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

M. J. Alvarado[1], C. R. Lonsdale[1], K. Cady-Pereira[1], B. Brown-Steiner[1], E. H. Fahy[1] and M. Shephard[2]

[1]Atmospheric and Environmental Research (AER)
[2]Environment and Climate Change Canada

2019 NASA Health and Air Quality Applications Program Review

Sept. 10th, 2019

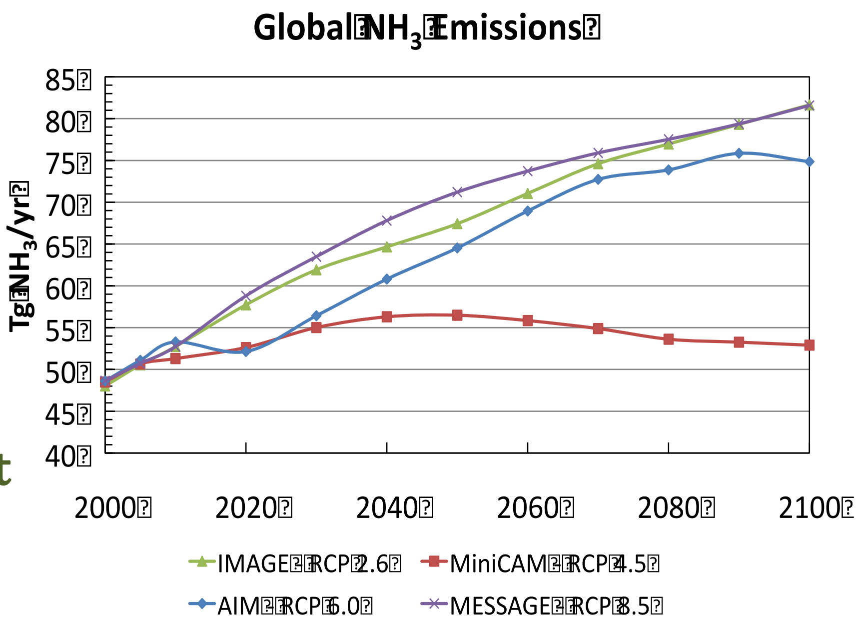
NH_3 is a $PM_{2.5}$ precursor and reactive N species

$NH_3 + HNO_3 \leftrightarrow NH_4NO_3$

$2\ NH_3 + H_2SO_4 \rightarrow (NH_4)_2SO_4$

- 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



SO_2, NO_X emissions decreasing due to controls, but NH_3 increasing!

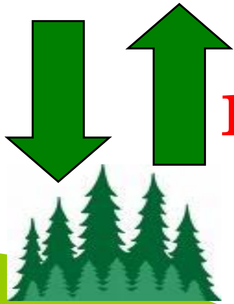
NH_3 sources are not well known

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

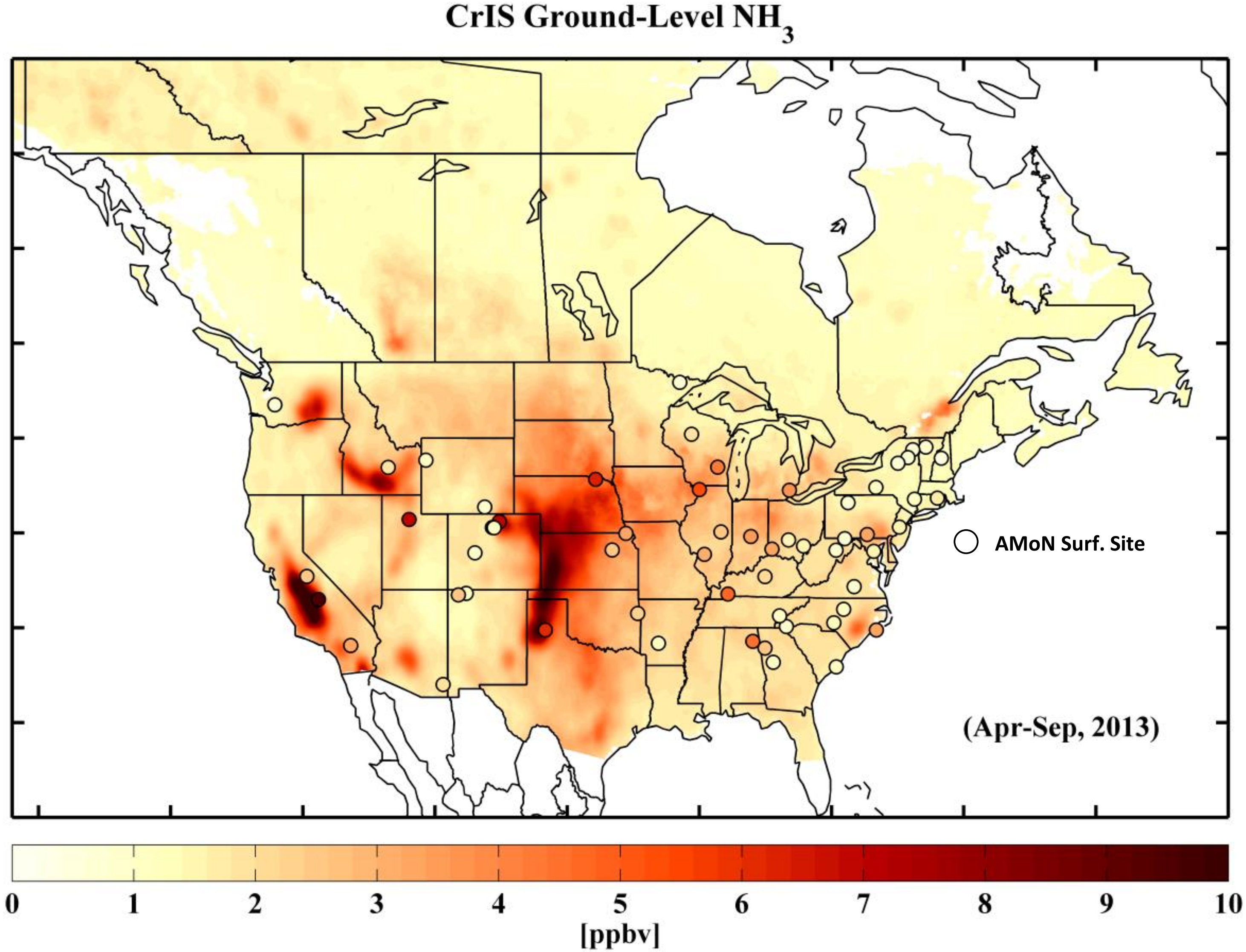
AGRICULTURE
- Animal waste (temperature dependent)
- Fertilizer application



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.



