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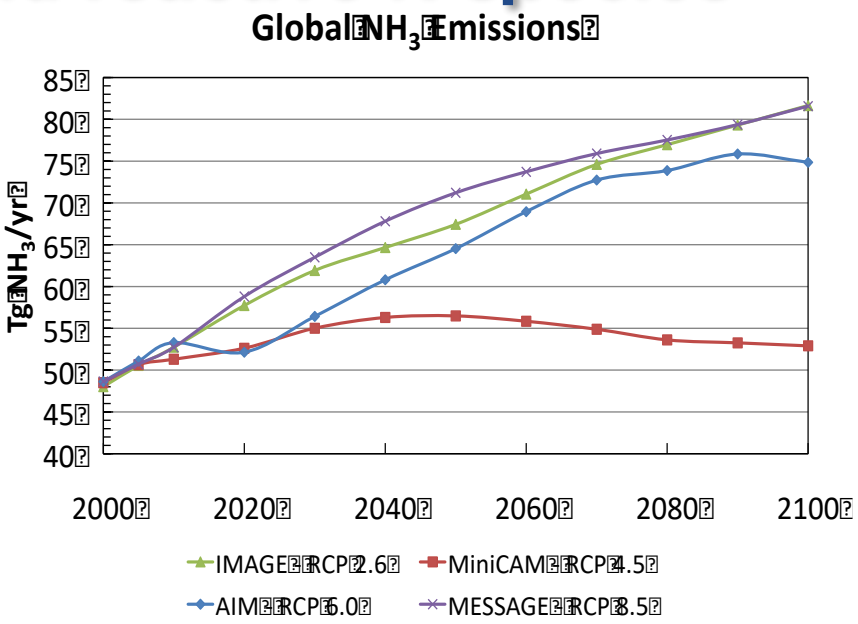
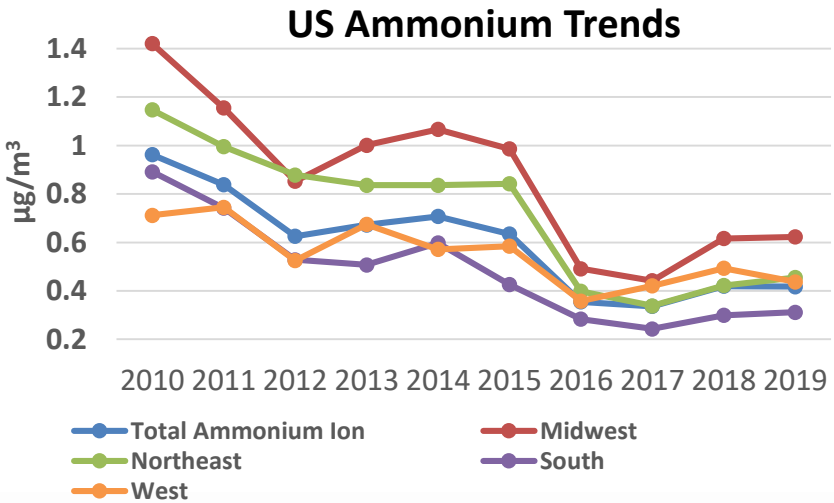
NH_3 is a $PM_{2.5}$ precursor and reactive N species

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

- 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





NH_3 sources are not well known

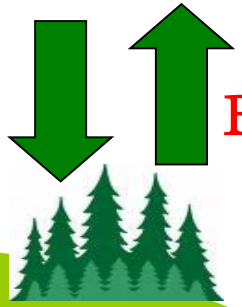
Biomass burning

Automobiles (catalytic converters)

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

Industry

- Fertilizer
- Coal Mining
- Power generation



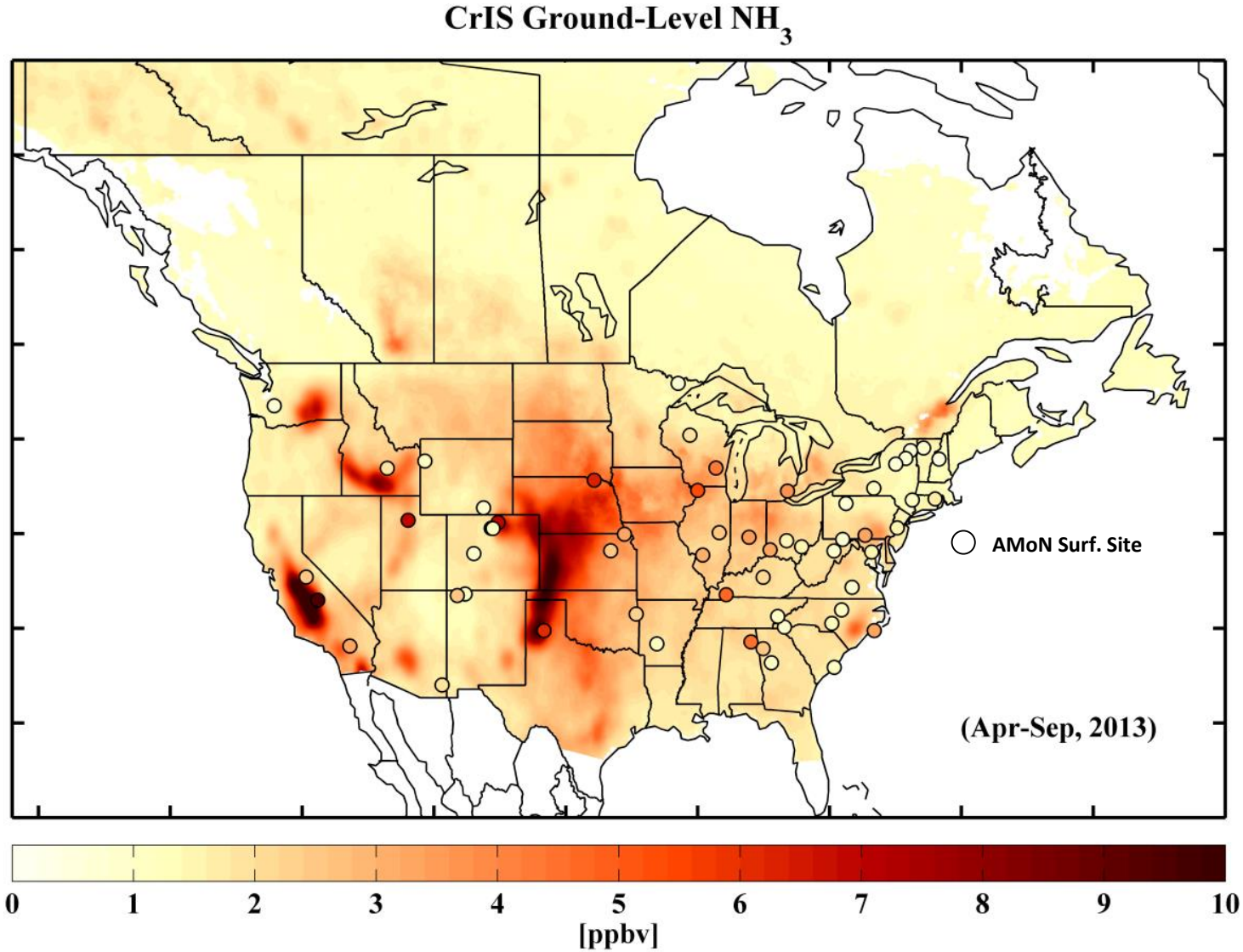
Bi-directional Flux

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.



