# 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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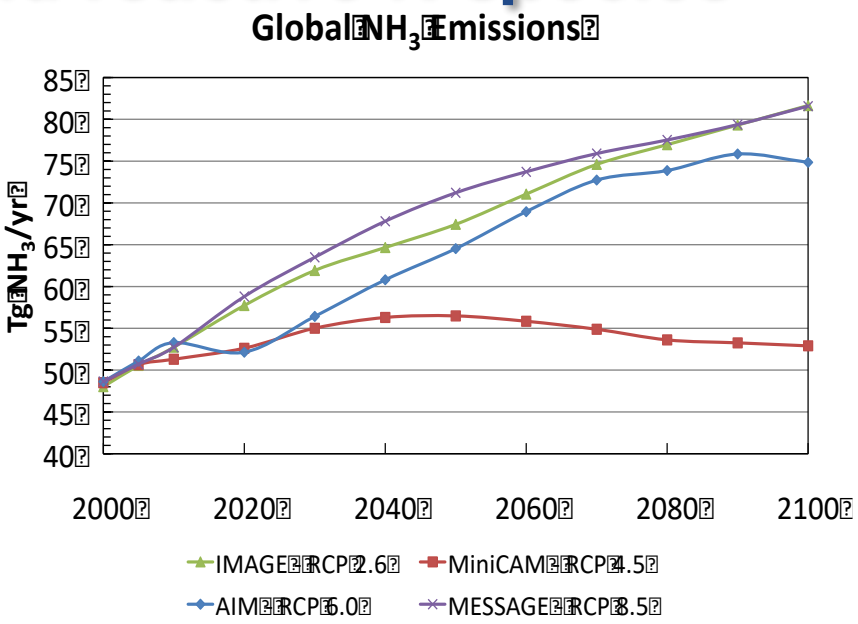
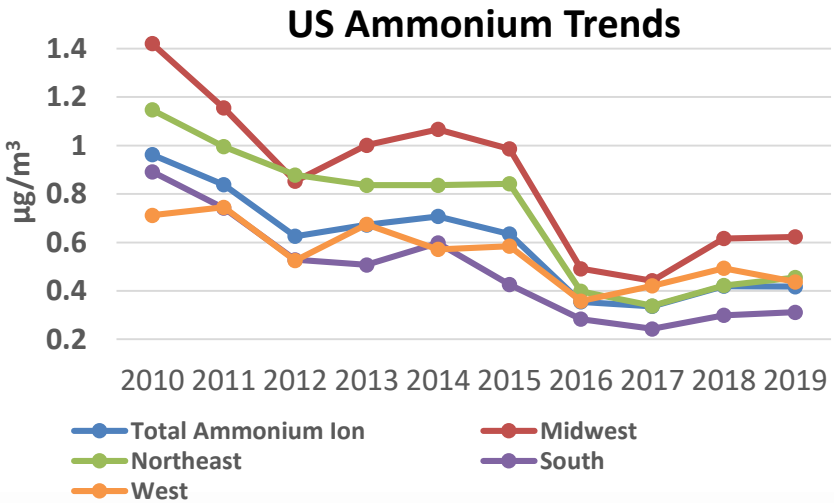
# $NH_3$ is a $PM_{2.5}$ precursor and reactive N species

$$NH_3 + HNO_3 \leftrightarrow NH_4NO_3$$
$$2\ NH_3 + H_2SO_4 \rightarrow (NH_4)_2SO_4$$

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

- $NH_3$ 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

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# $NH_3$ sources are not well known

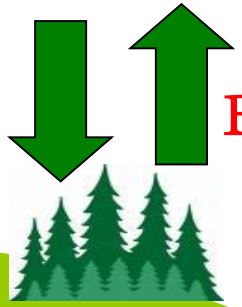
Biomass burning

Automobiles (catalytic converters)

- Large urban centers
  - 50% of $NH_3$ in LA area (Nowak et al., GRL, 2012)

Industry

- Fertilizer
- Coal Mining
- Power generation



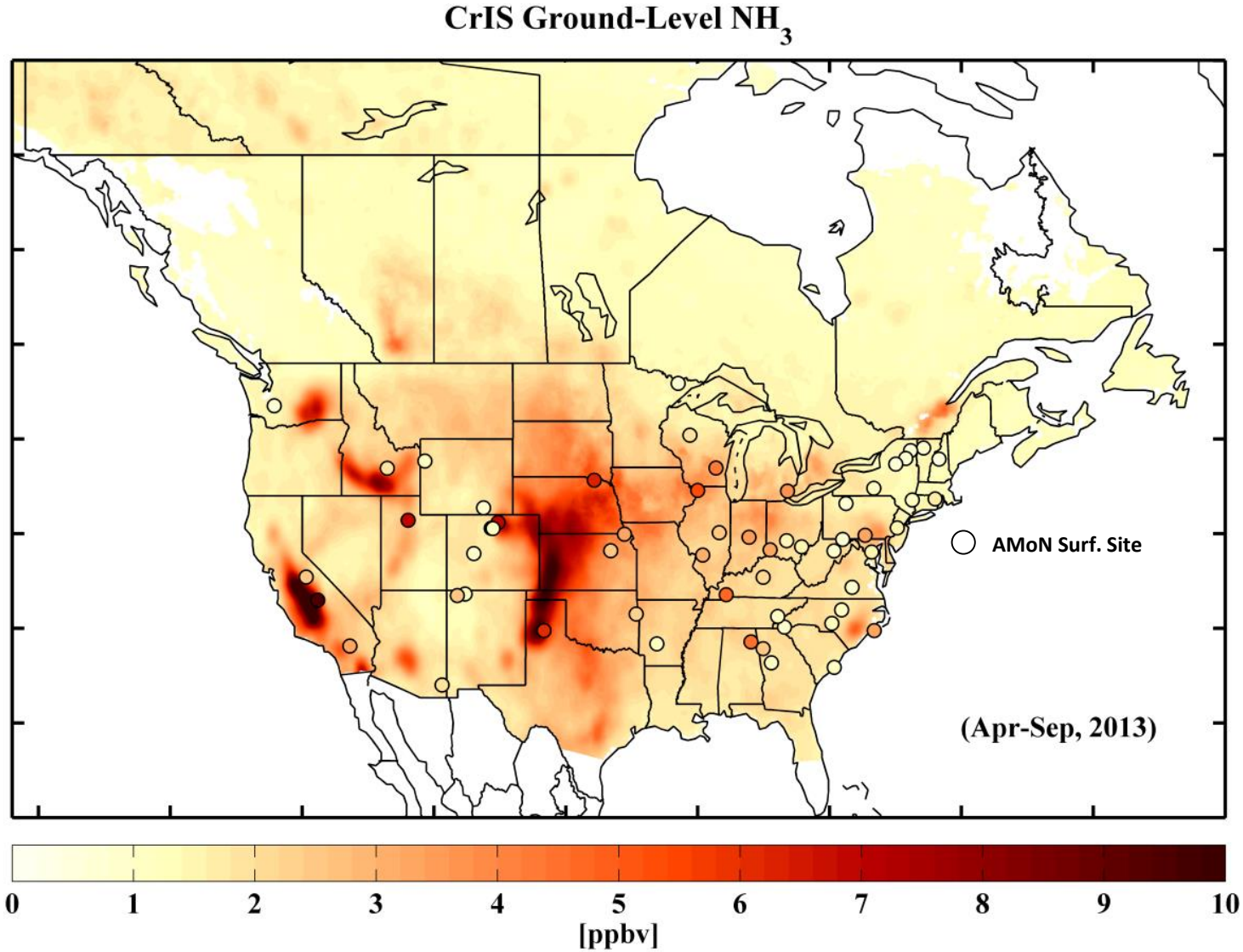
Bi-directional Flux

AGRICULTURE

- Animal waste (temperature dependent)
- Fertilizer application

# 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.



# Project Goal

**To use CrIS $NH_3$ retrievals to provide improved emission inventories of $NH_3$ to air quality (AQ) forecasters, AQ managers, and other stakeholders.**

