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Navigating Satellite Ammonia Measurements: Best Practices and Considerations

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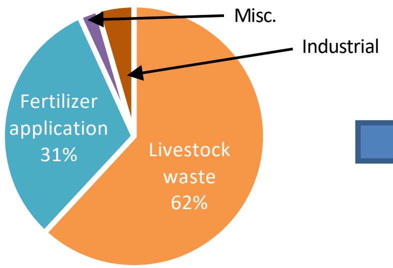
HAQAST2020

WEBINAR SERIES

Why ammonia (NH_3)?

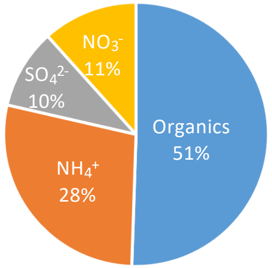
2011 U.S. NH_3 Emissions

Total = 3.44 × 10^9 kg



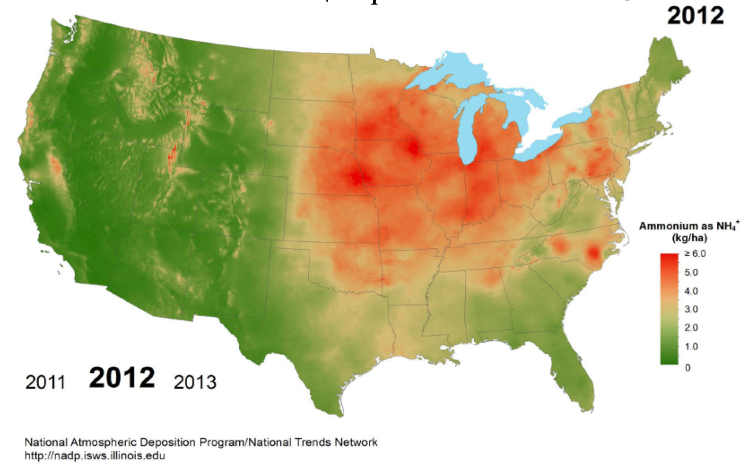
(EPA, 2011)

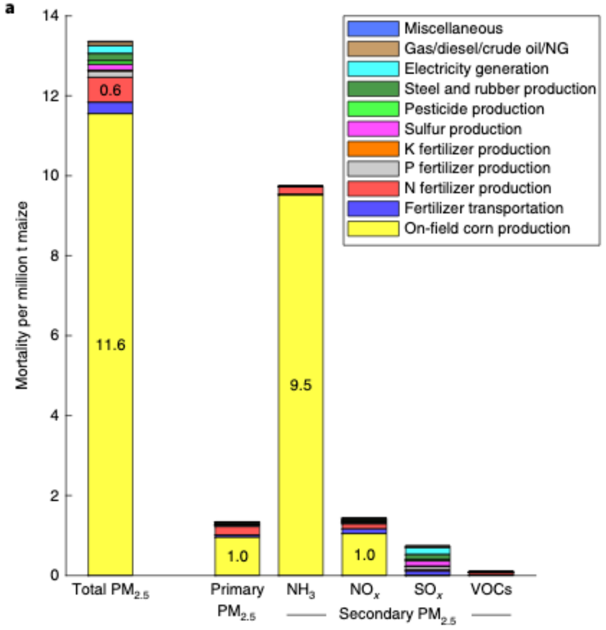
Aerosol composition by mole
Boulder, CO



Adapted from Jimenez et al. (2009)

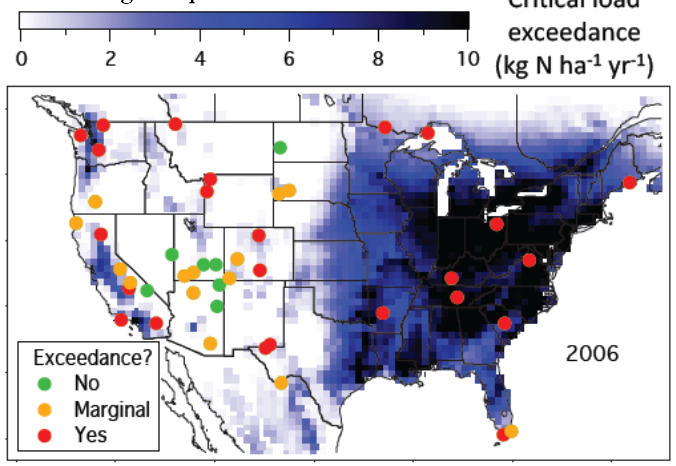
NH_4^+ deposition in US





Mortality from maize production *(Hill et al., 2019)*

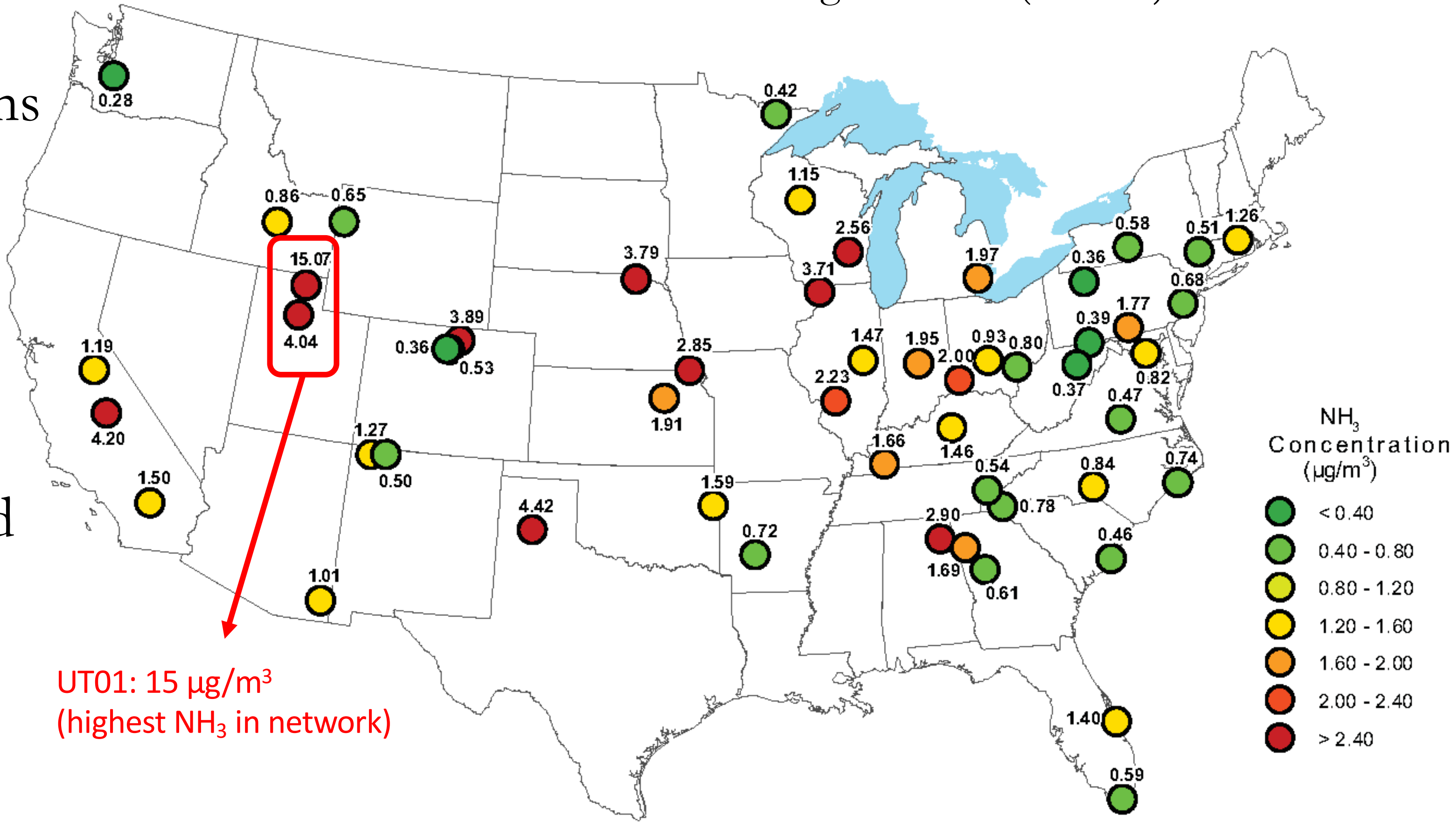
Excess nitrogen deposition in National Parks