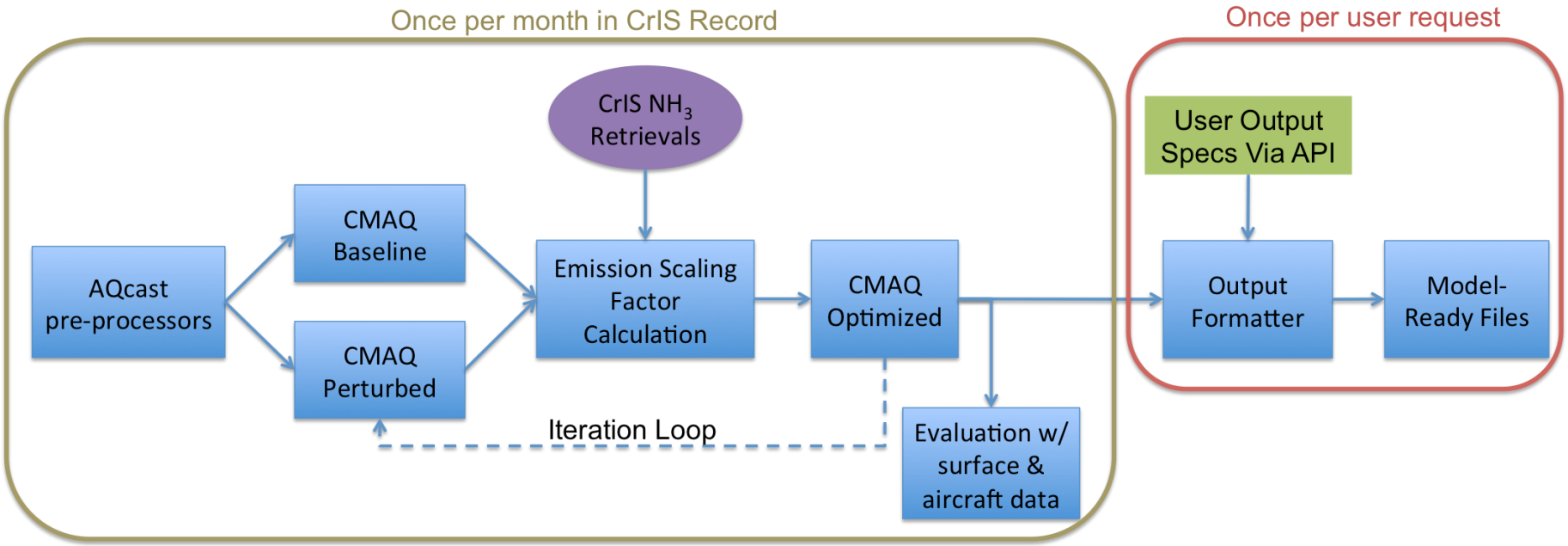
Project Goal

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

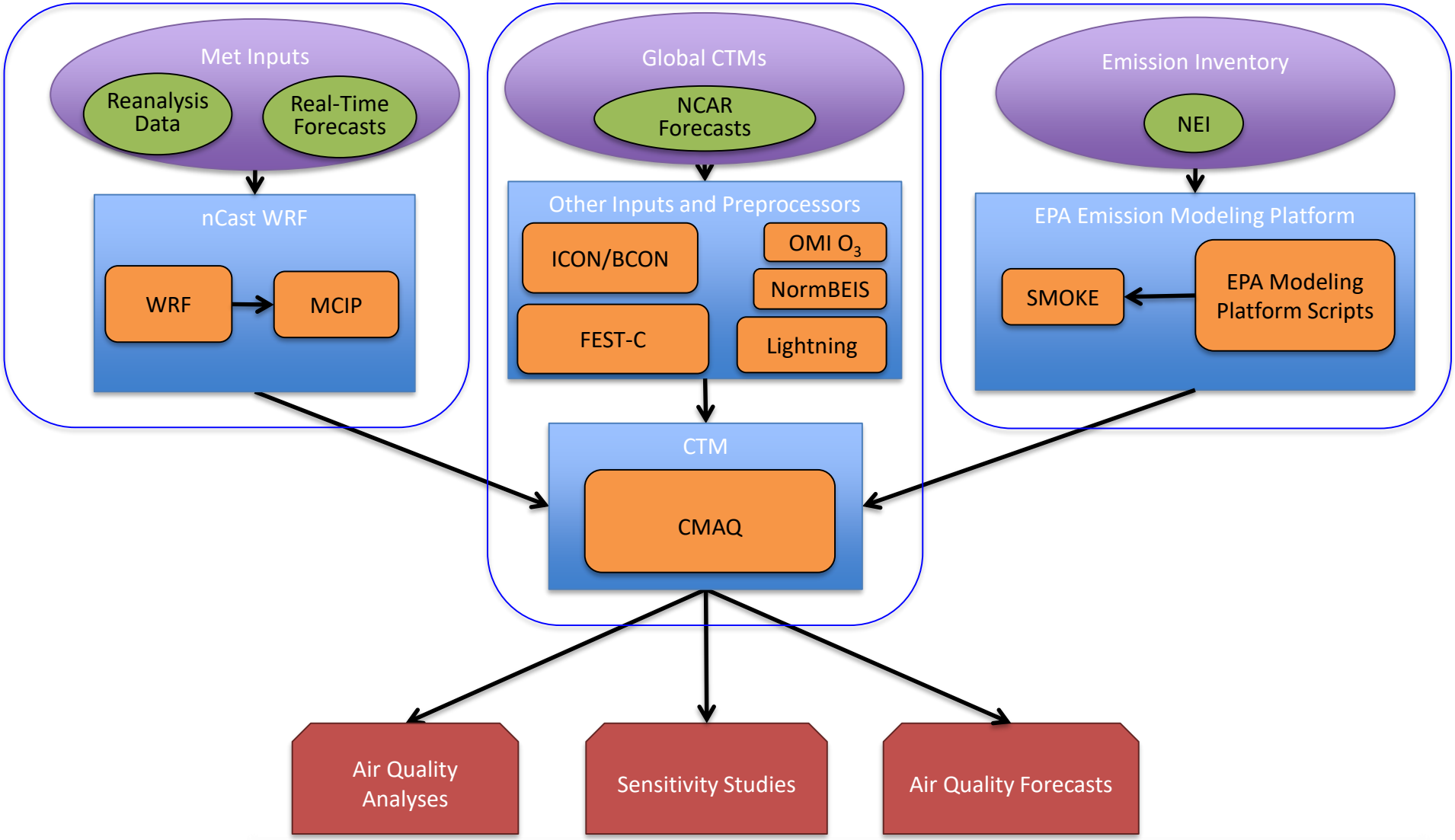
1. Integrate the NASA CrIS NH_3 retrieved product and our CMAQ-based inversion methodology into a prototype application system on the Amazon cloud (ARL 4)
2. Develop model-ready updated NH_3 emission files for CMAQ, CAMx, and GEM- MACH and beta-test them in the end-user applications (ARL 5)
3. Demonstrate 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)

