Using CrIS Ammonia Observations To Improve Decision Making on PM$_{2.5}$ Control Policies

M. J. Alvarado$^1$, N. Heath$^1$, C. Calkins$^1$, C. R. Lonsdale$^1$, K. Cady-Pereira$^1$, E. H. Fahy$^1$ and M. Shephard$^2$

$^1$Atmospheric and Environmental Research (AER)  
$^2$Environment and Climate Change Canada

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**NH₃ is a PM₂.₅ precursor and reactive N species**

- Increase incidence of cardiovascular and respiratory diseases
- Increase number of CCN

- NH₃ is also one of the most important reactive nitrogen species
  - Leads to soil acidification, water eutrophication (e.g. algal blooms)
  - Ammonia is the least well understood part of the nitrogen cycle

\[ \text{NH}_3 + \text{HNO}_3 \leftrightarrow \text{NH}_4\text{NO}_3 \]
\[ 2 \text{NH}_3 + \text{H}_2\text{SO}_4 \rightarrow (\text{NH}_4)_2\text{SO}_4 \]
NH₃ sources are not well known

Biomass burning

Industry
- Fertilizer
- Coal Mining
- Power generation

AGRICULTURE
- Animal waste (temperature dependent)
- Fertilizer application

Automobiles (catalytic converters)
- Large urban centers
- 50% of NH₃ in LA area (Nowak et al., GRL, 2012)

Bi-directional Flux
CrIS can identify NH$_3$ sources

- CrIS Satellite NH$_3$ warm season (Apr. – Sept., 2013) average surface map, with corresponding AMoN surface network measurements overlaid.

CrIS Ground-Level NH$_3$

(Apr-Sep, 2013)
Project Goal

To use CrIS NH₃ retrievals to provide improved emission inventories of NH₃ to air quality (AQ) forecasters, AQ managers, and other stakeholders.

Project Objectives

1. Integrate the NASA CrIS NH₃ retrieved product and our CMAQ-based inversion methodology into a prototype application system on the Amazon cloud (ARL 4)
2. Develop model-ready updated NH₃ emission files for CMAQ, CAMx, and GEM- MACH and beta-test them in the end-user applications (ARL 5)
3. Demonstrate that the prototype application improves the simulation of NH₃ and inorganic PM₂.₅ in end-user modeling and leads to better decision making (ARL 6)
4. Fully integrate the prototype application into end-user decision-making (ARL 7)
Technical Approach For This Project

Once per month in CrIS Record

Schematic of the AQcast processing set up for this project on the Amazon cloud. The steps on the left outline include monthly iterations of the CrIS data record. The steps on the right outline each user output request.

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AQcast CMAQ System for Continental US

**Met Inputs**
- Reanalysis Data
- Real-Time Forecasts

**nCast WRF**
- WRF
- MCIP

**Global CTMs**
- NCAR Forecasts
- Other Inputs and Preprocessors
  - ICON/BCON
  - FEST-C
  - OMI O3
  - NormBEIS
  - Lightning

**Emission Inventory**
- NEI

**EPA Emission Modeling Platform Scripts**
- SMOKE

**CTM**
- CMAQ

**Air Quality Analyses**
- Sensitivity Studies
- Air Quality Forecasts
AQcast Production Architecture
Technical Approach For This Project

Schematic of the AQcast processing set up for this project on the Amazon cloud. The steps on the left outline include monthly iterations of the CrIS data record. The steps on the right outline each user output request.
Accomplishments and Current ARL

• Current ARL = 4. Goal ARL = 7
• After much debugging, we have successfully implemented a prototype application on the Amazon Web Services (AWS) cloud. The current application is limited to the continental US due to difficulties with expanding emissions to cover Canada.
• We used this prototype this quarter to refine our inversion methodology by using the NH$_3$ column (with averaging kernel applied) as our comparison metric of the model results and CrIS satellite.
• We used June 2015 for these comparison to test our ability to run the application for an arbitrary month.
• Results of the prototype are good, as illustrated at later in this presentation.
## Project Challenges & Risks

<table>
<thead>
<tr>
<th>Risk</th>
<th>Mitigation Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spatial surrogate files for Canada were inconsistent with emission platform</td>
<td>We will update to the latest EPA emissions platform and then expand our application grid from CONUS to North America early in 2021.</td>
</tr>
<tr>
<td>Parental leave and resignation of Key Co-I</td>
<td>In July we hired Nick Heath, formerly a post-doc on the EPA CMAQ development team. He has made substantial progress in the last two months to get us back on schedule.</td>
</tr>
<tr>
<td>COVID-19 Delays</td>
<td>Lockdowns related to COVID-19 have meant the team is working from home and have delayed interactions with end users at conferences as well as project work.</td>
</tr>
</tbody>
</table>
Total Column is Better Metric Than Surface Concentration

Column, 15 K Contrast

Column, 5 K Contrast

Surface, 15 K Contrast

Surface, 5 K Contrast
Prototype Test – June 2015 Inversion

- Initial CMAQ simulation underestimated CrIS NH$_3$ columns.
- Prototype uses finite-difference mass balance inversion (Lamsal et al., 2011).
- Requires two CMAQ model runs per iteration to estimate sensitivity to emissions (beta).
- Calculate emission scaling factors and apply to next iteration.
Prototype Results – June 2015 Inversion