# Project Objectives

1. Integrate the NASA CrIS $NH_3$ retrieved product and our CMAQ-based inversion methodology into a prototype application system on the Amazon cloud (ARL 4)
2. Develop model-ready updated $NH_3$ 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 $NH_3$ and inorganic $PM_{2.5}$ 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)

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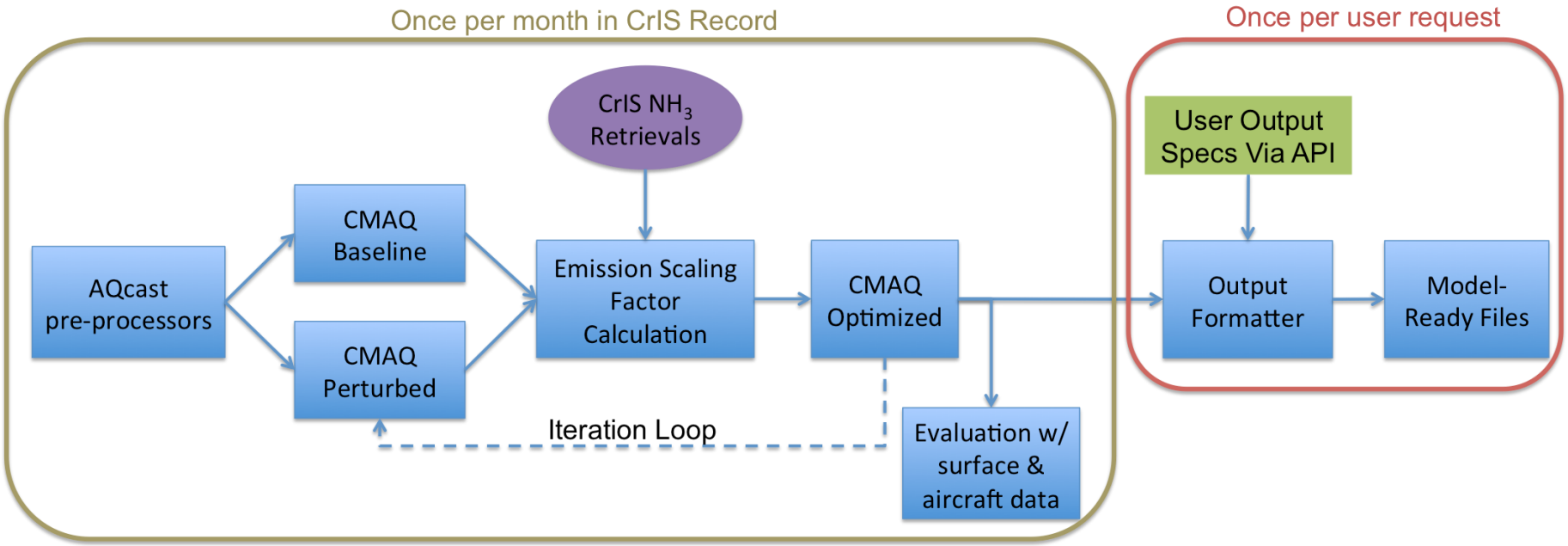
# Technical Approach For This Project




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.

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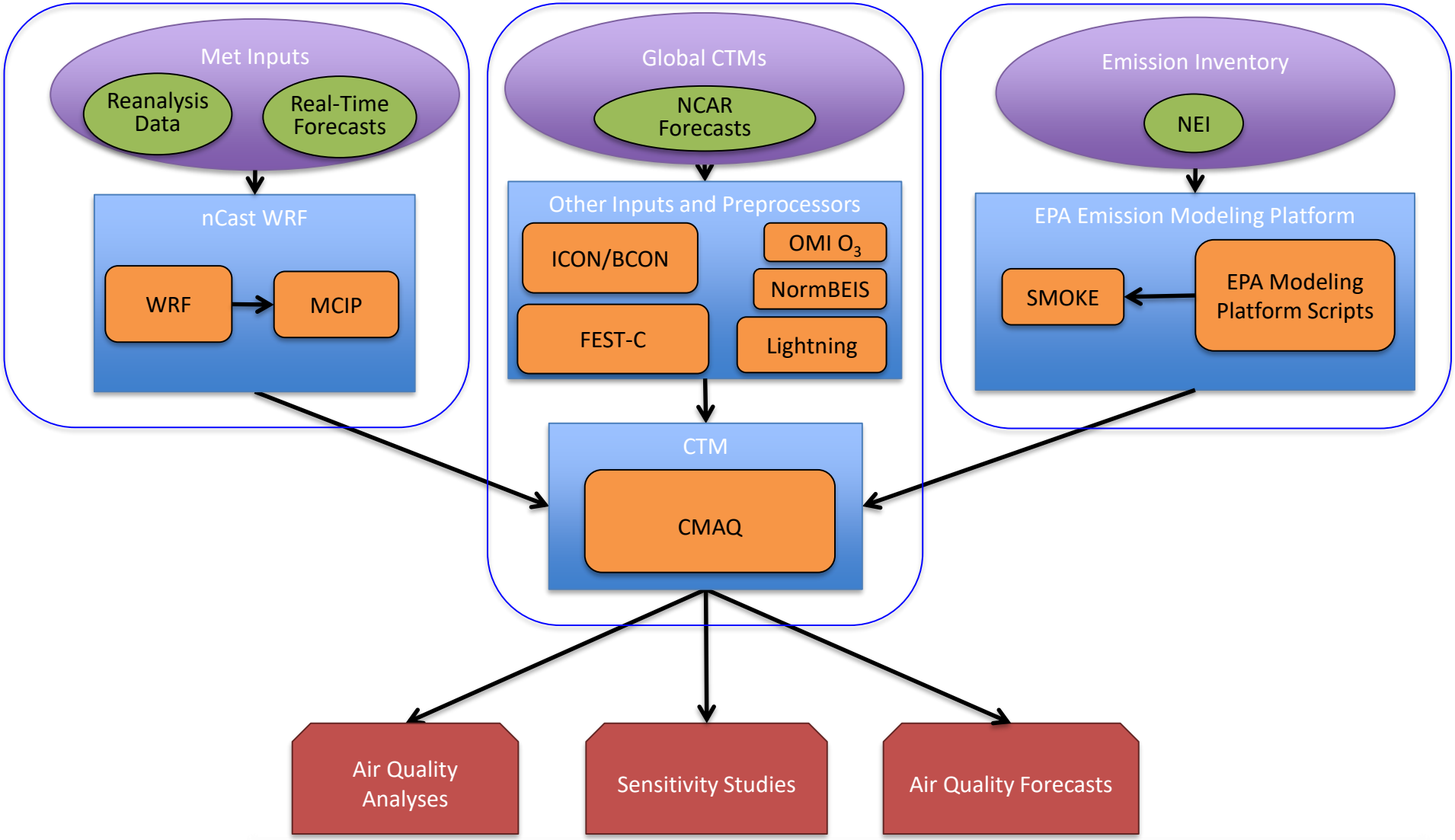
# AQcast CMAQ System for Continental US