Technical Approach For This Project

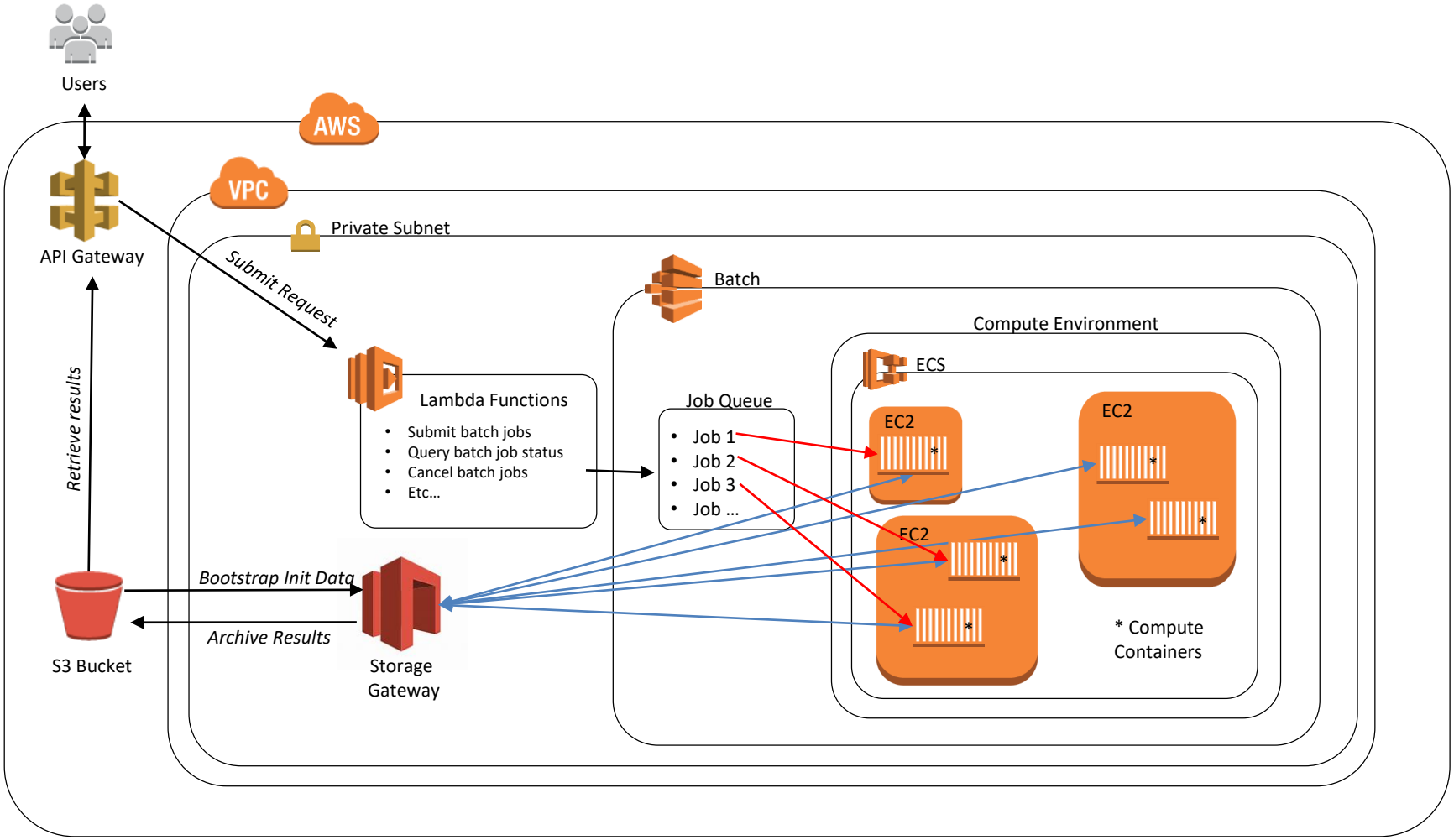


Schematic of the AQcast processing set up for this project on the Amazon cloud. The steps on the left outline include monthly iterations of the CrIS data record. The steps on the right outline each user output request.