Project Goal

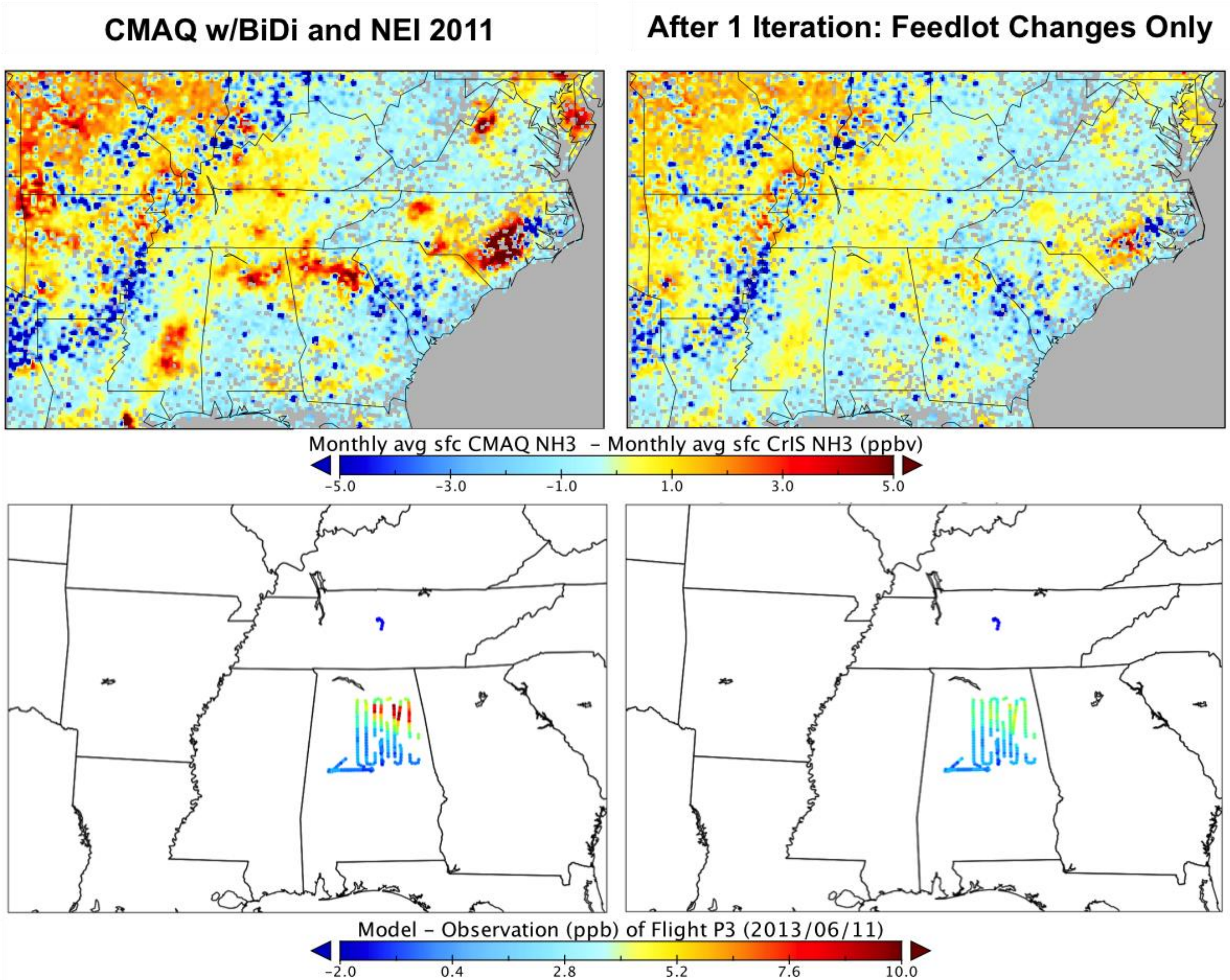
To use CrIS NH_3 retrievals to provide improved emission inventories of NH_3 to air quality (AQ) forecasters, AQ managers, and other stakeholders.

Project Objectives

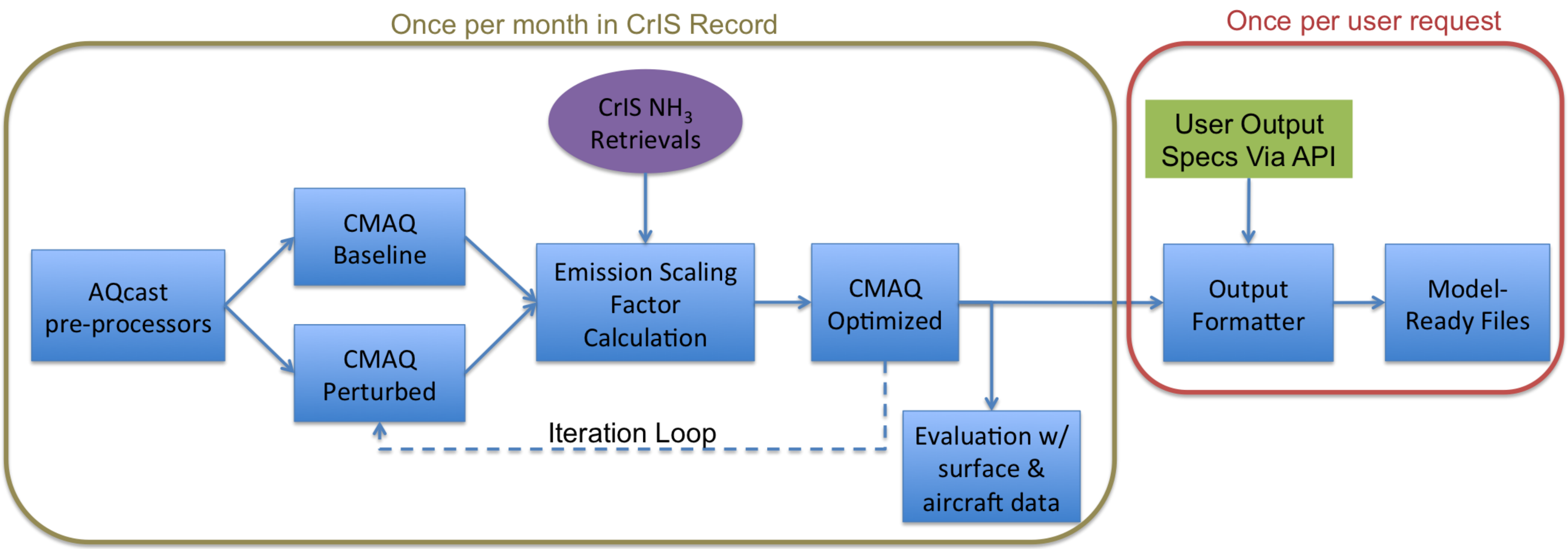
1. Integrate the NASA CrIS NH_3 retrieved product and our CMAQ-based inversion methodology into a prototype application system on the Amazon cloud (ARL 4)
2. Develop model-ready updated NH_3 emission files for CMAQ, CAMx, and GEM- MACH and beta-test them in the end-user applications (ARL 5)
3. Demonstrate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

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.