Existing observations

- large gaps exist between stations
- station siting problematic and may bias measurements
- large spatial gradients observed
- large temporal variations at many sites

Ammonia Monitoring Network (AMoN)



A closer look at the highest AMoN NH_3 site

Cache Valley, Utah

• site located immediately next to concentrated animal feeding operation!

Is this site representative of the region? What would it observe if, e.g., a few km away?

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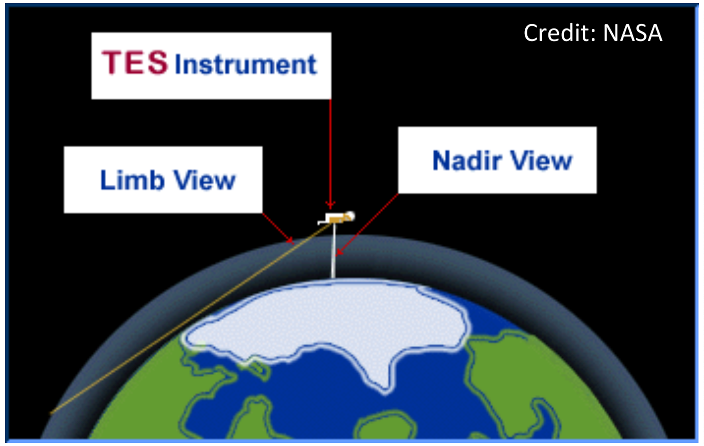
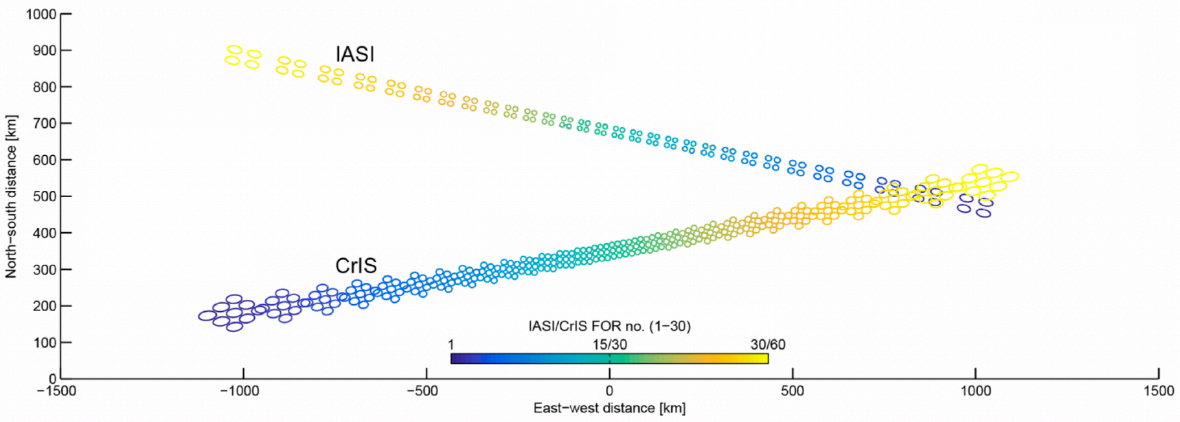
Satellites to the rescue!

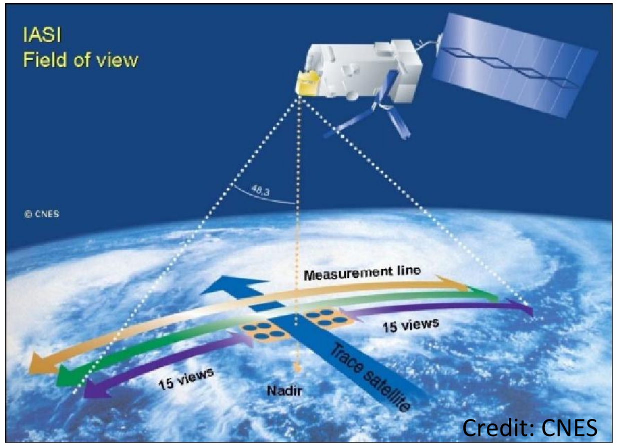
Infrared Atmospheric Sounding Interferometer (IASI)Cross-track Infrared Sounder (CrIS)

Tropospheric Emission Spectrometer (TES), Atmospheric Infrared Sounder (AIRS)

Instrument	Satellite	Day, equator crossing time (local)	Pixel size at nadir (km^2)	NH_3 data availability	Product	Spectral Resolution (cm^{-1})	Noise (K)	Swath width (km)	# pixels across swath	Data accessible to public
IASI	MetOp-A	9:30	12 × 12	2007-present	column	0.5	0.17	2200	60	Y
	MetOp-B	8:45	12 × 12	2013-present	column	0.5	0.17	2200	60	Y
CrIS	S-NPP	13:30	14 × 14	2014-present	profile	0.625	0.04	2200	90	late 2018
TES	Aura	13:30	5.3 × 8.5	2004-2015	profile	0.1	0.15	5.3	1	Y
AIRS	Aqua	13:30	13.5 × 13.5	2002-present	profile	0.5	0.2	1650	90	TBD