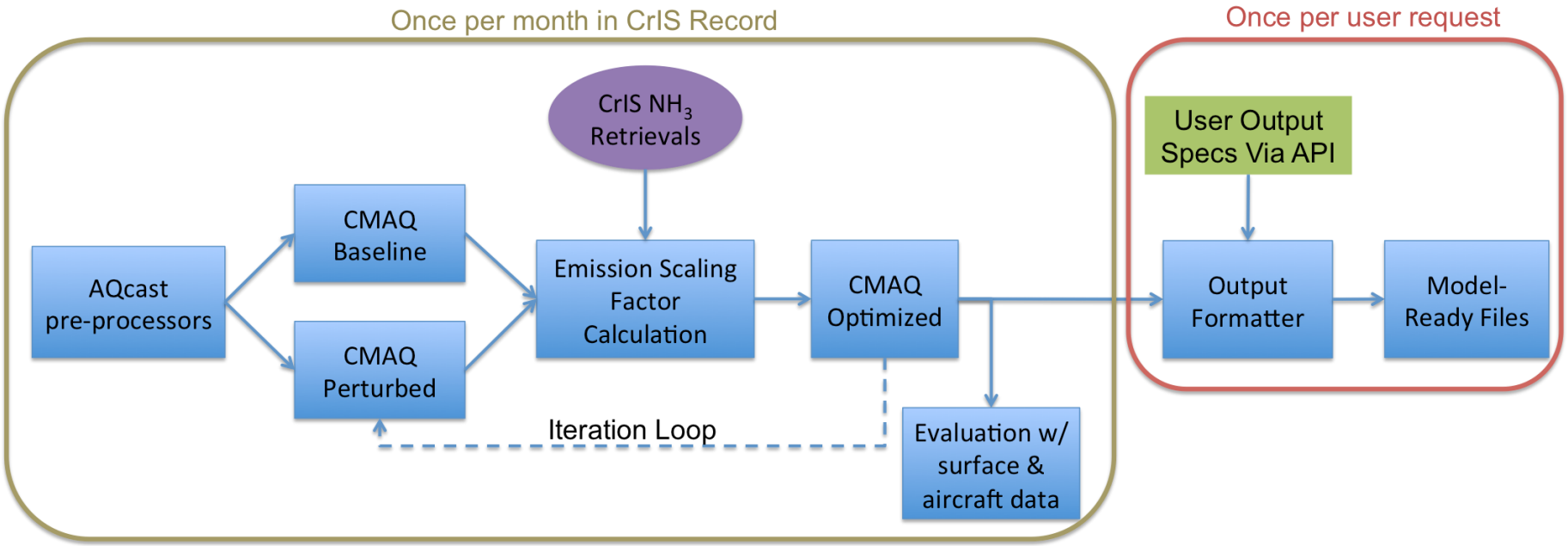
AQcast CMAQ System for Continental US



AQcast Production Architecture

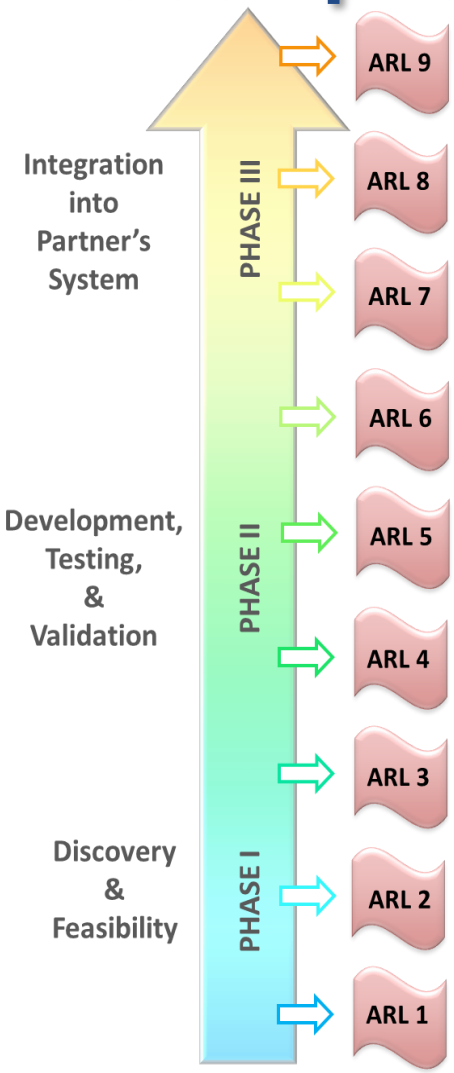


Technical Approach For This Project



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



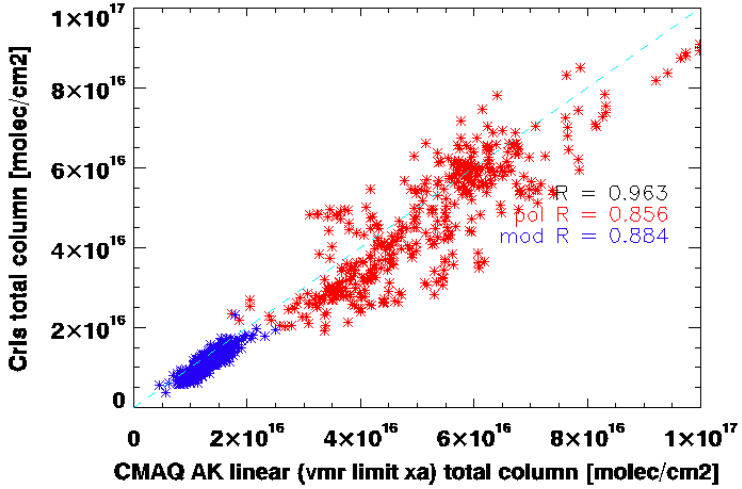
- Current ARL = 4. Goal ARL = 7
- After much debugging, we have successfully implemented a prototype application on the Amazon Web Services (AWS) cloud. The current application is limited to the continental US due to difficulties with expanding emissions to cover Canada.
- We used this prototype this 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

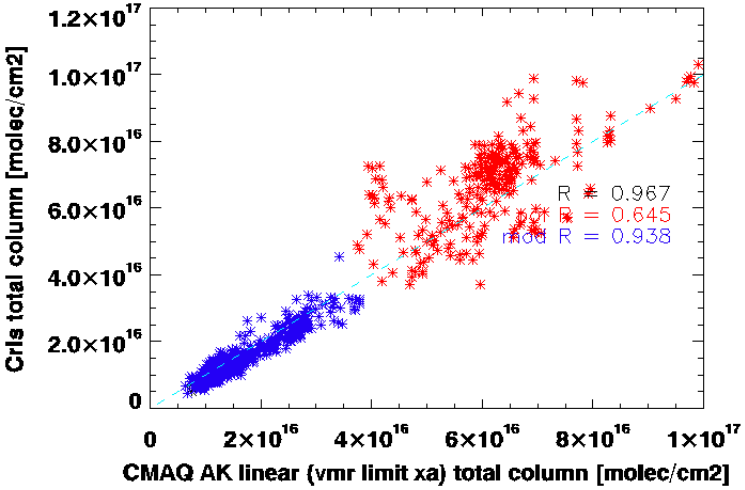
Risk	Mitigation Action
Spatial surrogate files for Canada were inconsistent with emission platform	We will update to the latest EPA emissions platform and then expand our application grid from CONUS to North America early in 2021.
Parental leave and resignation of Key Co-I	In July we hired Nick Heath, 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.