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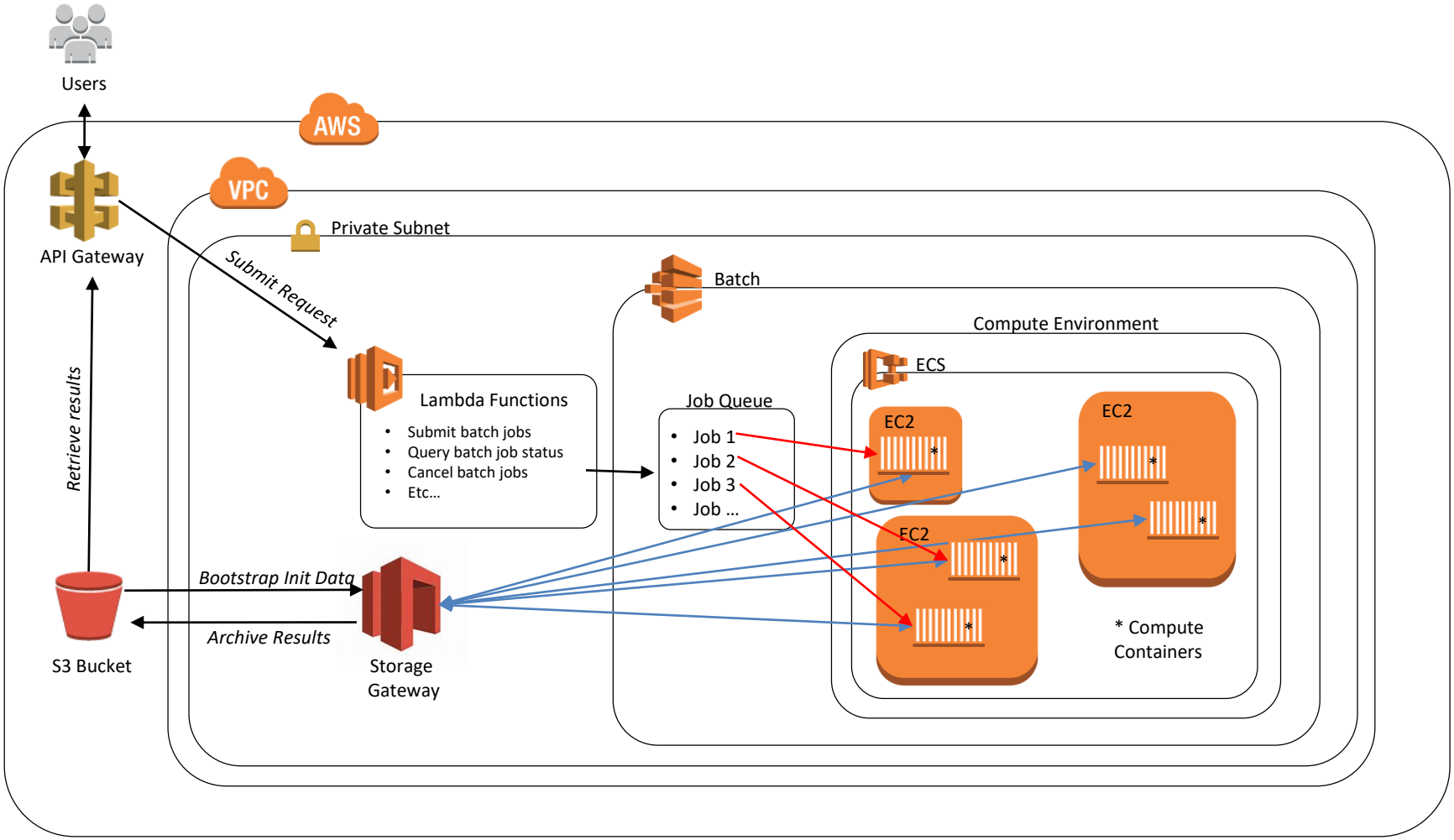
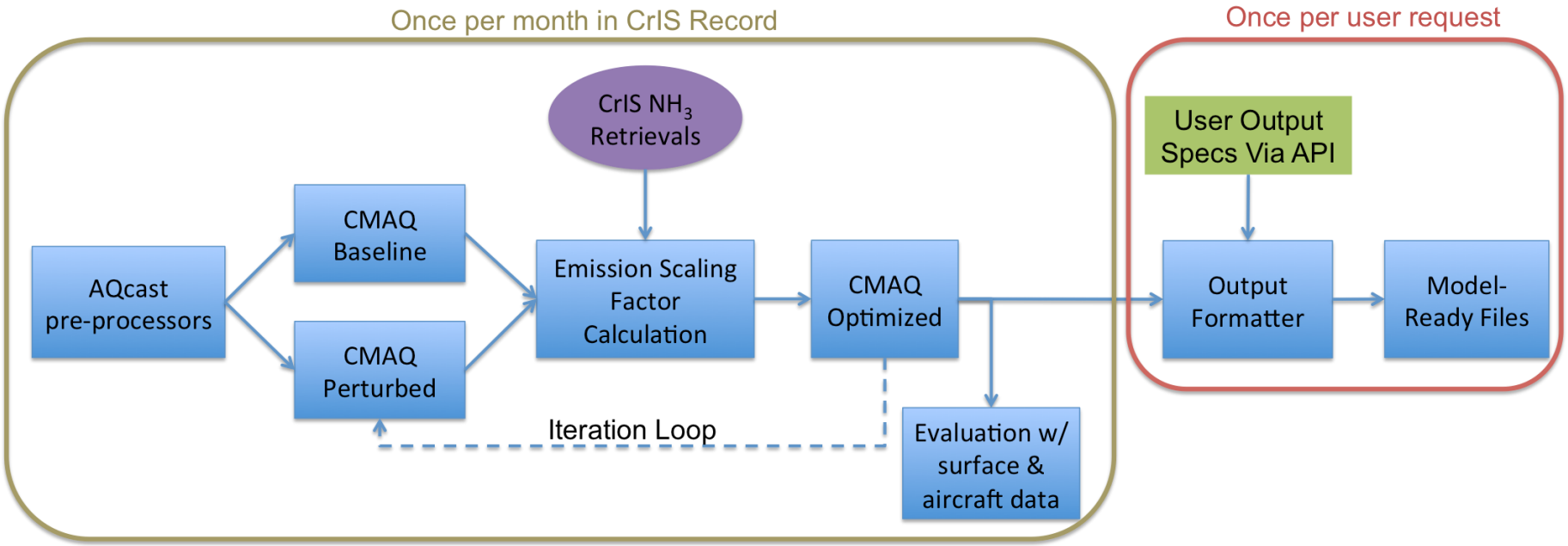
# AQcast Production Architecture