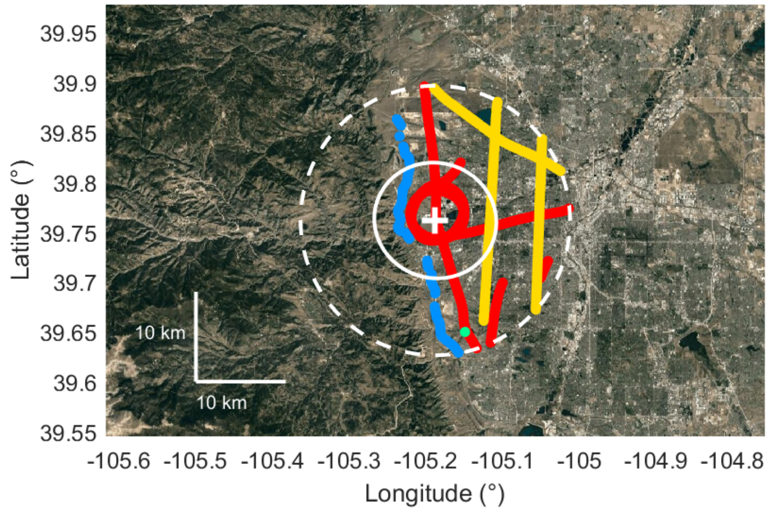


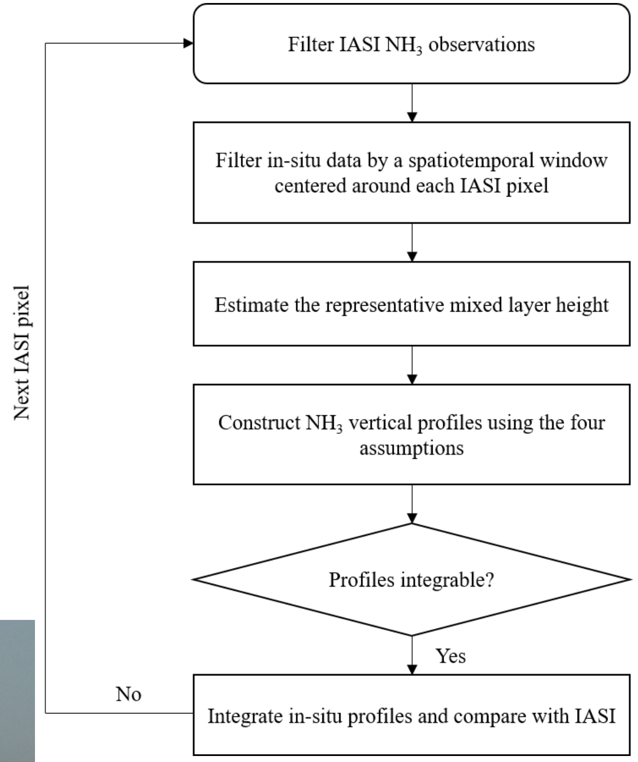
Satellite NH_3 considerations

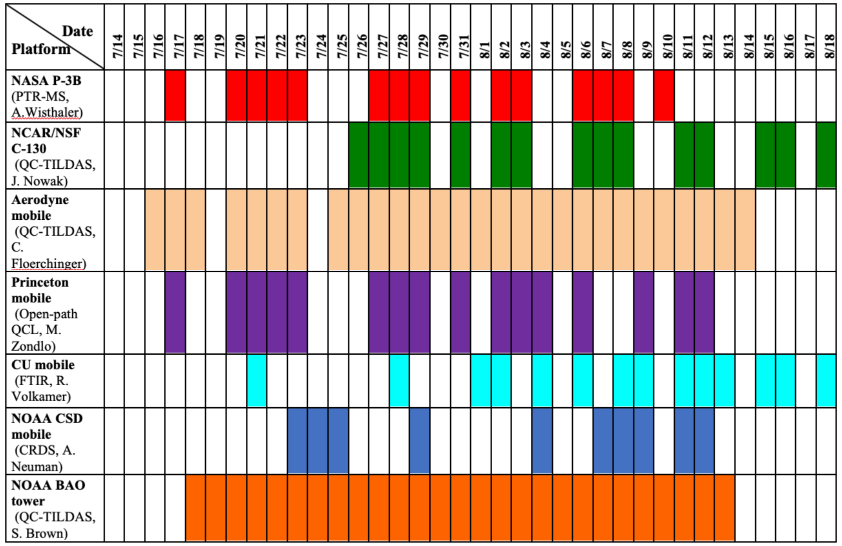
Logistical
- How accurate are these measurements?
- How representative is a single overpass time relative to other times of the day?
- To what extent do the different measurements agree with one another?

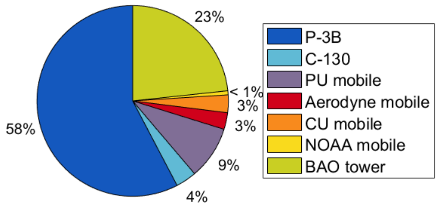
Practical
- For what applications are satellite NH_3 measurements truly groundbreaking?
- When and where should one exercise caution in their use?
- What are future opportunities with continued improvements?