Total Column is Better Metric Than Surface Concentration

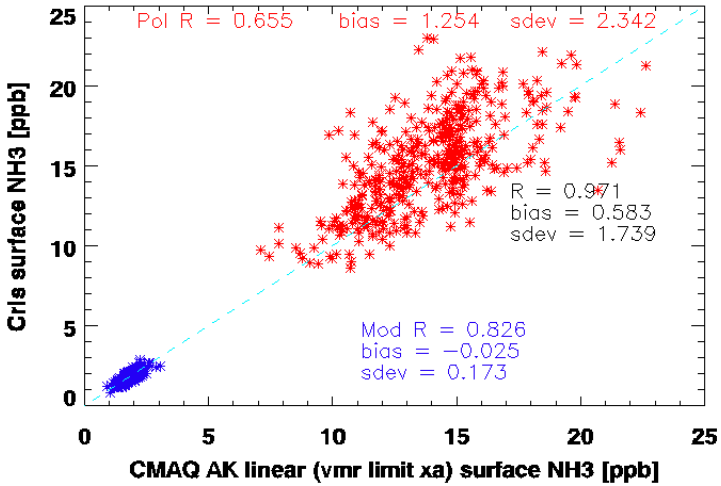
Column, 15 K Contrast



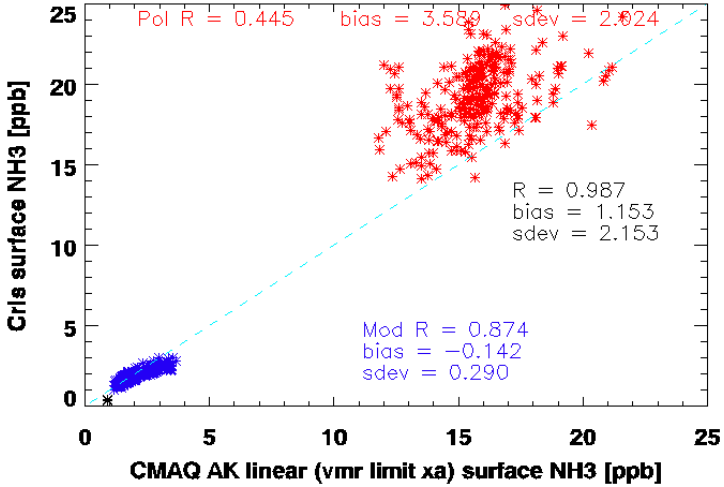
Column, 5 K Contrast



Surface, 15 K Contrast



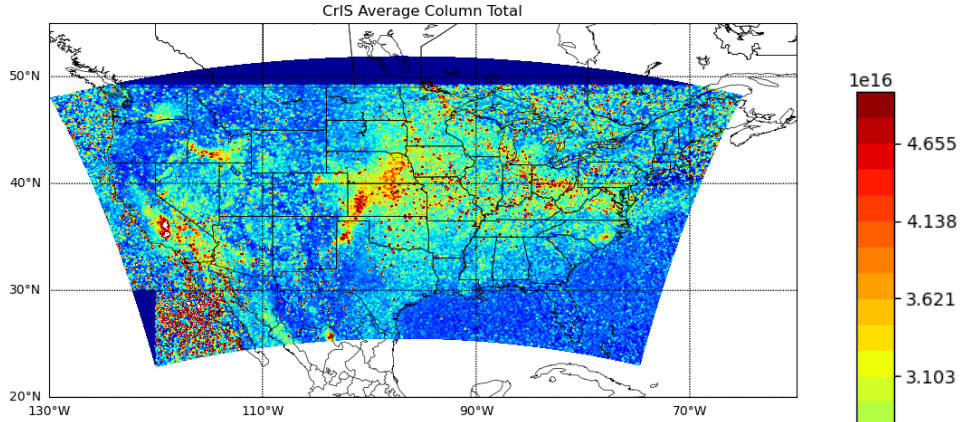
Surface, 5 K Contrast



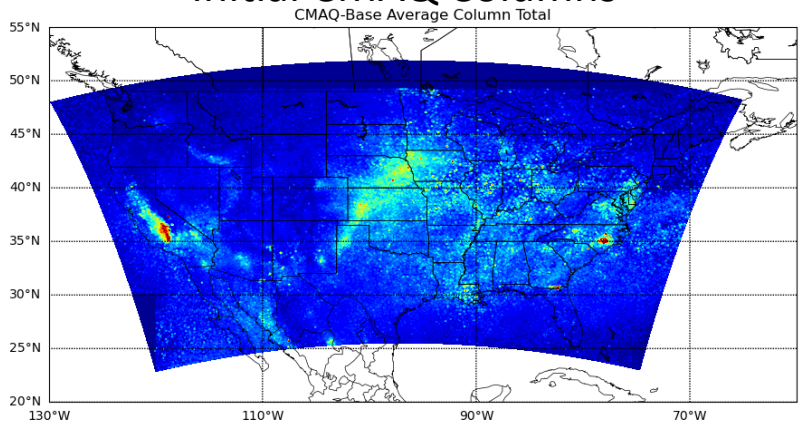
Prototype Test – June 2015 Inversion

- 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

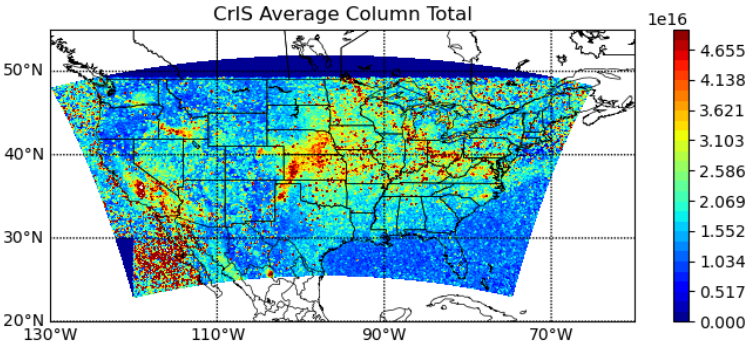


Initial CMAQ Columns

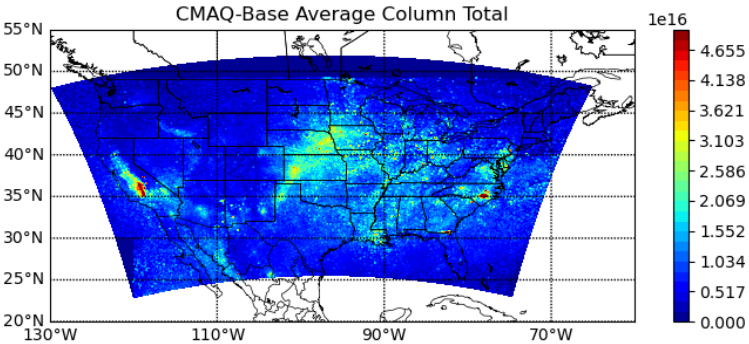


Prototype Results – June 2015 Inversion

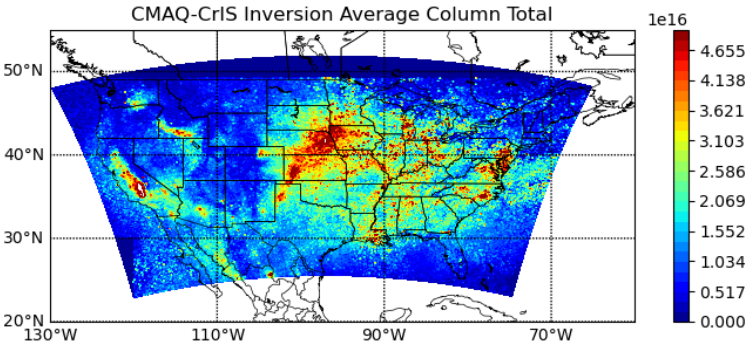
CrIS Columns



Initial CMAQ Columns



Posterior CMAQ Columns



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

Project Budget, Obligations & Costing Status

Project to Date (07/31/2020)					
Institution	**Budget**	**Obligated**	**Unobligated**	**Costed**	**Uncosted**
AER	$764,879	$513,349	$251,530	$513,349*	$0

Prior Year (01/01/2019-12/31/2019)					
Institution	**Budget**	**Obligated**	**Unobligated**	**Costed**	**Uncosted**
AER	$764,879	$513,349	$251,530	$346,100.51	$167,248.49