# 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.

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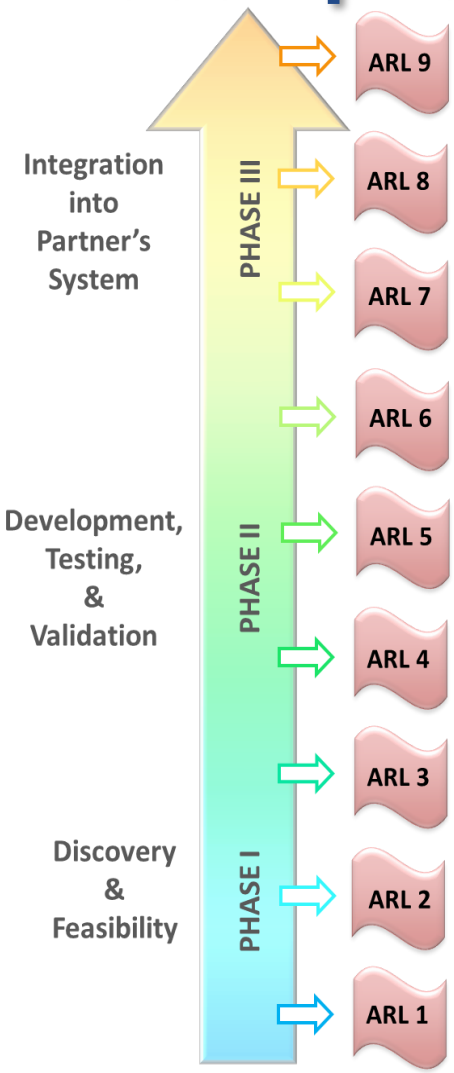
# Accomplishments and Current ARL




- 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.

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# Project Challenges & Risks

| Risk | Mitigation Action |
|---|---|
| Spatial surrogate files for Canada were inconsistent with emission platform | We will update to the latest EPA emissions platform and then expand our application grid from CONUS to North America early in 2021. |
| Parental leave and resignation of Key Co-I | 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. |
| COVID-19 Delays | 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. |

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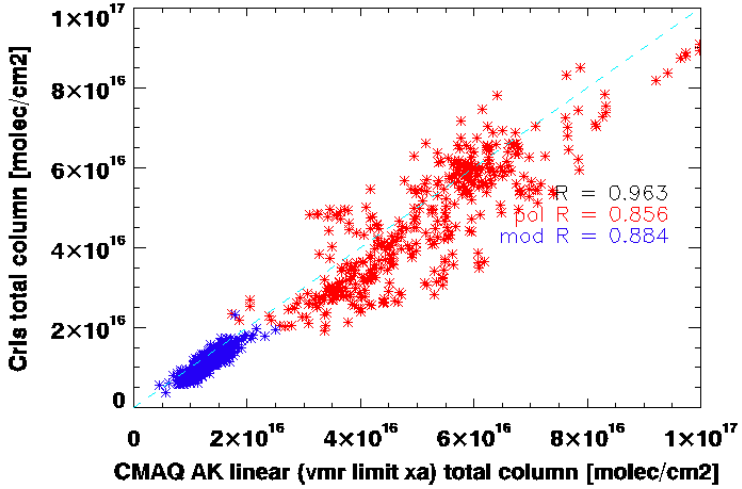
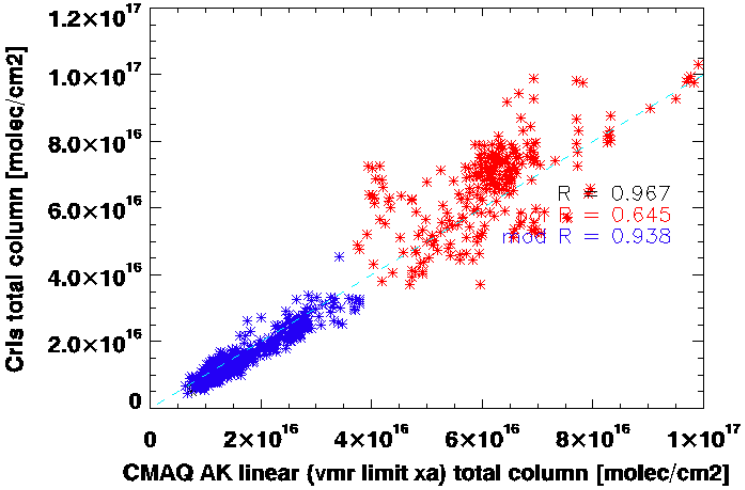
# Total Column is Better Metric Than Surface Concentration