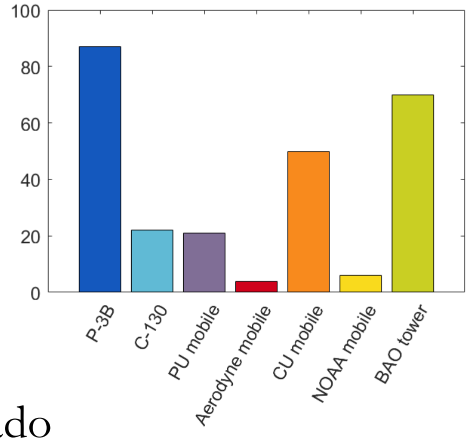
Validation of satellite NH_3











NASA DISCOVER-AQ field study, summer 2014 Colorado

NSF FRAPPE field study, summer 2014

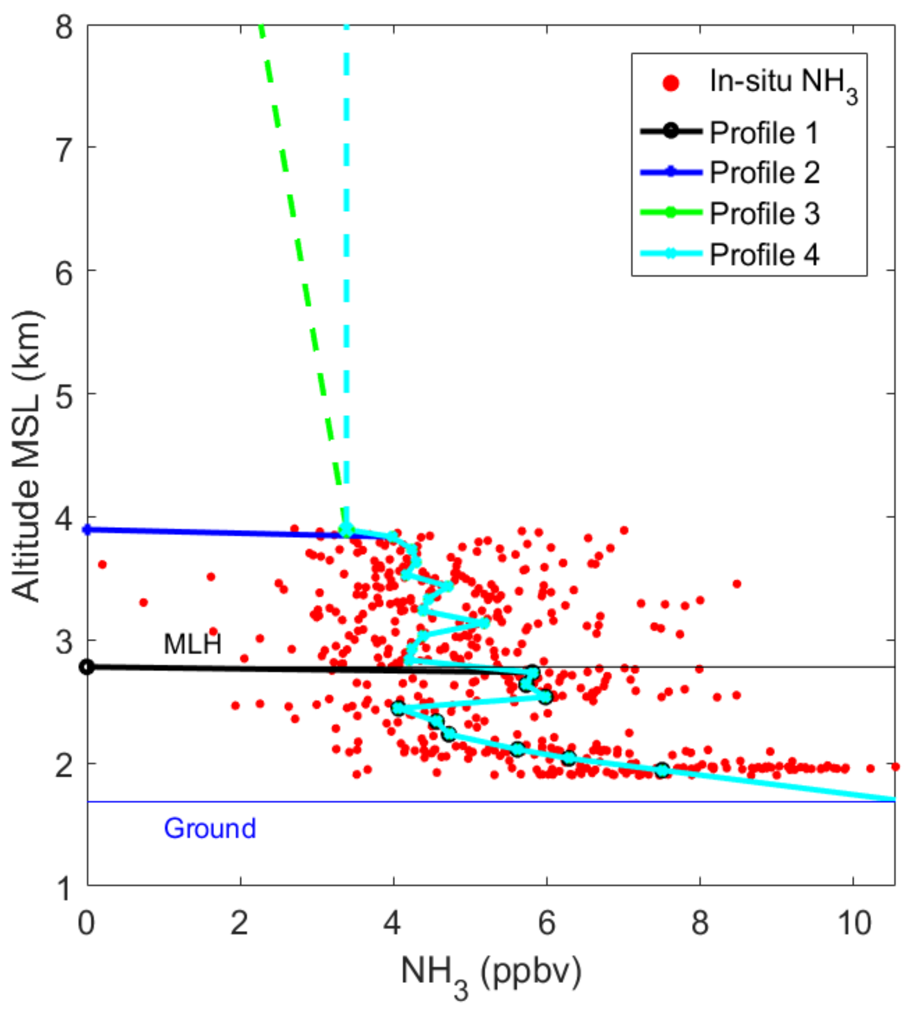
Individual vertical NH_3 profiles

- aircraft only went to ~ 4-5 km altitude
- choice of NH_3 from there to tropopause matters
- evaluated four profiles:
  1: NH_3 only in the mixed layer, zero above

  2: Use all aircraft data (sampling biases of instruments)

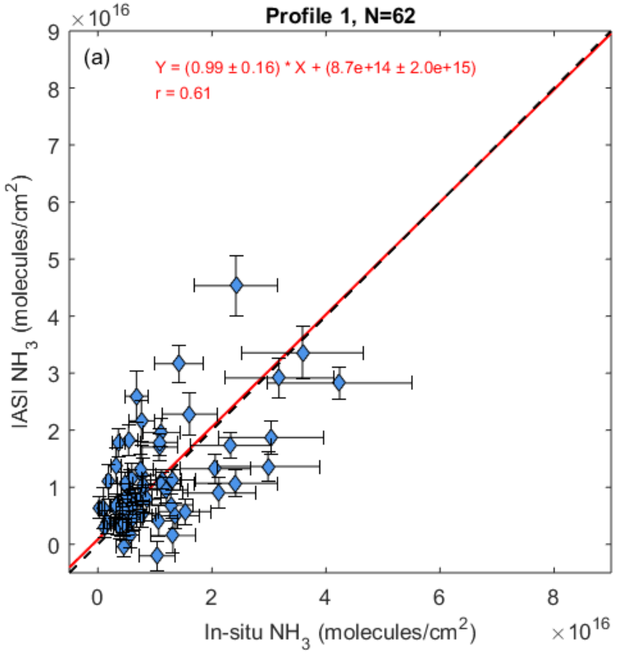
  3: Extrapolate highest altitude to zero at tropopause

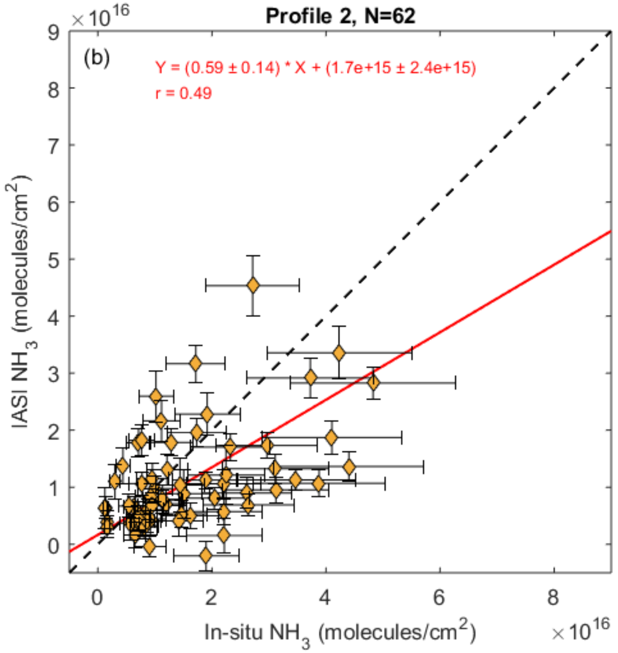
  4: Constant tropospheric values above aircraft (well-mixed)