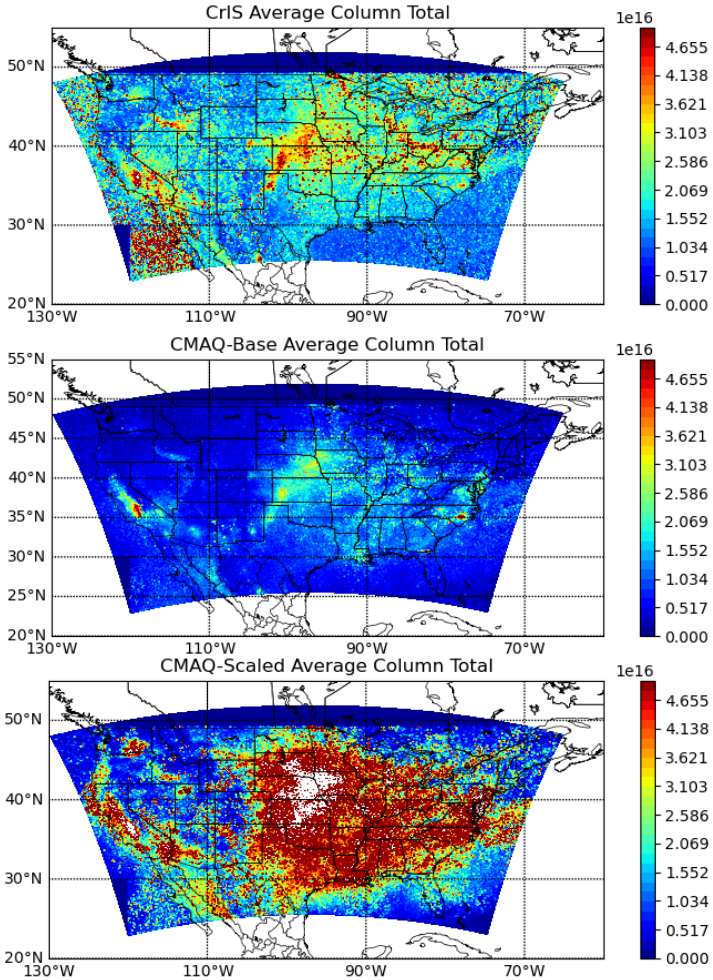
*We are using AER internal new hire funds for Co-I Heath to continue to make progress on the project until Year 3 funds are available.