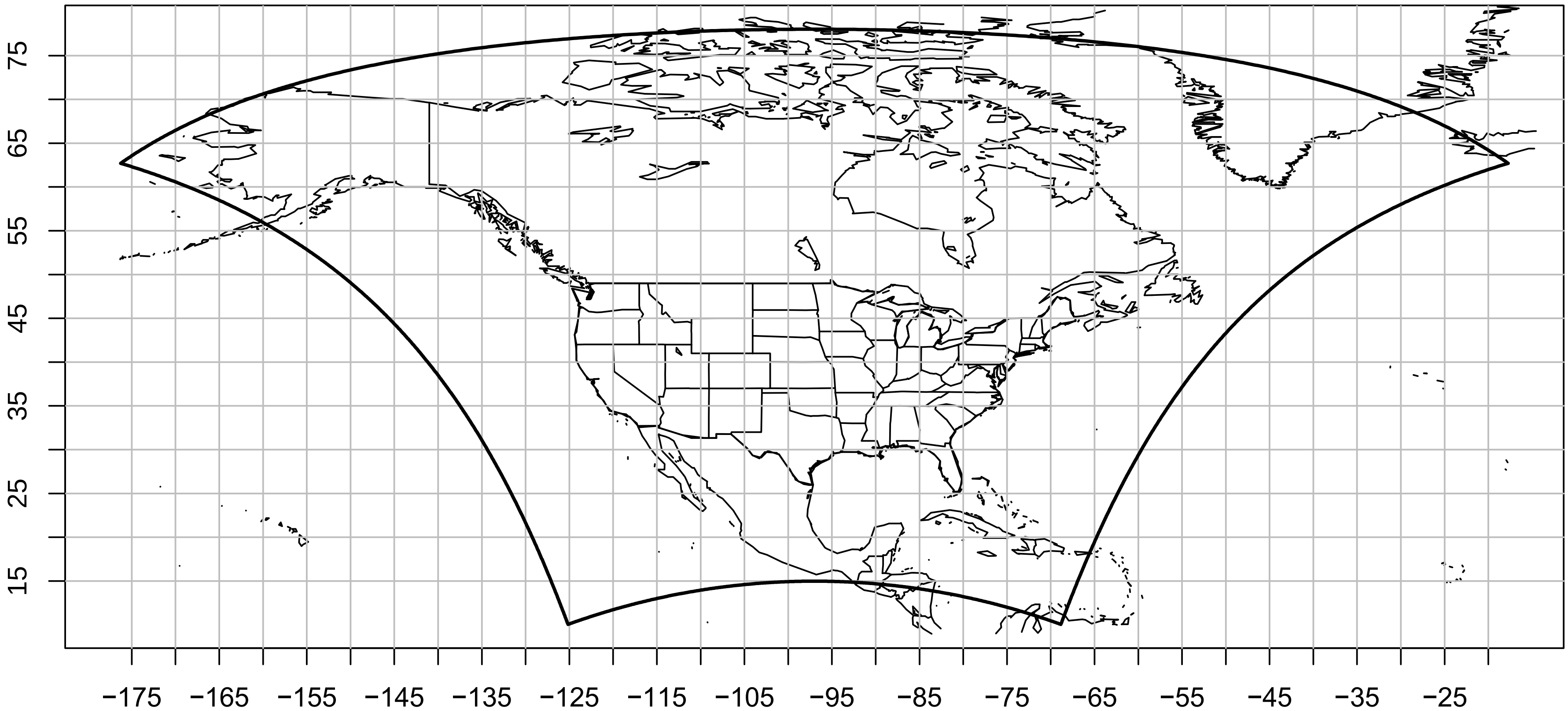


Technical Approach For This Project



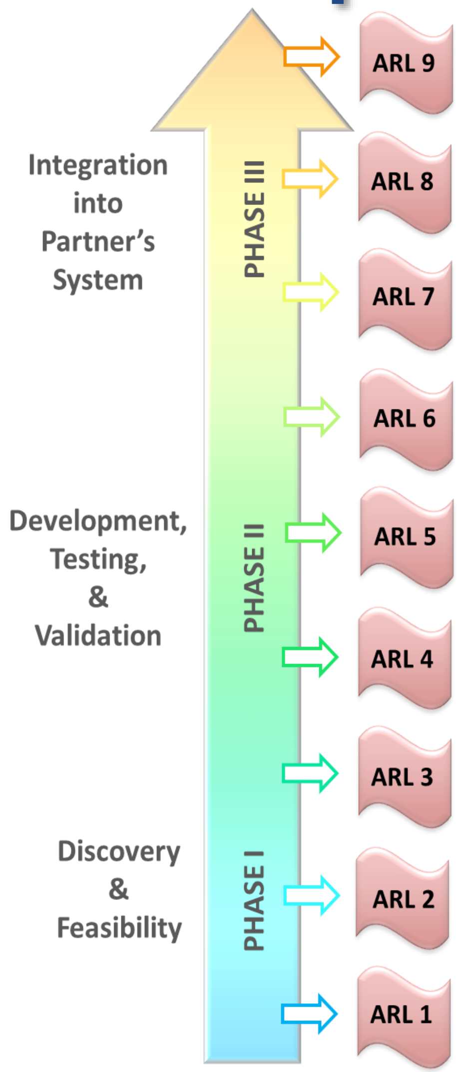
Schematic of the AQcast processing set up for this project on the Amazon cloud. The steps on the left outline include monthly iterations of the CrIS data record. The steps on the right outline each user output request.

NASA Applied Science Project Expanded North American Domain



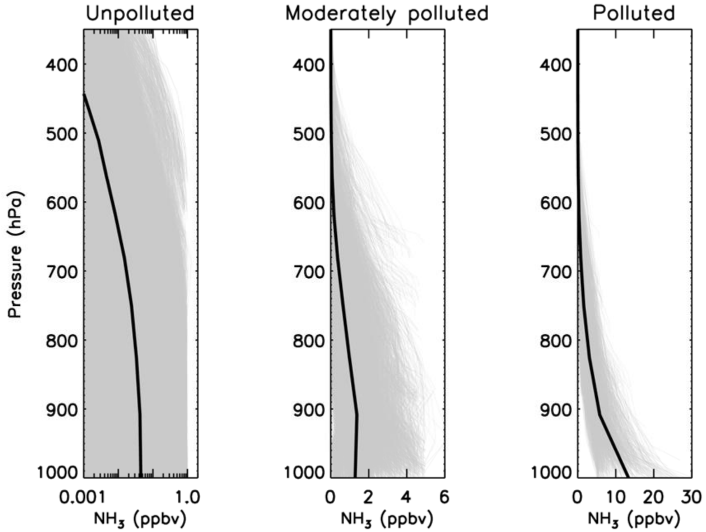
WRF version 3.8.1 with the YonSie University (YSU, Hong et al., 2006) non-local turbulent PBL scheme and the Noah land surface scheme (Chen and Dudhia, 2001) were used. Initial and boundary conditions for WRF were provided by the North American Regional Reanalysis (NARR, Mesinger et al., 2006),