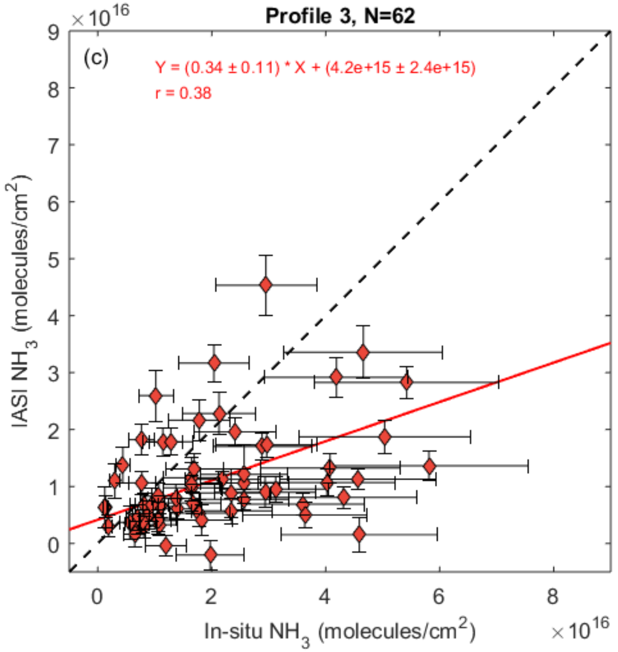


Validation vs. profile choices

Used ±15 km of IASI centroid, ± 1 hour of overpass time based upon mean wind







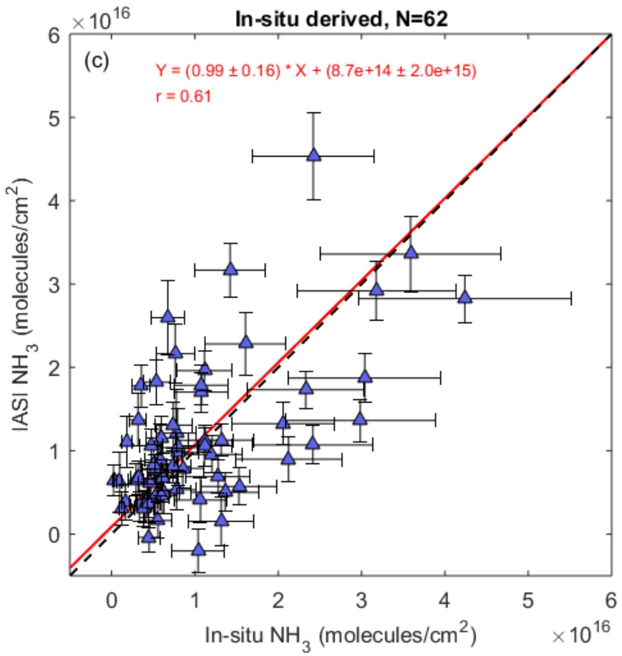
Assuming mixed layer contains most of NH_3 signal is consistent with its short lifetime

Also correlation best of all four approaches (also intercept and slope)

Validation results

Temporal window	20 min			60 min			180 min		
Spatial window	Within pixel	15 km	45 km	Within pixel	15 km	45 km	Within pixel	15 km	45 km
m	0.92 ±0.19	0.69 ±0.18	0.09 ±0.03	1.90 ±0.58	0.71 ±0.11	0.84 ±0.13	2.71 ±1.23	2.02 ±0.45	1.22 ±0.24
b	7.9e13 ±2.9e15	1.4e15 ±2.9e15	7.1e15 ±6.3e14	-7.1e15 ±5.2e15	1.4e15 ±1.4e15	4.8e14 ±1.1e15	-1.4e16 ±1.1e16	-7.5e15 ±4.0e15	-1.0e15 ±1.7e15
r	0.81	0.62	0.23	0.55	0.63	0.36	0.37	0.45	0.29
N	12	23	160	25	63	270	30	81	279
IASI mean	1.1e16 ±9.8e15	1.1e16 ±9.1e15	8.1e15 ±6.8e15	8.9e15 ±7.6e15	8.9e15 ±7.3e15	6.9e15 ±6.3e15	9.8e15 ±8.0e15	9.6e15 ±8.2e15	7.0e15 ±6.5e15
In-situ mean	1.2e16 ±1.0e16	1.4e16 ±1.2e16	1.1e16 ±1.9e16	8.4e15 ±5.2e15	1.0e16 ±9.0e15	7.7e15 ±6.8e15	8.8e15 ±5.2e15	8.5e15 ±5.9e15	6.6e15 ±6.1e15