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

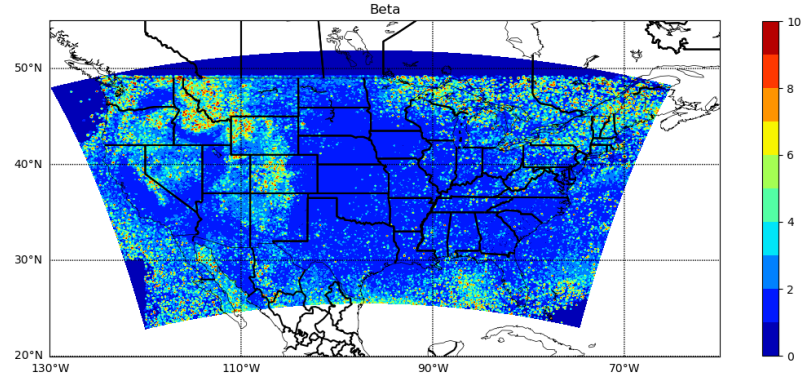


CrIS

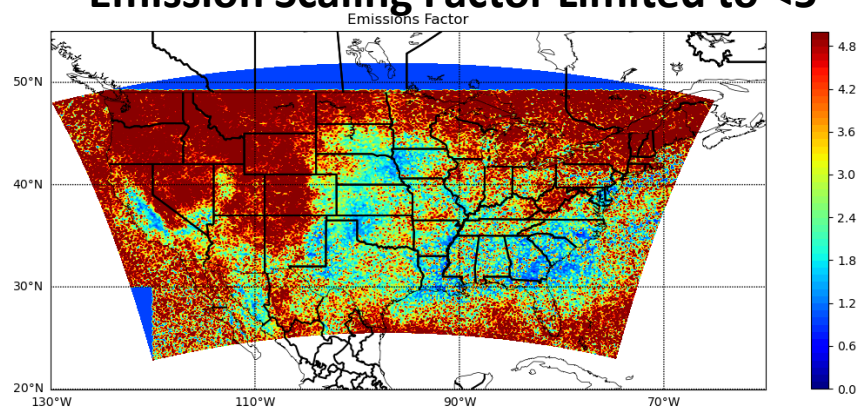
Initial CMAQ

Posterior CMAQ

"Beta" – Sensitivity of Column to Emissions

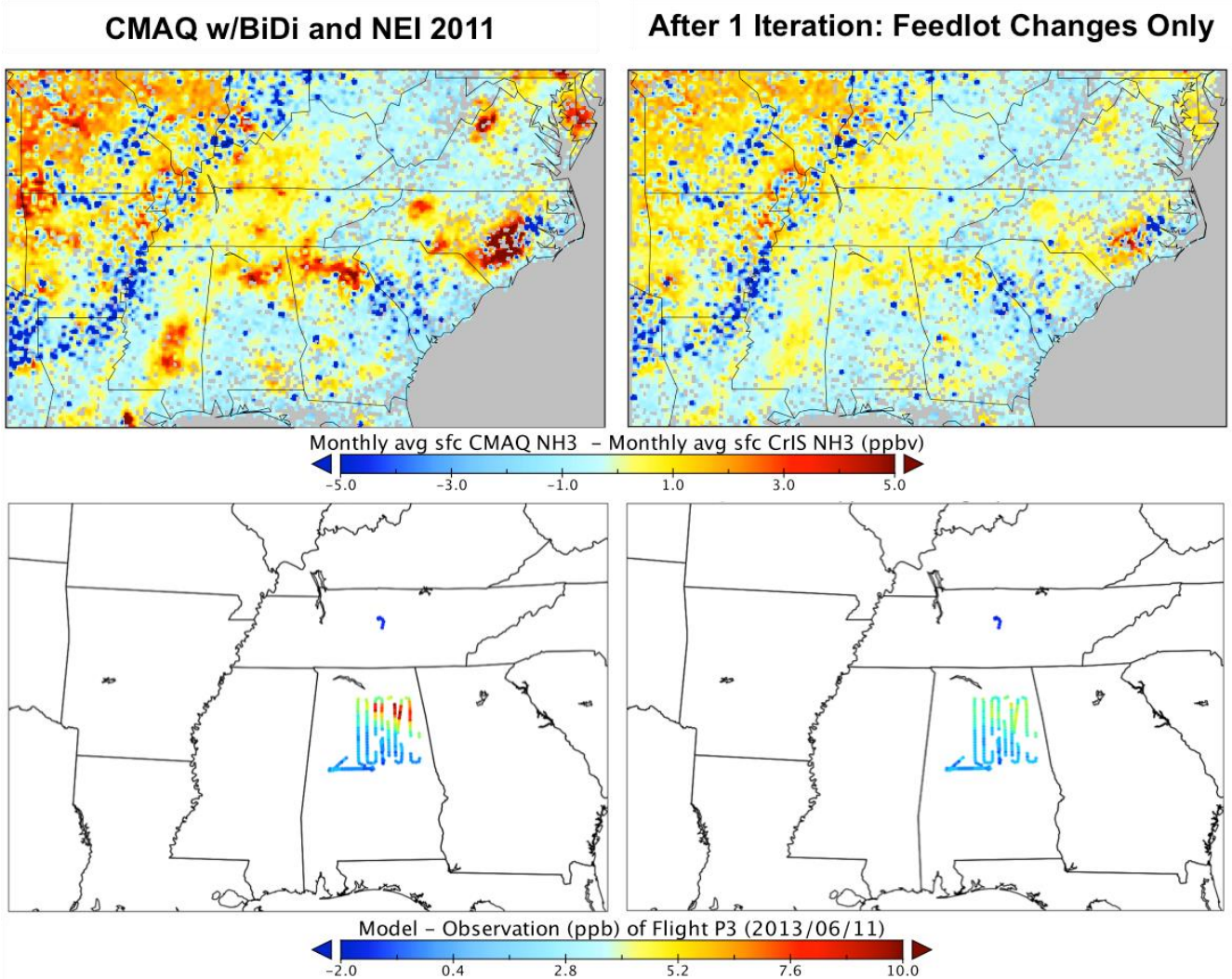


Emission Scaling Factor Limited to <5



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)

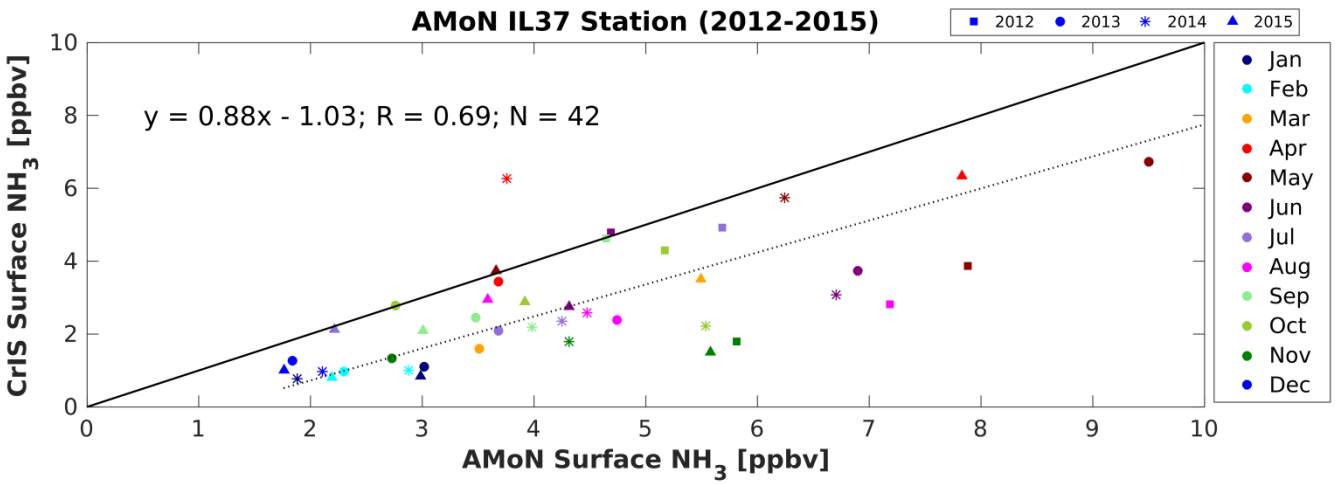
- CrIS can monitor global NH_3 with high spatial coverage from 2011 and over the next decade or more

	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

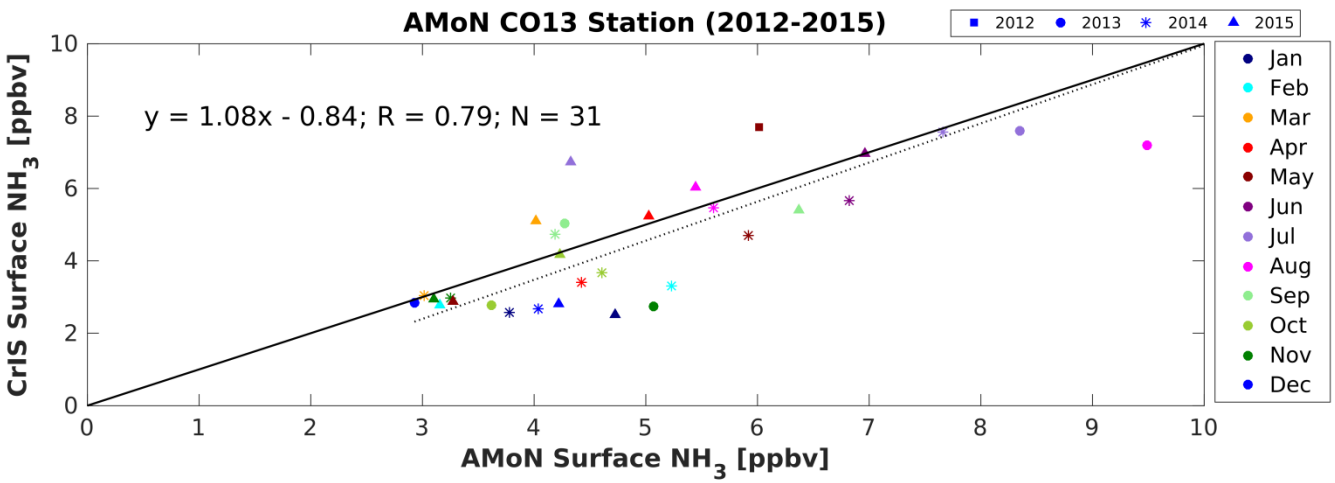
CrIS Satellite Ammonia Monitoring and Evaluation

Multi-year monthly comparisons of CrIS surface NH_3 with AMoN obs.