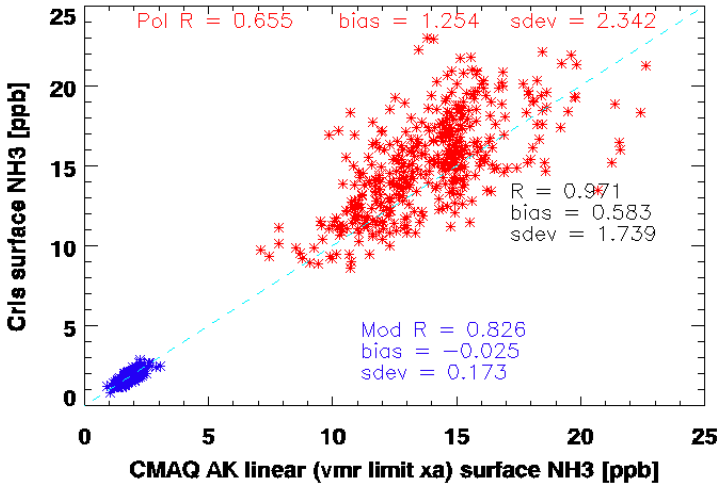
## Column, 15 K Contrast



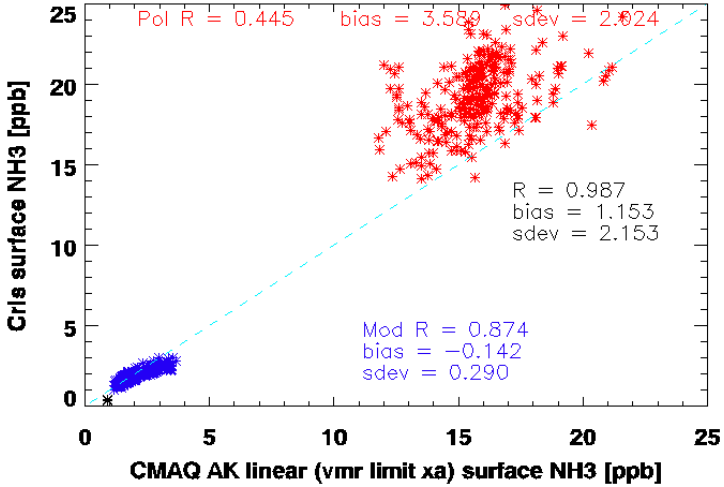

## Column, 5 K Contrast




## Surface, 15 K Contrast



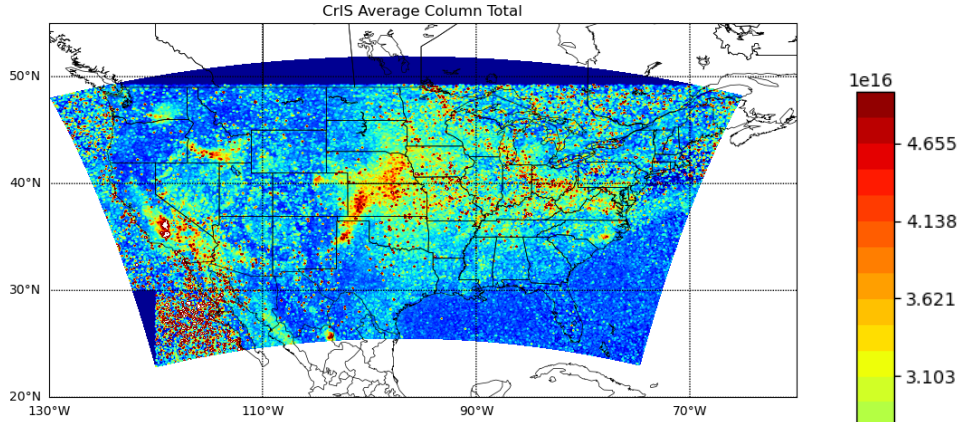

## Surface, 5 K Contrast



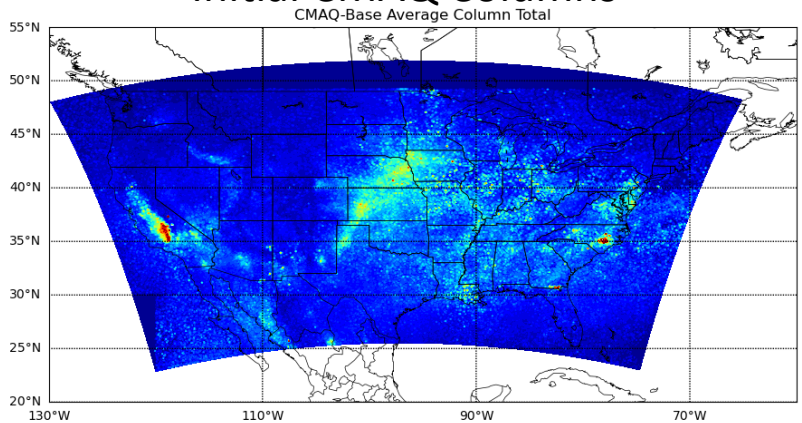
# Prototype Test – June 2015 Inversion

- 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.

CrIS Columns

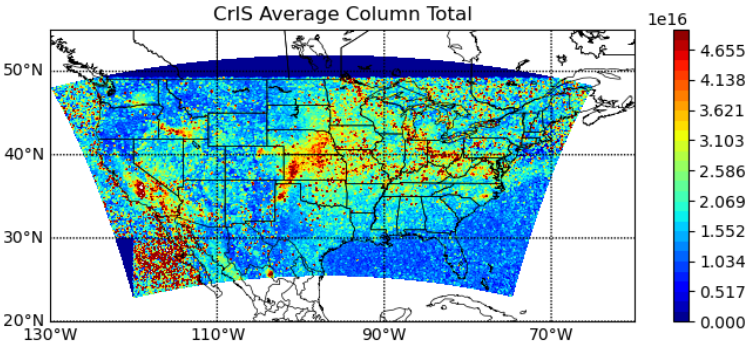



Initial CMAQ Columns

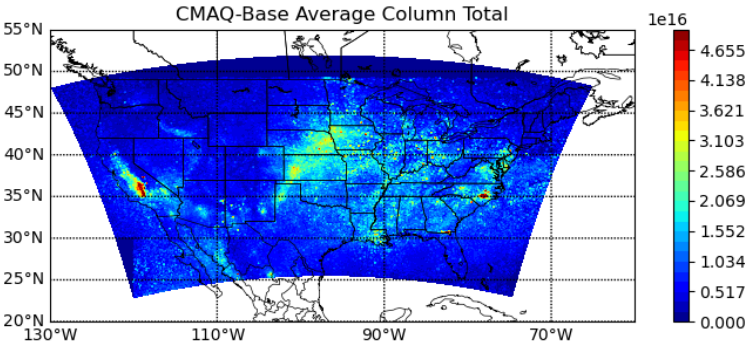


# Prototype Results – June 2015 Inversion

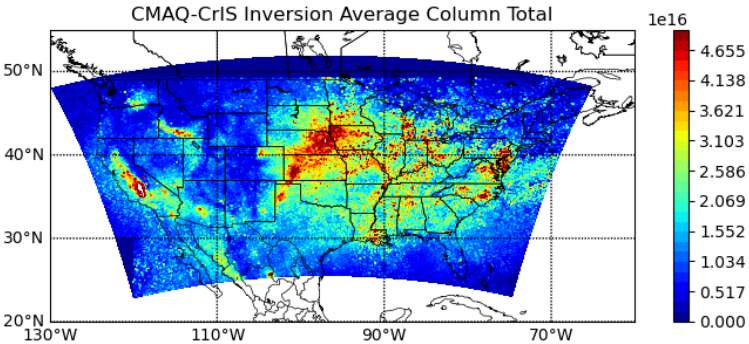
**CrIS Columns**




**Initial CMAQ Columns**




**Posterior CMAQ Columns**

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# Next Steps

| Milestone Statement | Date |
|---|---|
| Automate production of model-ready files and demonstrate the potential to improve the end user's modeling (ARL 5). | 12/2020 |
| Confirm that the files can easily be used by the end user (ARL 5). | 12/2020 |
| Evaluate the new emissions using surface and aircraft data (ARL 6). | 06/2021 |
| Demonstrate that the application improves the end user's modeling (ARL 6). | 06/2021 |
| Incorporate application into end user's standard modeling (ARL 7). | 11/2021 |
| Transfer software to end users (ARL 7) | 11/2021 |

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# 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.

