- Contributing Ramboll colleagues:
 - Dr. Chris Lindhjem, Tejas Shah, Yesica Alvarez, Sai Sreedhar Varada, Dr. Greg Yarwood



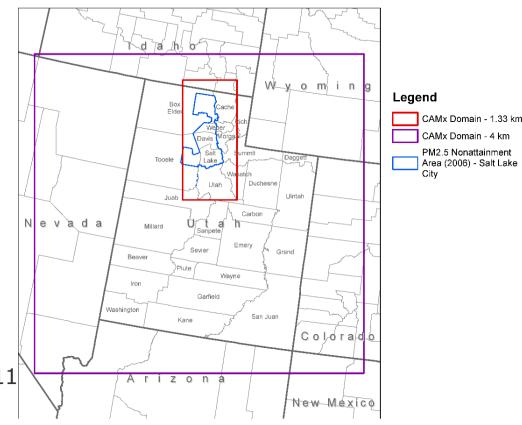
Overview

- Winter PCAP episodes can violate Federal 24-hour PM_{2.5} air quality standard
 - Buildup of ammonium nitrate (from NOx) and carbon (from smoke)
- UDAQ applies a photochemical model to assess/project PM_{2.5} levels
 - Model under predicts ammonium nitrate from lack of ammonia (NH₃)
 - Ad hoc blanket NH₃ emissions increase helps to alleviate under predictions
 - BUT: a major model uncertainty that may affect accuracy of projected $PM_{2.5}$
- We investigated causes for the modeled NH₃ shortfall
 - Benefitted from USU's 2019 WaFACO study
 - Reviewed emission inventories and measured concentration patterns
 - Investigated modeling uncertainties/deficiencies
 - Increased modeled NH₃ emissions from vehicles
 - Updated the model, re-evaluated modeling results and projected attainment-year PM_{2.5}



UDAQ Models and Datasets

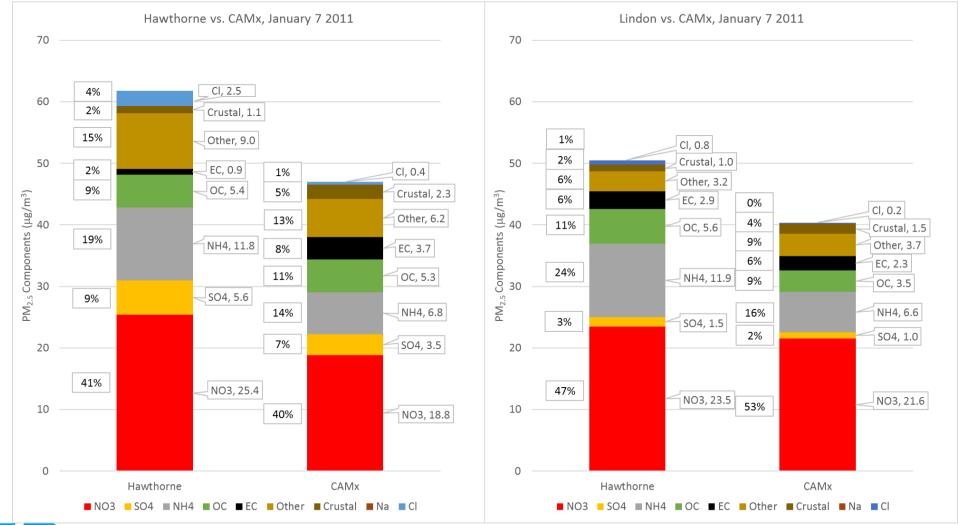
- Photochemical Model CAMx v6.3
 - PCAP event during January 1-10, 2011
 - Models dispersion, chemistry, surface sink for:
 - Gas precursors and oxidants: NOx, VOC, SO₂, CO, NH₃, ozone
 - PM_{2.5} components: sulfate, nitrate, carbon, salts, dust, other
 - Project PM_{2.5} levels to 2019 attainment year
- Meteorology WRF v3 (Crossman and Foster, 2016)
 - Hourly/gridded winds, temperature, humidity, clouds, etc.
- Emissions SMOKE v3.6.5
 - Hourly/gridded/chemically speciated based on Triennial 2011 and 2014 annual county-level inventories
 - Projected to future years: activity growth, vehicle fleet turnover, stationary source controls