Accomplishments and Current ARL



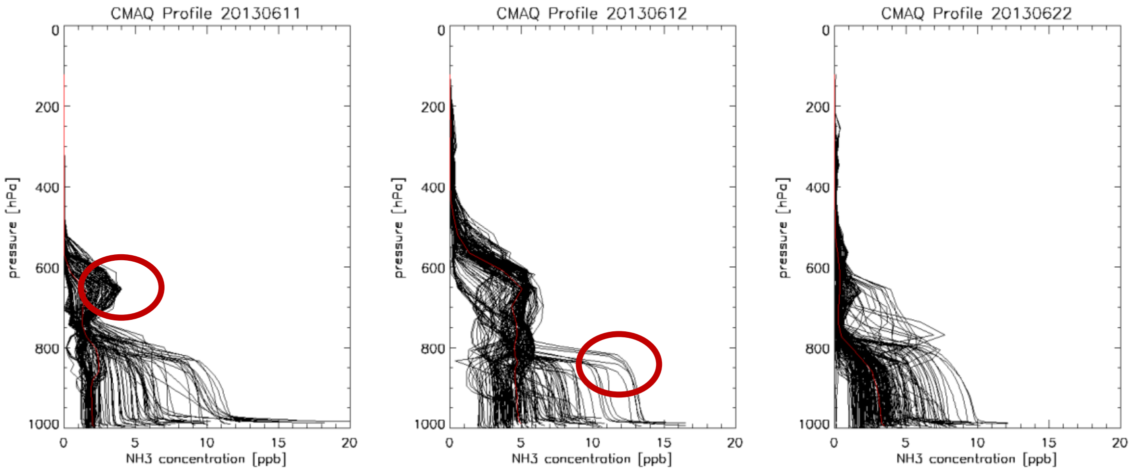
- Current ARL = 3 *(08-16-2019)* Goal ARL = 7
- Completed AWS Lambda function to unify components.
- Developed Python functions to process CrIS data and perform CMAQ model comparison and emission update.
- Automated the re-gridding of final emissions to CAMx, CMAQ, and GEM-MACH domains.
- Performed WRF simulations and created emission spatial surrogates for our expanded North American domain.
- Performed a model-retrieval closure study to determine the best metrics to use in the CMAQ inverse modeling.
- We are currently debugging CMAQ preprocessors and SMOKE emissions runs over the N. Am. domain in the prototype system. ***Once this is completed, we will have met ARL 4.***

How best to evaluate CMAQ with CrIS?



CrIS and TES *a priori* profiles (top left) were developed from GEOS-Chem simulations of 2005 (Shephard et al., ACP, 2011).

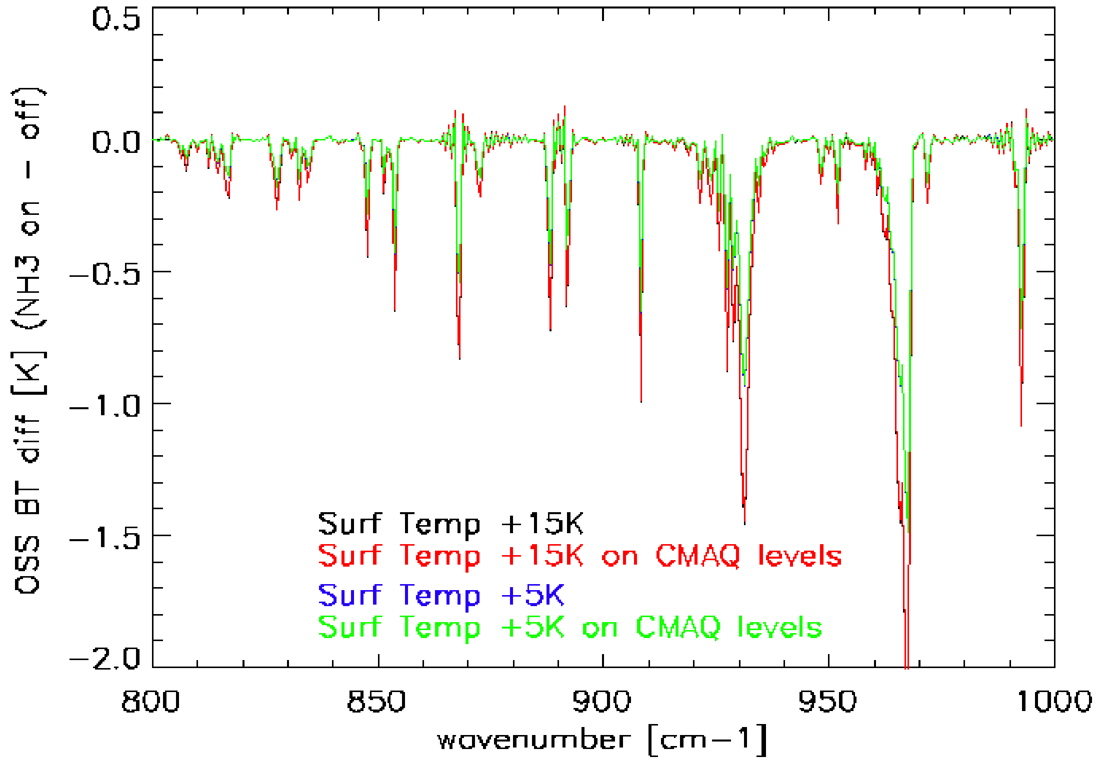
- However, CMAQ profiles (bottom left) have a very different shape.
- Key Question: ***What is the best metric for comparing CrIS and CMAQ?***



Above: ~850 CMAQ NH_3 profiles from SENEX following P3 aircraft track

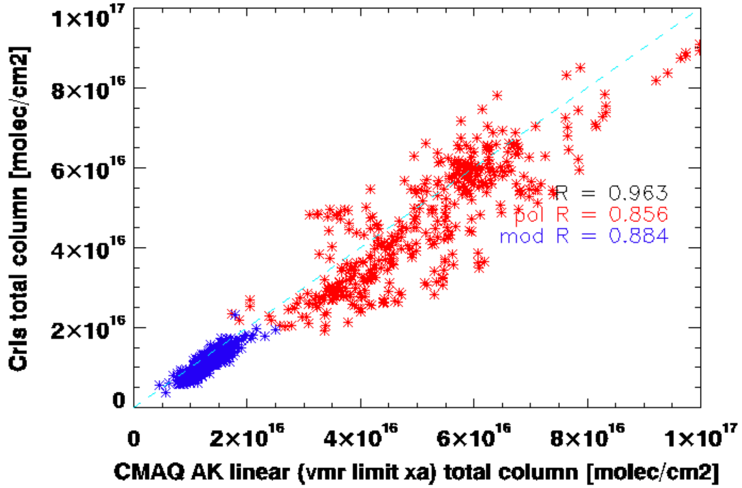
Method: Retrieval Closure Study

- Ran OSS radiative transfer model on CMAQ profiles and applied CrIS noise to simulated spectrum.
- Ran CrIS NH_3 retrieval code on simulated spectrum.
- Compared retrieved profile with original CMAQ profile and with CMAQ profile with different averaging kernels applied.