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# ADDITIONAL SLIDES

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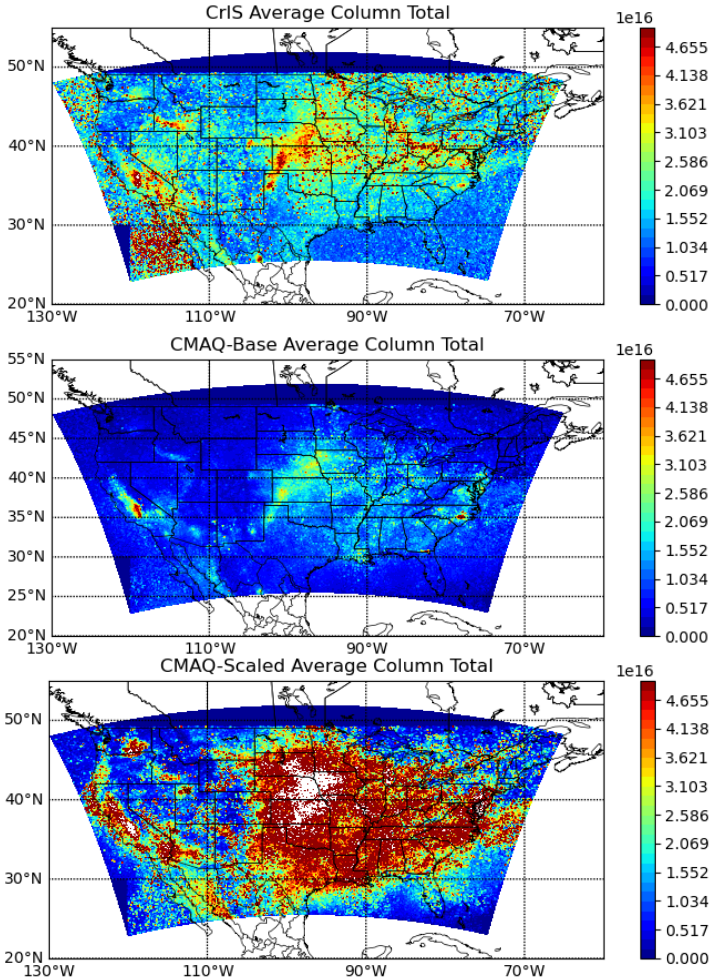
# Limiting Scaling Factor to Prevent Overcorrection