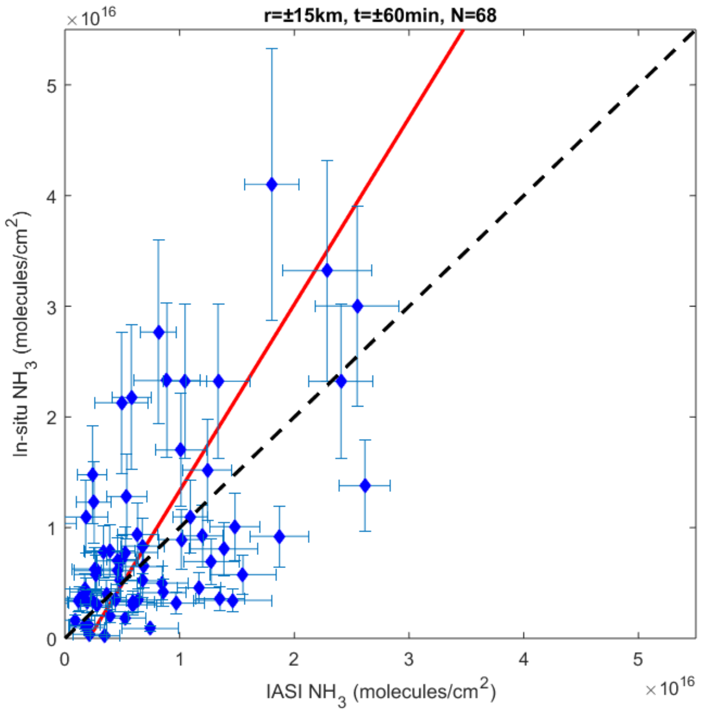
±15 km, ± one hour

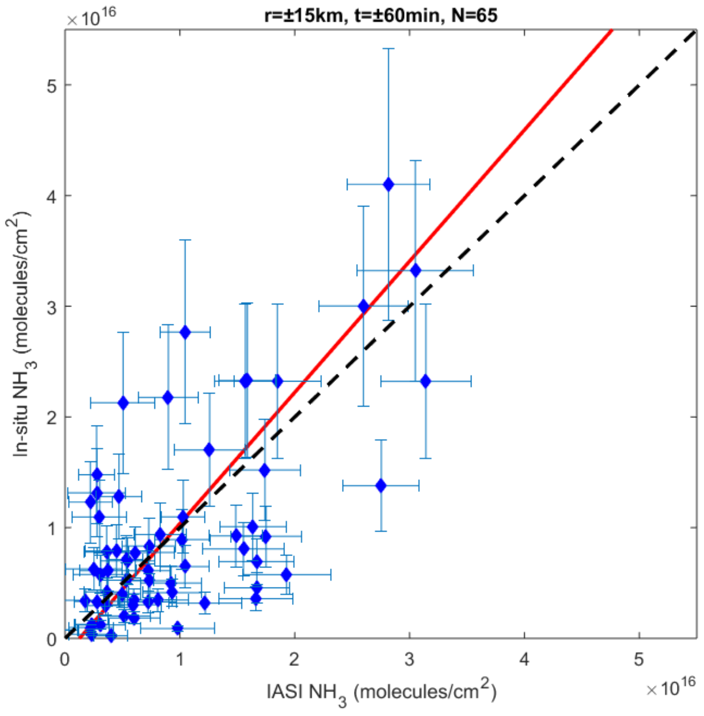


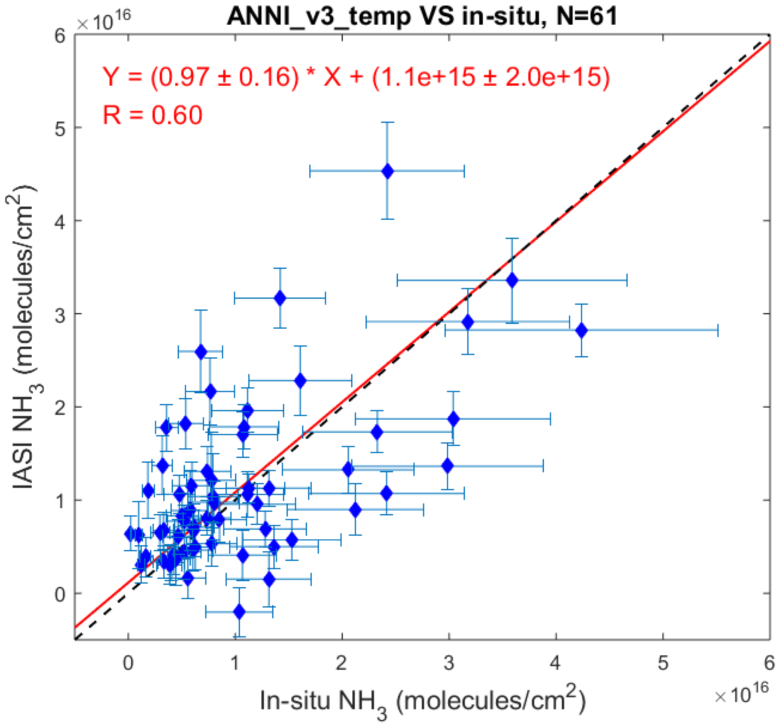
Temporal window matters: decreasing correlation as window expands

Spatial window matters: as one increases the window, correlation degrades

IASI: version improvements over time







CrIS products, though newer and less mature, are also showing significant improvements over time

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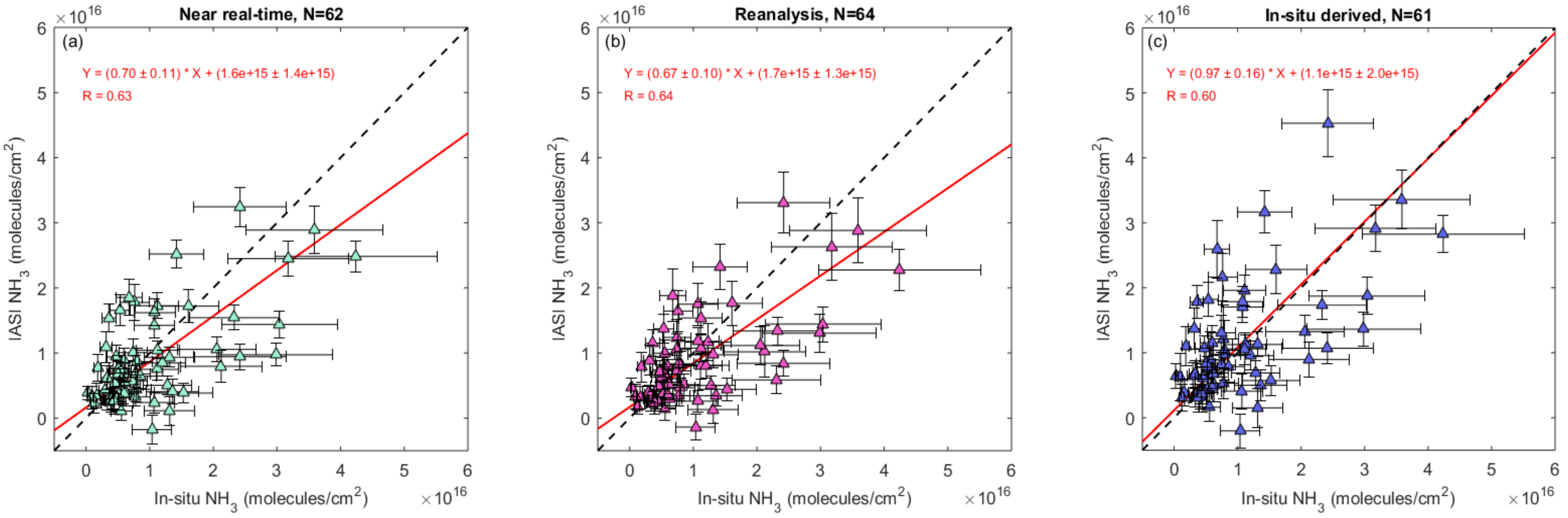
Sensitivity to accurate temperature profiles

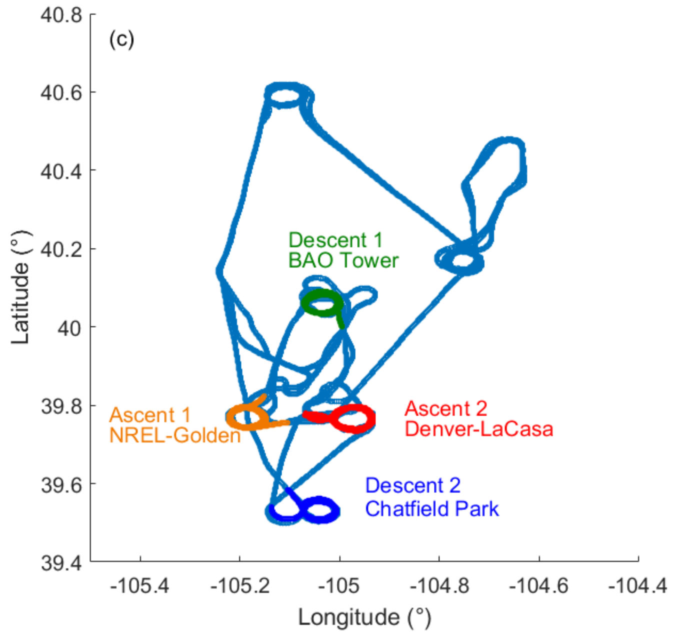
Validation using different temperature inputs with the last one using actual temperatures