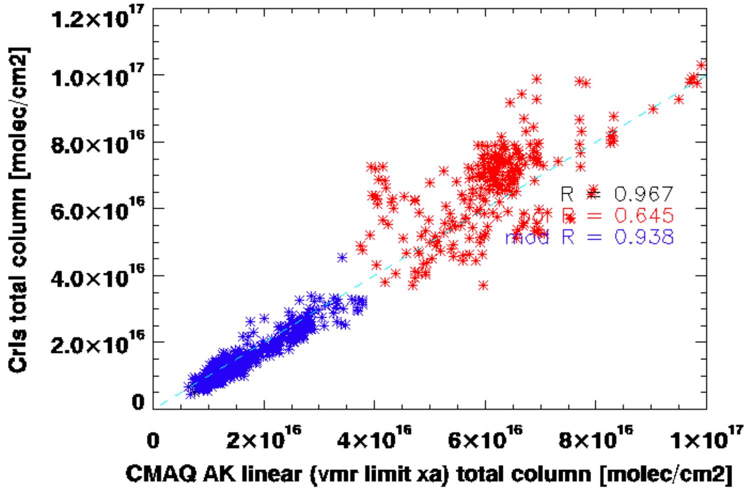


Total Column is Better Metric Than Surface Concentration

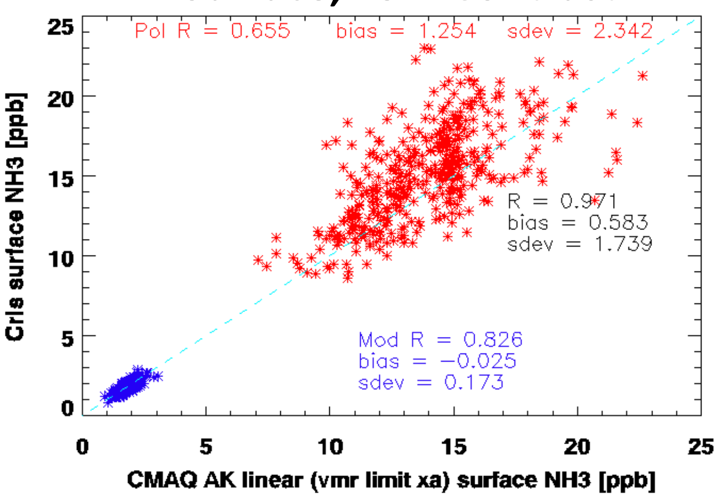
Column, 15 K Contrast



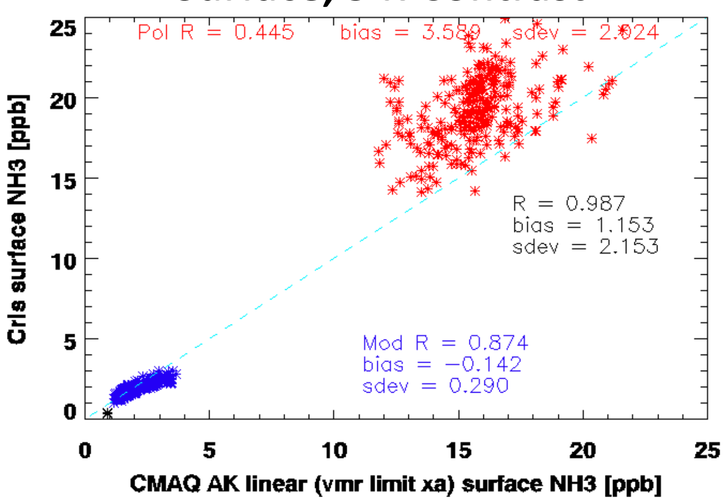
Column, 5 K Contrast



Surface, 15 K Contrast



Surface, 5 K Contrast



Project Challenges & Risks

Rank	Risk	Mitigation Action
1	CMAQ preprocessors and SMOKE for expanded domain (Technical)	We are working to debug the associated preprocessors and will reduce the size of our simulation domain if needed.
2	Parental Leave of Key Co-I (Management)	We have identified a suitable replacement for the Co-I for the duration of their parental leave and had the two working side-by-side for the last month.

Summary

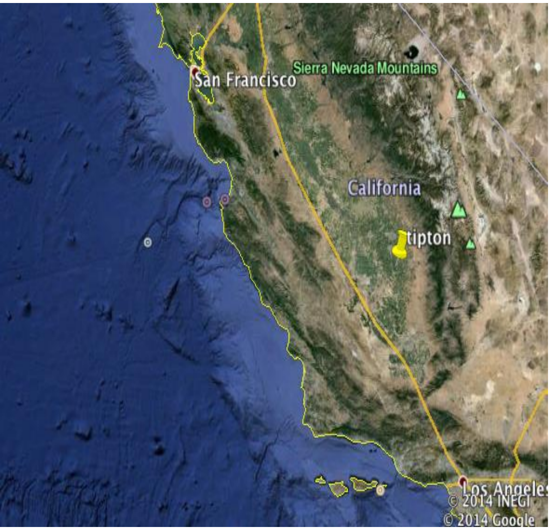
- This work will provide improved emission inventories of NH_3 to air quality (AQ) forecasters, AQ managers, and other stakeholders.
- The current set up for our NASA Applied Science project includes:
  - WRF, SMOKE, EPA Emission Platform, and CMAQ along with its pre-processors
  - A North American WRF/CMAQ domain
  - Using AWS batch which saves the infrastructure as software and allows you to create identical machines and easily maintain them
- We performed a model-retrieval closure study to determine the best metrics to use in the CMAQ inverse modeling, concluding that the total column of NH_3 from CrIS should be compared with the total column from CMAQ after an observation operator with a linear averaging kernel (instead of a log AK) is applied.
- Expect to achieve ARL 4 soon after SMOKE and CMAQ pre-processor debugging is completed. Goal ARL for overall project is 7.

ADDITIONAL SLIDES

Monitoring NH_3 is difficult

NH_3 is highly reactive
➔ highly variable in space and time

NH_3 from an Open path Quantum Cascade Laser (QCL) on a moving platform in the San Joaquin Valley during DISCOVER-AQ 2013.