UDAQ PM_{2.5} Base Year Modeling Peak PM_{2.5} Day on January 7, 2011







Ramboll Investigative Modeling

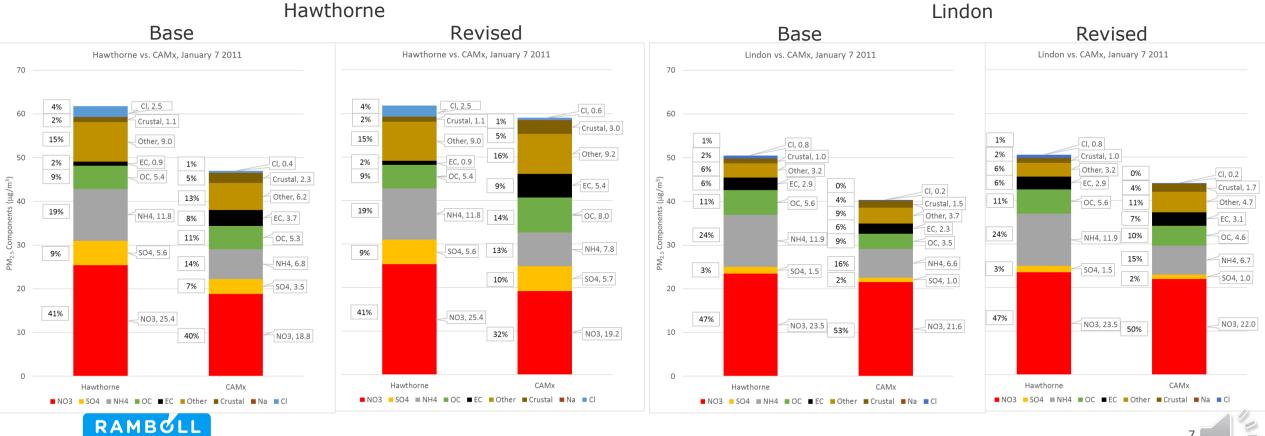
- Physical Processes
 - Vertical Mixing Reduce to improve simulated PM_{2.5} and gas concentrations, decrease apparent NH₃ shortfall
 - Bi-directional NH₃ Surface Exchange A source of NH₃ shortfall?
 - Snow cover squelches NH₃ deposition and re-emission, and daytime snow melt enhances deposition
- Emission Processes
 - On-Road Gasoline Vehicle NH₃ Emissions Scale-up ~2x as supported by scientific literature
 - On-Road Gasoline Vehicle NH₃ Emissions in Cold Weather Scale-up ~40% as supported by scientific literature
 - NOx Emissions Does remaining NOx under prediction bias affect PM_{2.5}?
 - Scale up of non-point NOx by 20% results in lower ammonium nitrate highly non-linear system!
- Chemical Processes
 - Inorganic PM Chemistry Does alternative chemistry affect PM_{2.5}? No significant impacts
 - Halogen Chemistry Do more chlorides impact PM_{2.5}? Negligible effects on total PM_{2.5} but higher particulate chloride
 - Snow Albedo Increase to observed levels have small effects on PM_{2.5}
 - Cloud Chemistry How does cloud over prediction impact PM_{2.5}?
 - Little photolysis sensitivity and an unwanted reduction in aqueous sulfate production





Revised Base Year Modeling

- Improved agreement for total PM_{2.5} mass over all site-days; especially inorganic compounds
- Largest relative errors remain for species that have small to negligible PM_{2.5} contributions



PM_{2.5} Projections to 2019

- 2017 and 2019 (attainment year) emission inventory from UDAQ
- We applied the same model updates as described previously
- EPA's Software for Modeled Attainment Test (SMAT) projects observed 2016-2018 design values (DV) to 2019 based on modeled projections
- Our 2019 $PM_{2.5}$ DV projections are similar to UDAQ's; all sites attain 35 μ g/m³ standard

| AIRS ID | Site Name, County | 2016-2018 DVb | UDAQ 2019 DVf | Ramboll 2019 DVf |
|-----------|-------------------------|---------------|------------------|---------------------|
| 490030003 | Brigham City, Box Elder | 32.4 | 33.5 | 33.4 |
| 490110004 | Bountiful, Davis | 28.5 | 28.3 | 28.6 |
| 490353006 | Hawthorne, Salt Lake | 33.4 | 34.0 | 33.2 |
| 490353010 | Rose Park, Salt Lake | 34.9 | 35.4 | 35.0 |
| 490494001 | Lindon, Utah | 31.1 | 29.8 | 30.6 |
| 490495010 | Spanish Fork, Utah | 28.4 | 28.9 | 28.5 |
| 490570002 | Ogden, Weber | 30.2 | 30.7 | 30.2 |



Conclusions

- Simulated urban PM_{2.5} responded well to increased on-road gasoline vehicle NH₃ emissions
 - Scale-up by a factor of ~2 is supported by scientific literature
 - UDAQ NH₃ injection added ~65% to Salt Lake County emissions, while the NH₃ scale-up added ~40%
- Final model resulted in improved agreement with PM_{2.5} measurements in urban areas
 - NH₃ (based on 2019 WaFACO) and sulfate are simulated well
 - Nitrate remains under predicted by \sim 30% (but consistent with other western US PM_{2.5} modeling)
 - Carbon (mostly from smoke) is over predicted and smoke speciation may need adjustment
 - Continued $PM_{2.5}$ under predictions at rural sites where agricultural NH_3 sources are important
- Projected PM_{2.5} DVs using the updated model were similar to UDAQ's projections
 - No sites projected to exceed the standard





Conclusions

- Modeling indicates basin is in "NOx-disbenefit" condition during PCAP events, in agreement with recent field studies
 - NOx-saturated and oxidant-lean
 - NOx emission reductions can raise oxidant levels and secondary PM formation rates
 - Has implications for accurately projecting PM_{2.5} based on anticipated emission inventory changes
- Modeling indicates basin is near balance between NH₃-limited and nitrate-limited conditions, in agreement with recent field studies
 - BUT: PM_{2.5} response is affected by remaining model uncertainties and biases



Recommendations

- Model a more recent PM_{2.5} episode to analyze contemporary air quality and update projections
- Carry key updates identified in this project into any new PM_{2.5} modeling
- Investigate improvements for meteorological simulations of PCAP episodes
- Improve NH₃ emission inventory and spatial allocation for livestock and landfills
- Investigate causes for under estimates of NOx and chloride
- Improve speciation for wood smoke among organic/elemental carbon and other components
- Investigate the role of snow in modulating surface-atmosphere NH₃ exchange
- Investigate impacts of all updates on PM_{2.5} response to future projected and/or alternative emissions scenarios