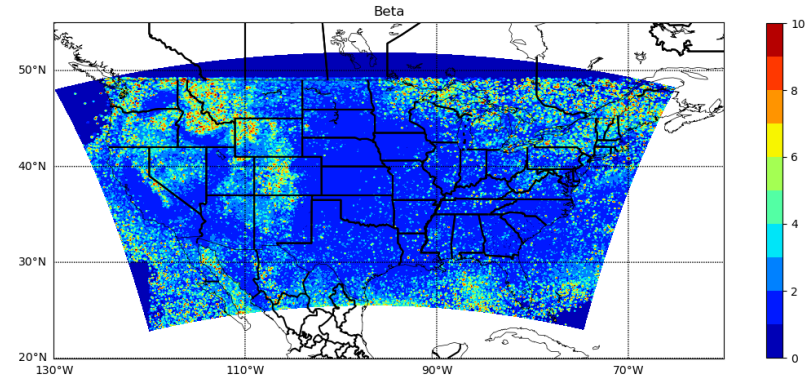



CrIS

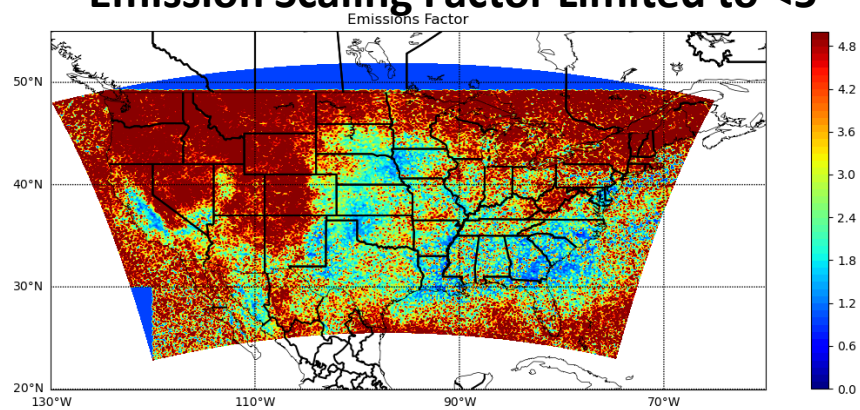
Initial CMAQ

Posterior CMAQ

## "Beta" – Sensitivity of Column to Emissions

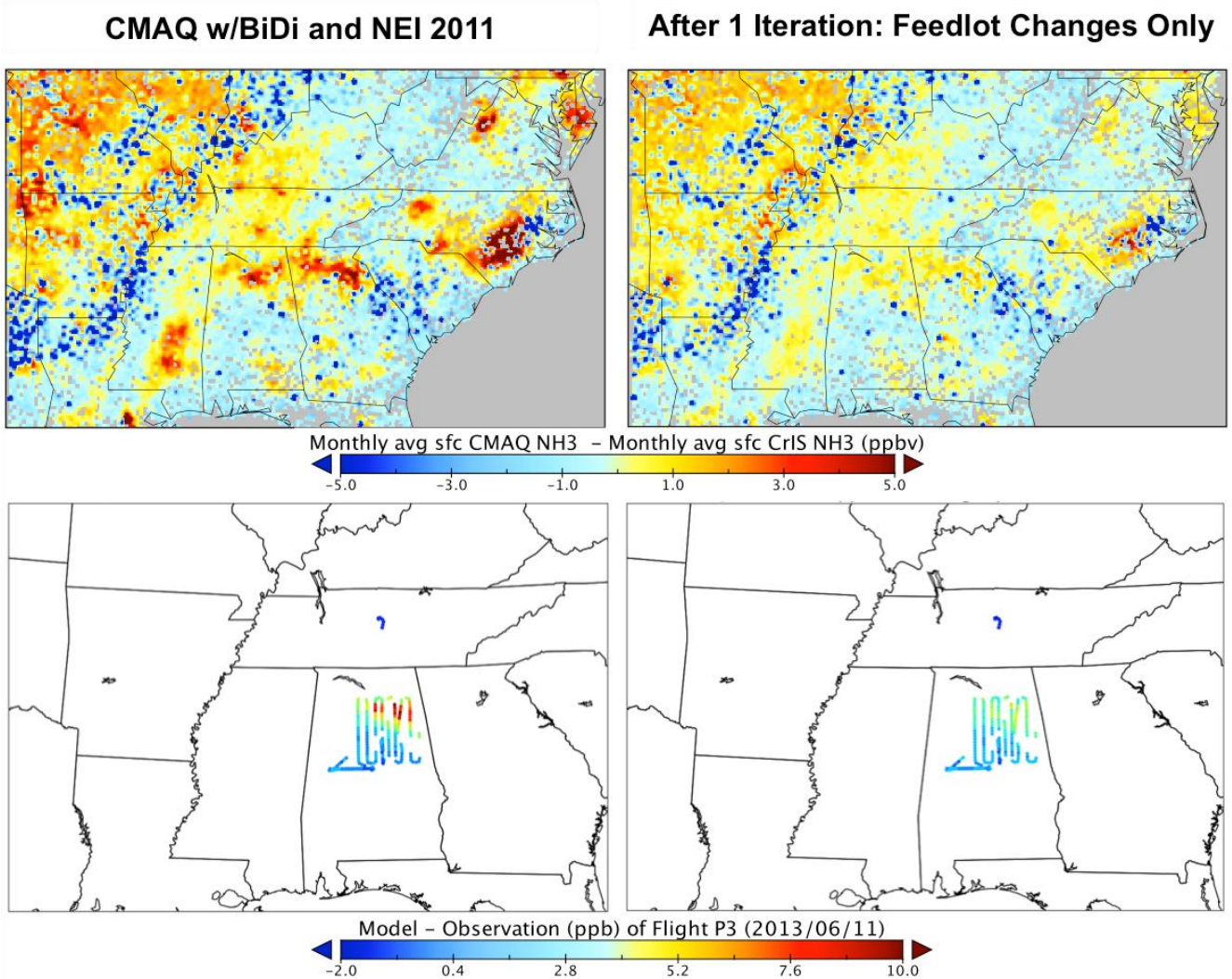



## Emission Scaling Factor Limited to <5



# 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

| | TES | CrIS |
|---|---|---|
| Satellite | AURA | NPP and JPSS-1 |
| Available Data | July 2004 - Jan. 2019 | October 2011-present |
| Resolution | 0.06 $cm^{-1}$ | 0.625 $cm^{-1}$ |
| Footprint | 5x8 km rectangle | 14 km diameter circle |
| Repeat cycle | Once every 16 days | Daily |
| Equatorial crossing | 1:30 am and 1:30 pm | 1:30 am and 1:30 pm |
| Noise in $NH_3$ window | 0.09 – 0.12 K | 0.03 – 0.06 K |

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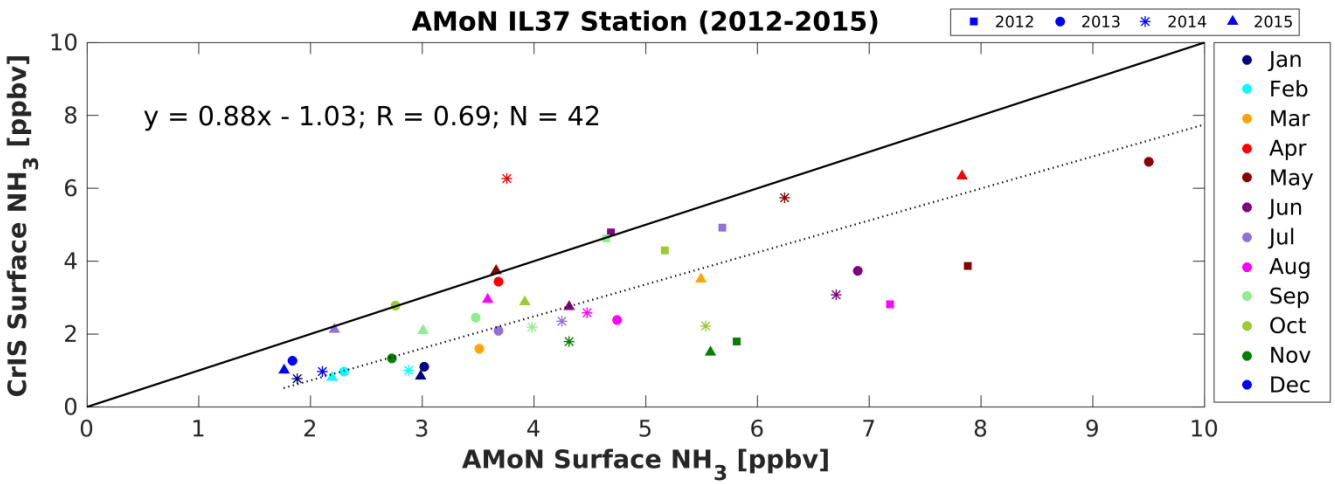
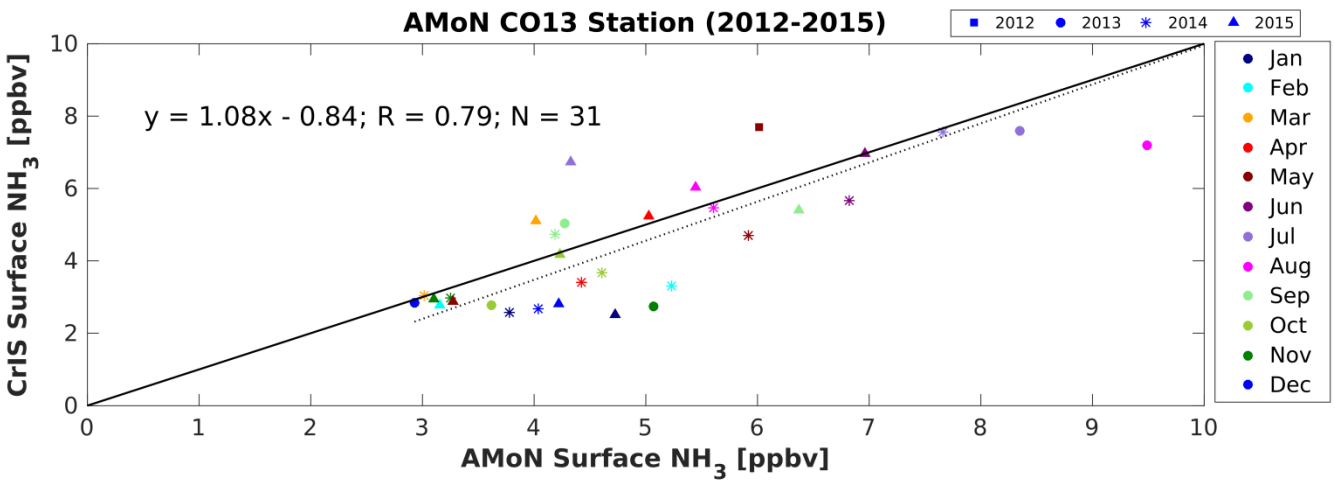
# CrIS Satellite Ammonia Monitoring and Evaluation