Stockton, Illinois



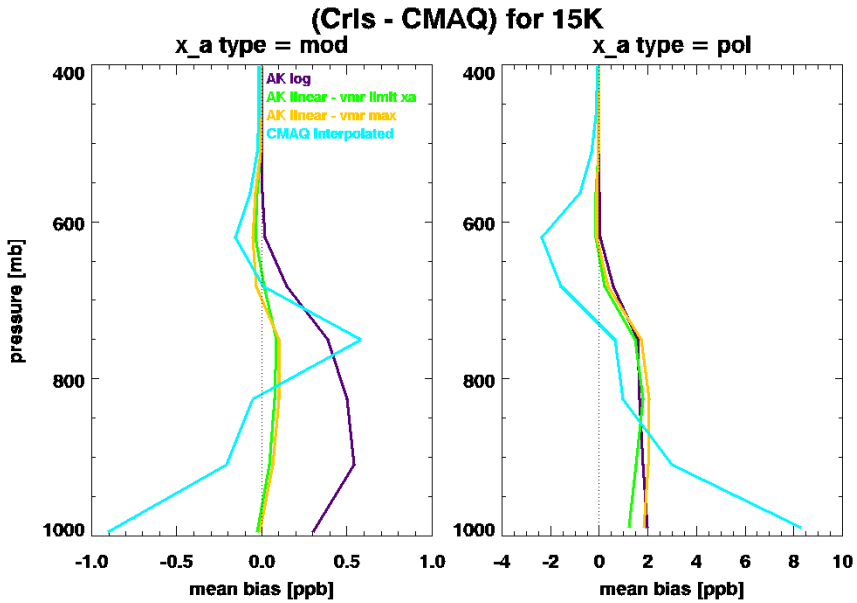
Fort Collins, Colorado



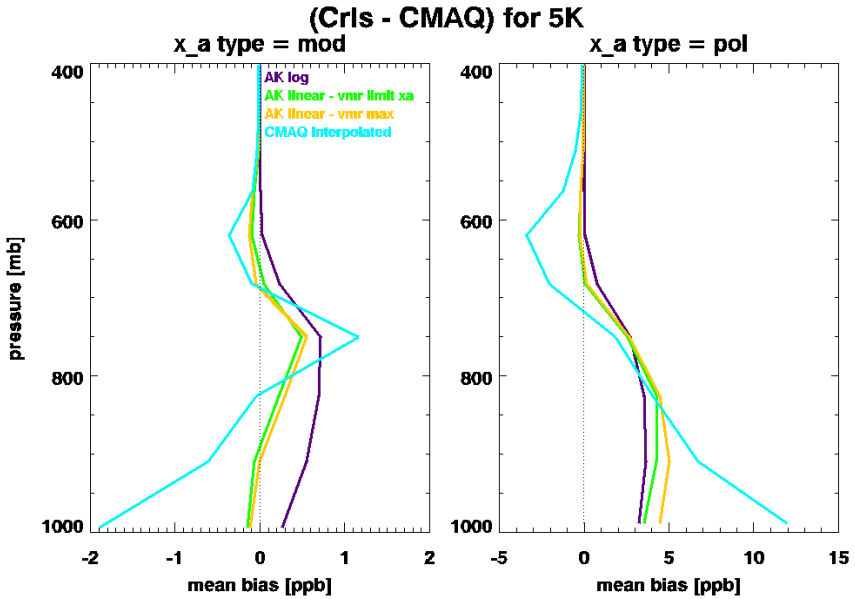
Initial assessment shows that the satellite and AMoN surface observations agree well despite sampling differences

Linear AKs Have Less Bias for Moderately Polluted Cases

Mean Bias for +15K



Mean Bias for +5K



CMAQ No AK

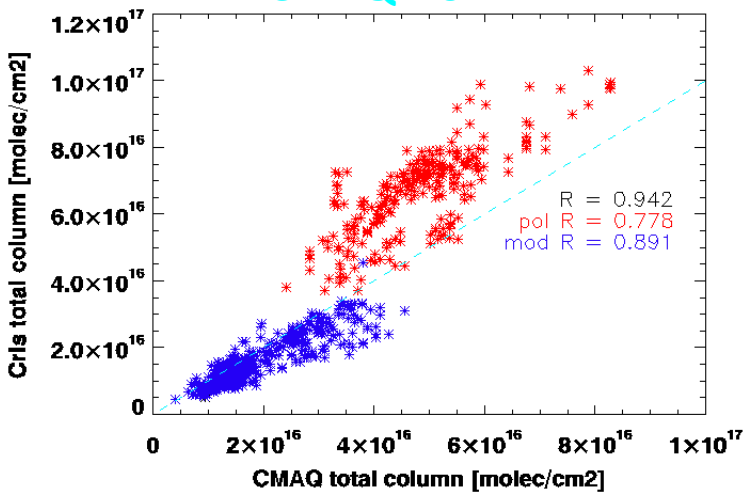
CMAQ AK log

CMAQ AK linear – vmr limit xa

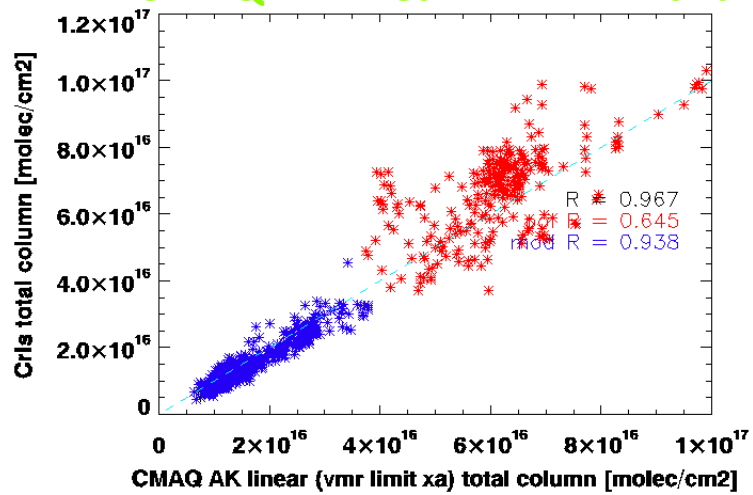
CMAQ AK linear – vmr max

Simulated CrIS NH_3 Col. Vs. CMAQ

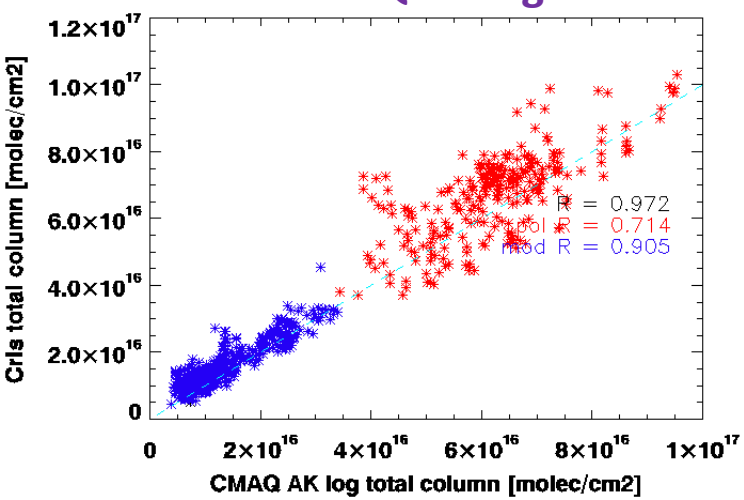
CMAQ No AK



CMAQ AK linear – vmr limit xa



CMAQ AK log



CMAQ AK linear – vmr max