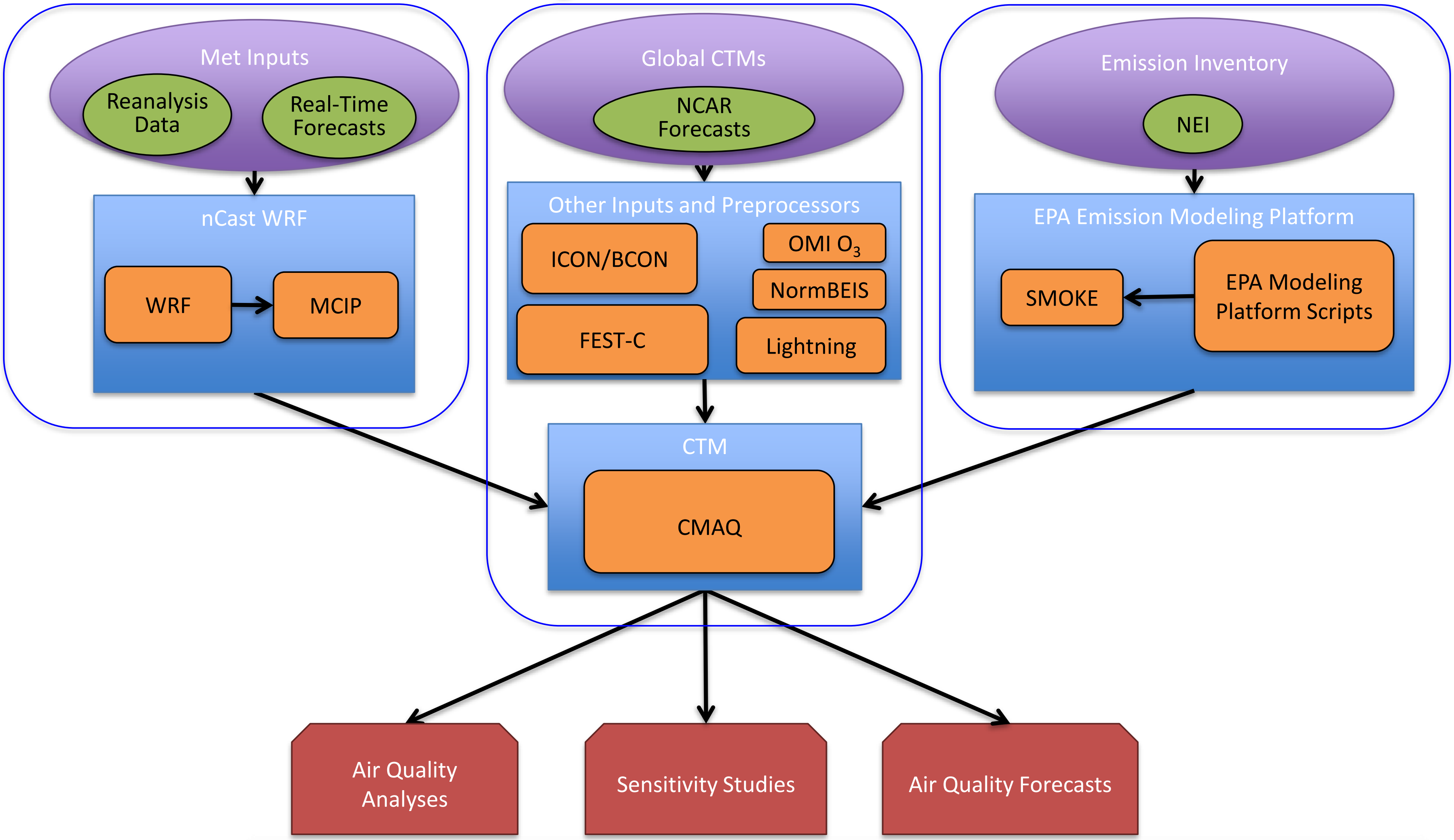
Miller et al., AMT 2013

Cross-track Infrared Sounder (CrIS)

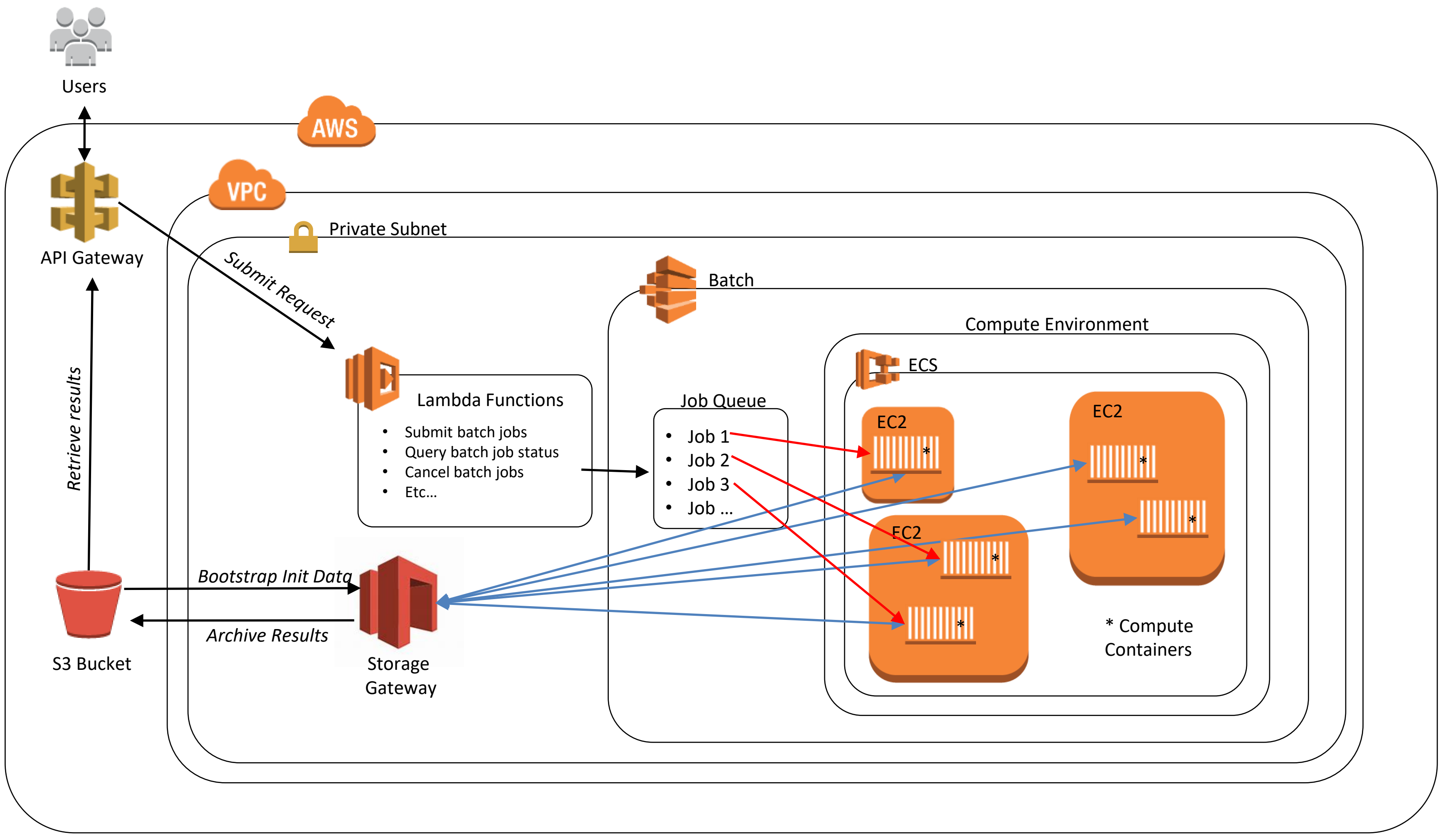
- CrIS can monitor global NH_3 with high spatial coverage from 2011 and over the next decade or more