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

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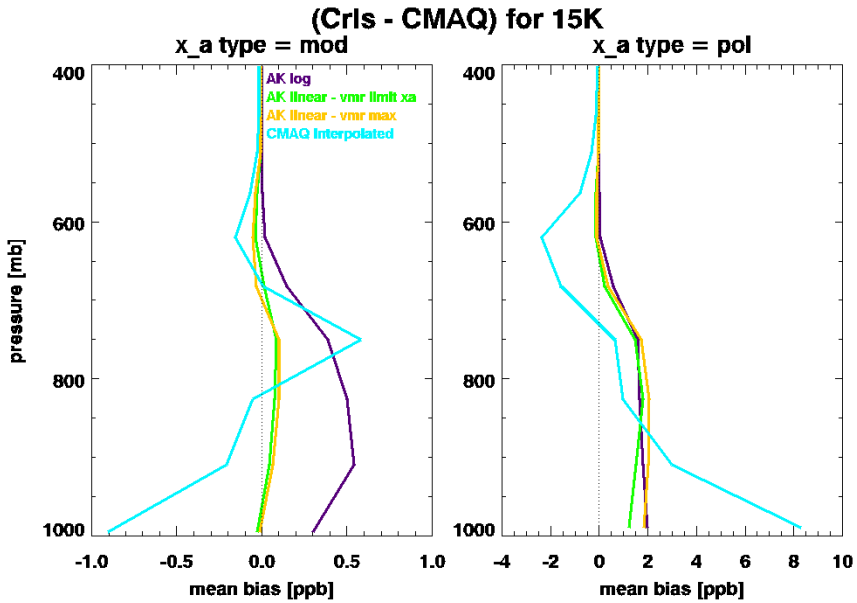
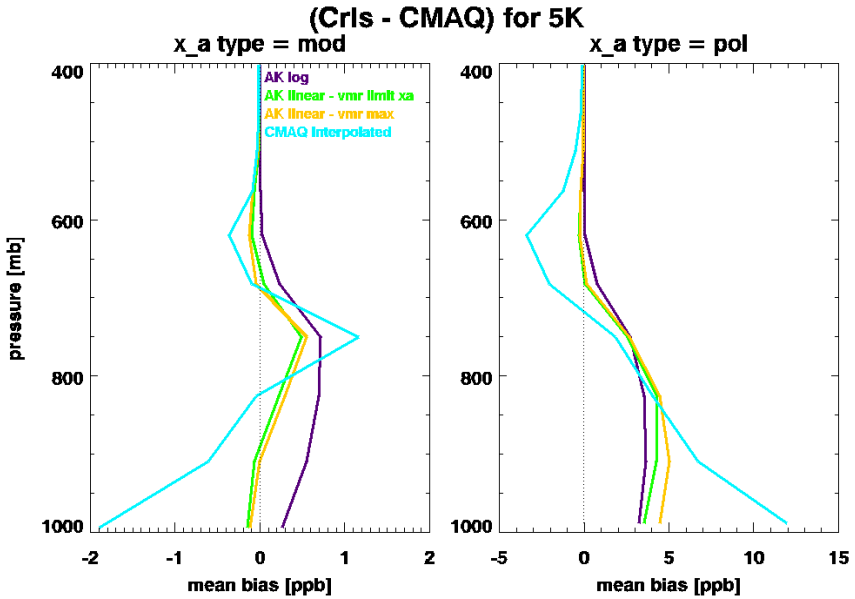
# Linear AKs Have Less Bias for Moderately Polluted Cases

## Mean Bias for +15K




## Mean Bias for +5K




**CMAQ No AK**

**CMAQ AK log**

**CMAQ AK linear – vmr limit xa**

**CMAQ AK linear – vmr max**

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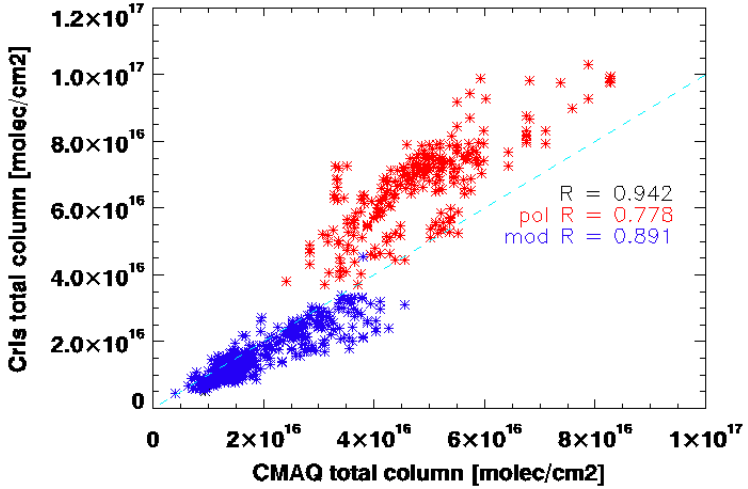
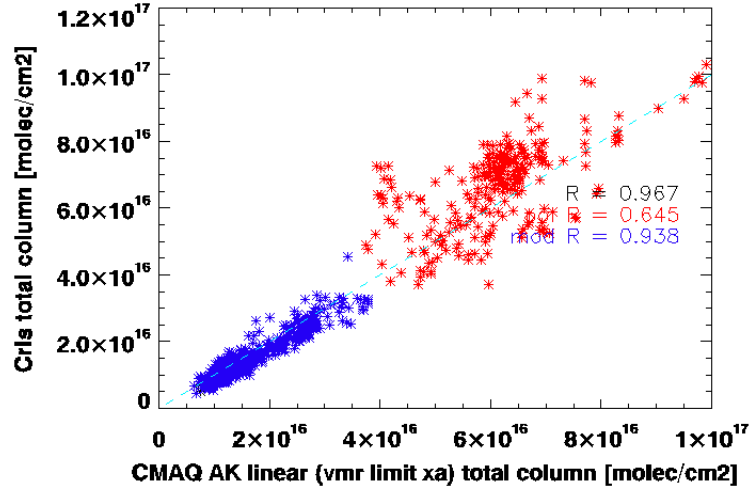
# Simulated CrIS $NH_3$ Col. Vs. CMAQ

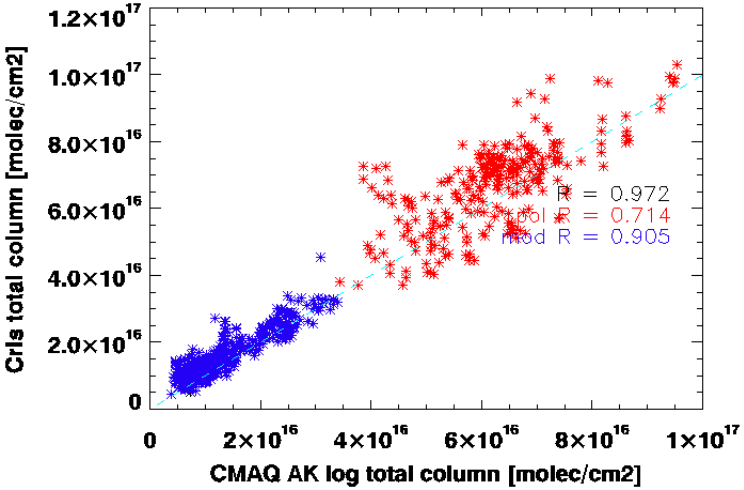
## CMAQ No AK



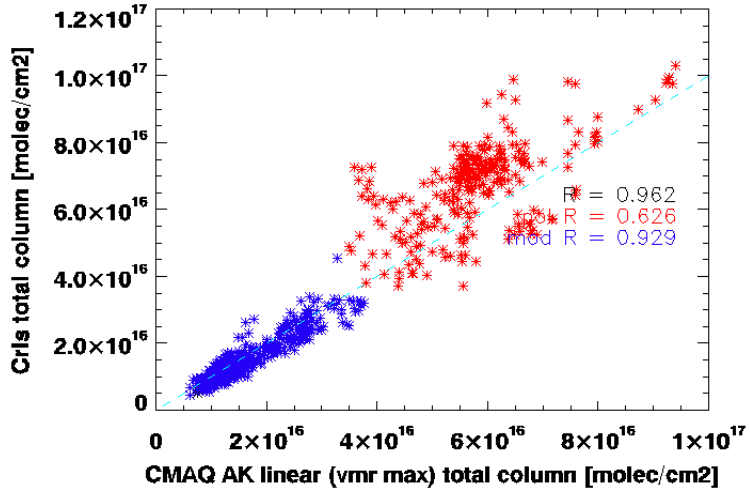

## CMAQ AK linear – vmr limit xa




## CMAQ AK log




## CMAQ AK linear – vmr max

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