CrIS Columns

Initial CMAQ Columns

Posterior CMAQ Columns
## Next Steps

<table>
<thead>
<tr>
<th>Milestone Statement</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Automate production of model-ready files and demonstrate the potential to improve the end user’s modeling (ARL 5).</td>
<td>12/2020</td>
</tr>
<tr>
<td>Confirm that the files can easily be used by the end user (ARL 5).</td>
<td>12/2020</td>
</tr>
<tr>
<td>Evaluate the new emissions using surface and aircraft data (ARL 6).</td>
<td>06/2021</td>
</tr>
<tr>
<td>Demonstrate that the application improves the end user’s modeling (ARL 6).</td>
<td>06/2021</td>
</tr>
<tr>
<td>Incorporate application into end user’s standard modeling (ARL 7).</td>
<td>11/2021</td>
</tr>
<tr>
<td>Transfer software to end users (ARL 7)</td>
<td>11/2021</td>
</tr>
</tbody>
</table>
## Project Budget, Obligations & Costing Status

### Project to Date (07/31/2020)

<table>
<thead>
<tr>
<th>Institution</th>
<th>Budget</th>
<th>Obligated</th>
<th>Unobligated</th>
<th>Costed</th>
<th>Uncosted</th>
</tr>
</thead>
<tbody>
<tr>
<td>AER</td>
<td>$764,879</td>
<td>$513,349</td>
<td>$251,530</td>
<td>$513,349*</td>
<td>$0</td>
</tr>
</tbody>
</table>

### Prior Year (01/01/2019-12/31/2019)

<table>
<thead>
<tr>
<th>Institution</th>
<th>Budget</th>
<th>Obligated</th>
<th>Unobligated</th>
<th>Costed</th>
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<tbody>
<tr>
<td>AER</td>
<td>$764,879</td>
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<td>$251,530</td>
<td>$346,100.51</td>
<td>$167,248.49</td>
</tr>
</tbody>
</table>

*We are using AER internal new hire funds for Co-I Heath to continue to make progress on the project until Year 3 funds are available.*
Summary

• This work will provide improved emission inventories of NH$_3$ to air quality (AQ) forecasters, AQ managers, and other stakeholders.

• We performed a closure study to determine the best metric for the CMAQ inverse modeling, concluding that the total column from CMAQ should be used after the observation operator is applied.

• We demonstrated the prototype application for continental US using simulations for June 2015 and the column metric described above. The prototype works and suggests that NH$_3$ emissions are dramatically underestimated in CMAQ.

• Next steps include expanding domain to cover Canada, evaluating the impact of improved emissions estimates on end user modeling, and incorporating the final application in end user’s modeling.

• Achieved ARL 4. Goal ARL for overall project is 7.
ADDITIONAL SLIDES
Limiting Scaling Factor to Prevent Overcorrection

CrIS

CMAQ-Base Average Column Total

CMAQ-Scaled Average Column Total

Initial CMAQ

“Beta” – Sensitivity of Column to Emissions

Posterior CMAQ

Emission Scaling Factor Limited to <5
Proof-of-Concept Inversion Method

• Finite-difference mass balance (Lamsal et al., GRL, 2011).
• Requires two model runs per iteration to estimate sensitivity to emissions.
• Calculate emission scaling factors and apply to next iteration.
Cross-track Infrared Sounder (CrIS)

- CrIS can monitor global NH$_3$ with high spatial coverage from 2011 and over the next decade or more

<table>
<thead>
<tr>
<th></th>
<th>TES</th>
<th>CrIS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Satellite</td>
<td>AURA</td>
<td>NPP and JPSS-1</td>
</tr>
<tr>
<td>Resolution</td>
<td>0.06 cm$^{-1}$</td>
<td>0.625 cm$^{-1}$</td>
</tr>
<tr>
<td>Footprint</td>
<td>5x8 km rectangle</td>
<td>14 km diameter circle</td>
</tr>
<tr>
<td>Repeat cycle</td>
<td>Once every 16 days</td>
<td>Daily</td>
</tr>
<tr>
<td>Equatorial crossing</td>
<td>1:30 am and 1:30 pm</td>
<td>1:30 am and 1:30 pm</td>
</tr>
<tr>
<td>Noise in NH$_3$ window</td>
<td>0.09 – 0.12 K</td>
<td>0.03 – 0.06 K</td>
</tr>
</tbody>
</table>
CrIS Satellite Ammonia Monitoring and Evaluation

Multi-year monthly comparisons of CrIS surface NH$_3$ with AMoN obs.

Stockton, Illinois

Fort Collins, Colorado

Initial assessment shows that the satellite and AMoN surface observations agree well despite sampling differences.
Linear AKs Have Less Bias for Moderately Polluted Cases

Mean Bias for +15K
(Cris - CMAQ) for 15K

Mean Bias for +5K
(Cris - CMAQ) for 5K

CMAQ No AK
CMAQ AK log

CMAQ AK linear – vmr limit xa
CMAQ AK linear – vmr max
Simulated CrIS NH$_3$ Col. Vs. CMAQ

- CMAQ No AK
- CMAQ AK log
- CMAQ AK linear – vmr limit xa
- CMAQ AK linear – vmr max