	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

AQcast CMAQ System for Continental US



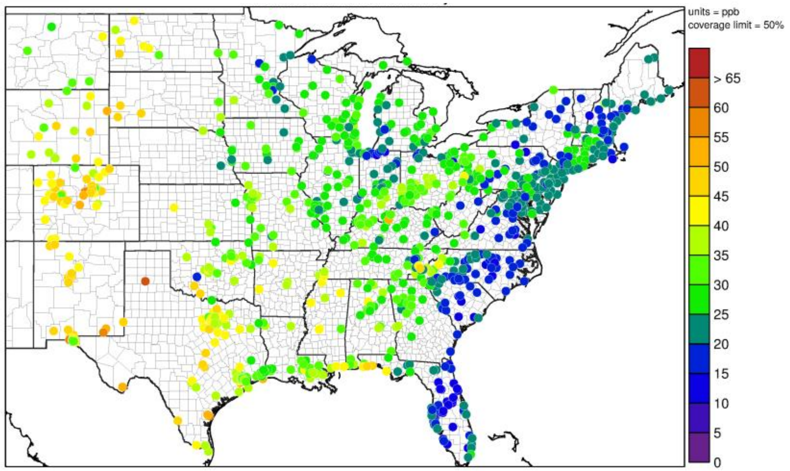
AQcast Production Architecture



Other AQcast Updates for 2019:

- Add **AMET** to evaluate outputs against monitoring network data.
- New components for source attribution and sensitivity runs (**OSAT, PSAT**).
- **Flexible grid settings** by adding spatial surrogate generation tools to Amazon Batch

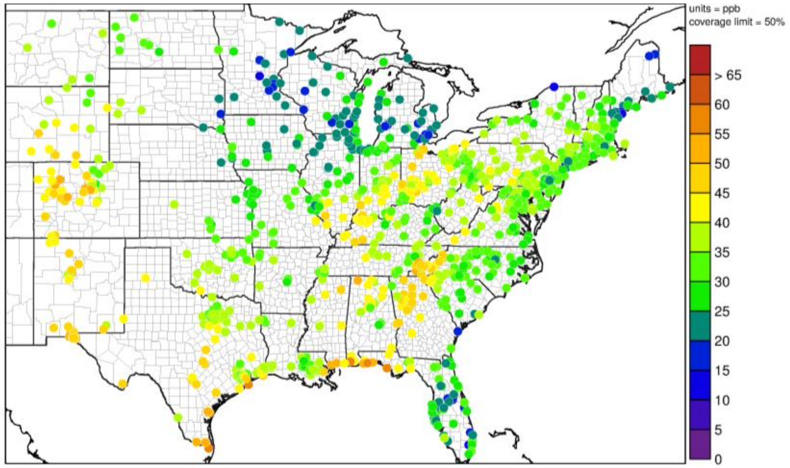
Observed 1-hr Max. O_3 (SENEX)



AERMOD on the Cloud

- Reads and converts fence line and building data from GIS shapefiles.
- Automatically collects and processes met and terrain data.
- Automatically identifies sensitive receptors.
- Creates data summaries and graphics of maximum concentrations.

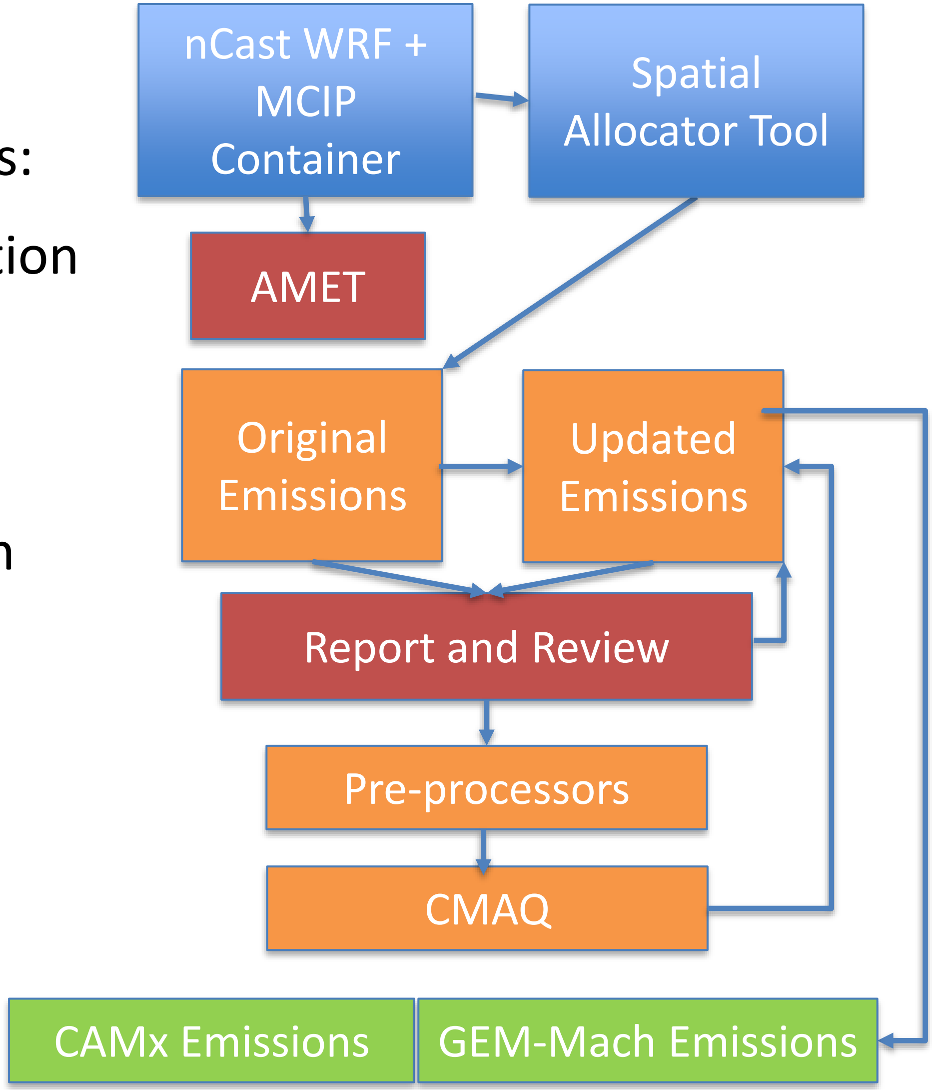
Modeled 1-hr Max. O_3 (SENEX w/ NEI 2011)



Application Work Flow

Modeling work flow currently includes:

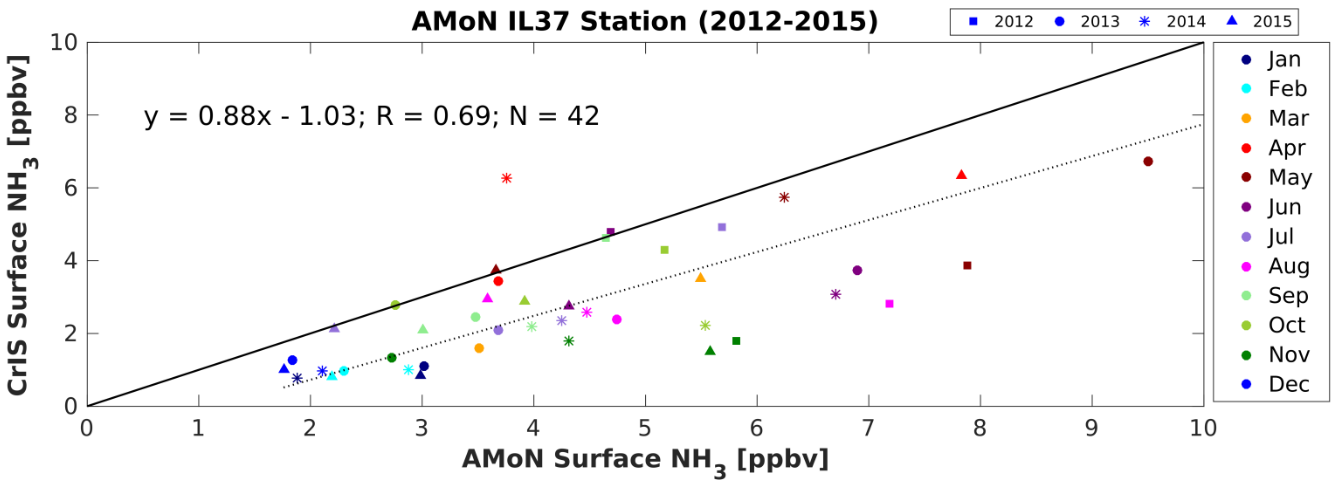
- North American met configuration
- AMET evaluation
- Spatial allocator shapefiles
- Multiple emission configuration options
- Pre-processor configuration
- Multiple CCTM configuration options



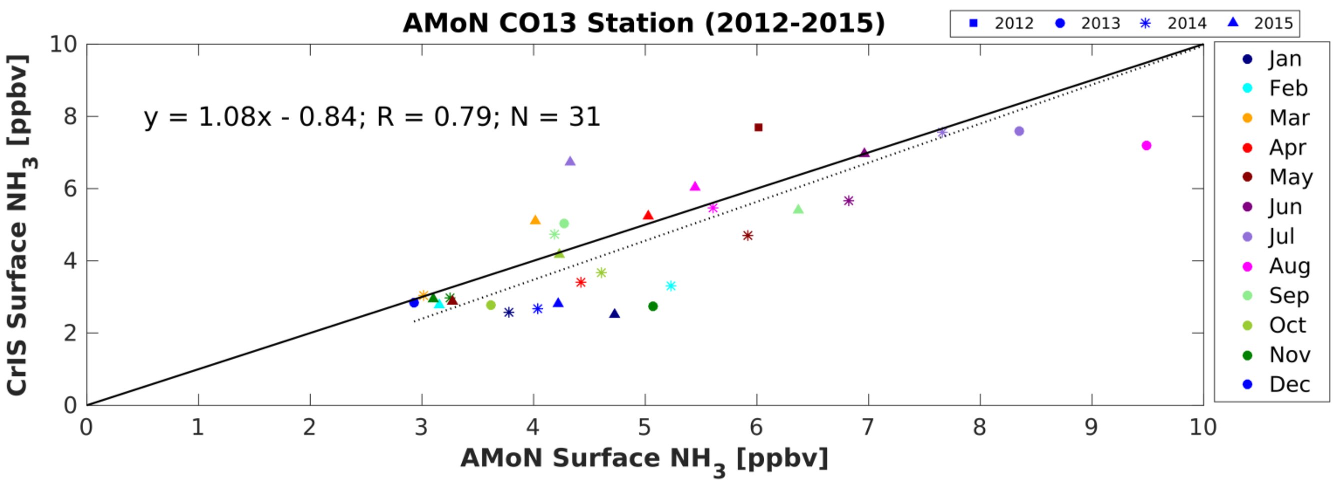
CrIS Satellite Ammonia Monitoring and Evaluation

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

Stockton, Illinois



Fort Collins, Colorado

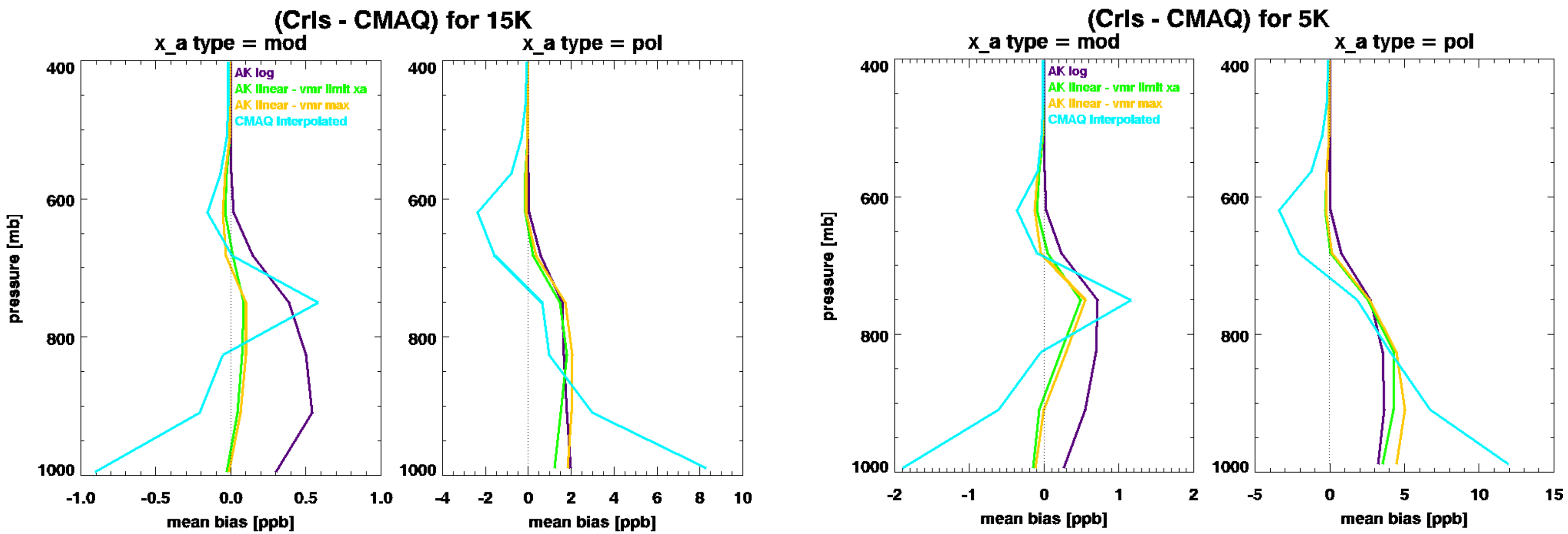


Initial assessment shows that the satellite and AMoN surface observations agree well despite sampling differences

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