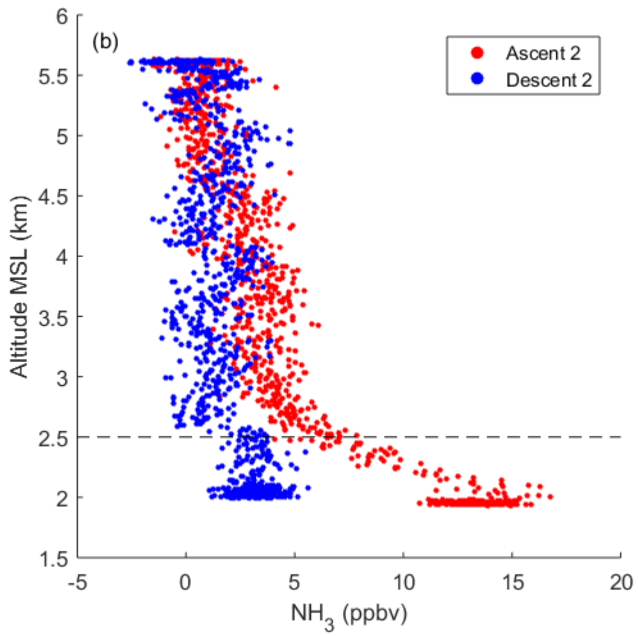


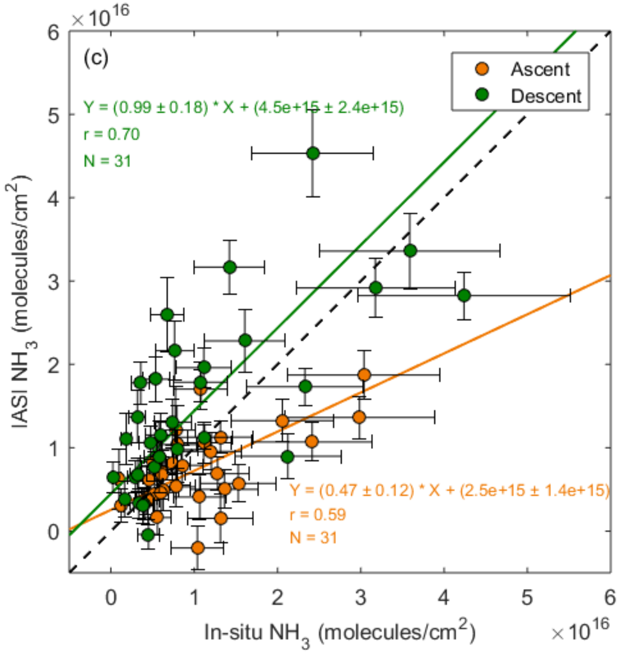
Accurate knowledge of temperature retrievals in the boundary layer really matters!

- inversions, winter time may be difficult to trust completely for any satellite NH_3

...but in-situ measurements have biases!







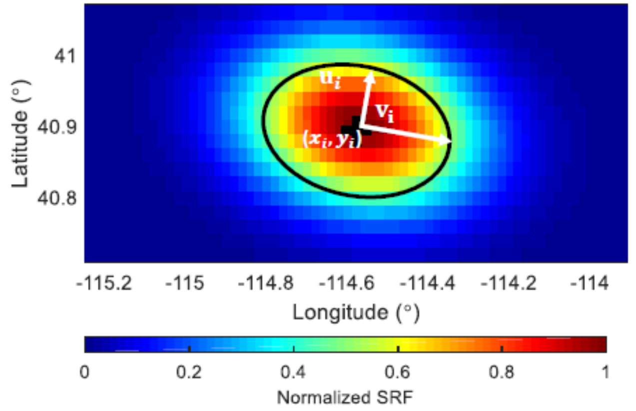
- differences when plane ascends vs. descending – artifacts from "sticky" ammonia problematic for validation
- great need for validation under different conditions (thermal contrast), more measurements

Achieving high spatial resolution (2 km)

2-D Gaussian function to approximate the spatial response function

(SRF determines the spatial response of the satellite pixel with respect to its center)

(Sun et al., AMT, 2018)



Spatial response function $\mathbf{SRF(i,j)}$

+

Uncertainty $\boldsymbol{\sigma(i)}$

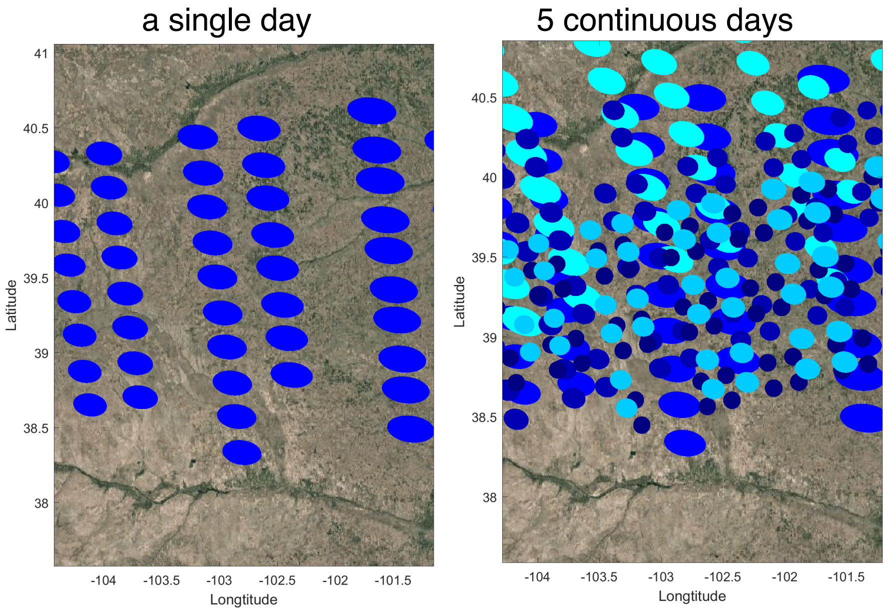
Weighted mean at grid j

$$C(j) = \frac{\sum_i \frac{SRF(i,j)}{\sigma(i)} \Omega(i)}{\sum_i \frac{SRF(i,j)}{\sigma(i)}}$$

$\Omega(i)$: the vertical column density measured at pixel i

$\sigma(i)$: the uncertainty of vertical column density measured at pixel i

Satellite tracks on:



Overlapping satellite pixels from different times are grid-averaged

Weighted mean in each grid is used to plot the NH_3 map

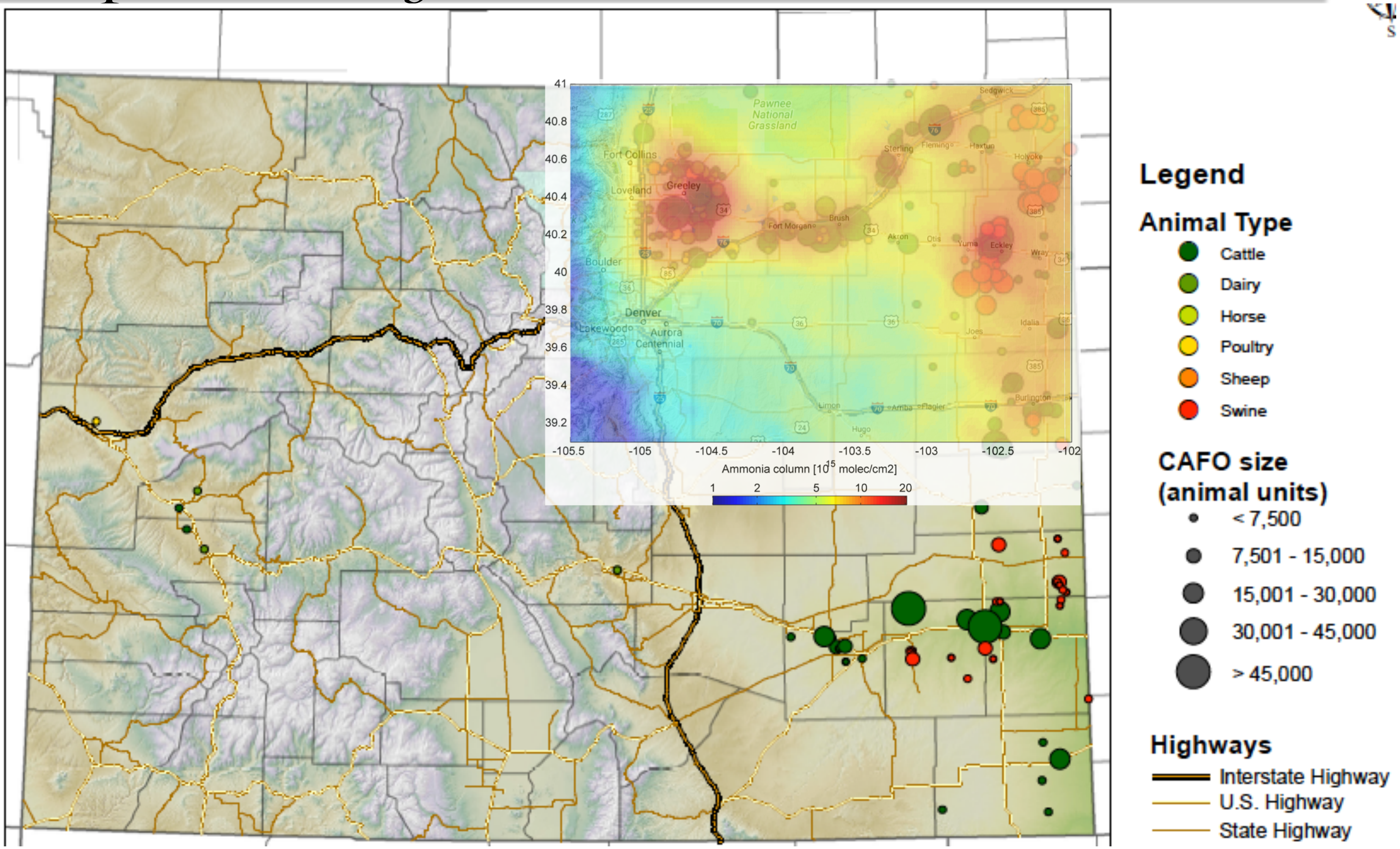
Trade temporal for spatial resolution for few km resolution

Example: NH_3 columns and feedlots

- Concentrated animal feeding operations (CAFOs) in northeastern Colorado

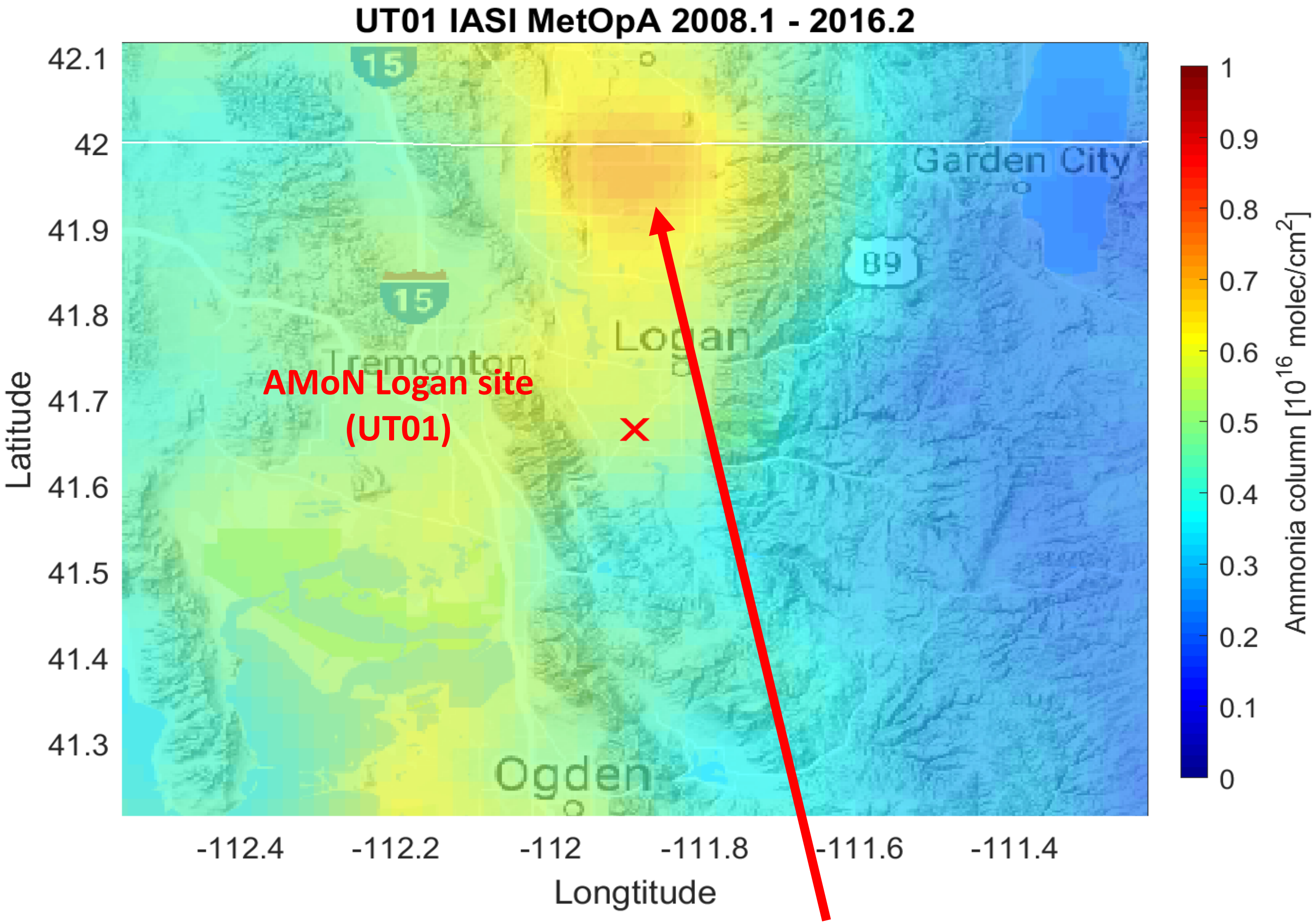
- Oversampling IASI algorithm over the same location

- Striking co-location of high NH_3 with columns



Example: revisiting the highest AMoN site

- UT01 has the highest NH_3 in AMoN
- site may not be representative of the area if farm upwind of site
- NH_3 actually higher in the northern portions of the valley vs. southern
- How does this compare nationally to other NH_3 hospots?



NH_3 column maximized in northern portion of Valley

Average annual NH_3 column abundances

+ AMoN sites
  (white=ongoing)
  (black=not operational)

<u>NH_3 Hotpot Characteristics</u>

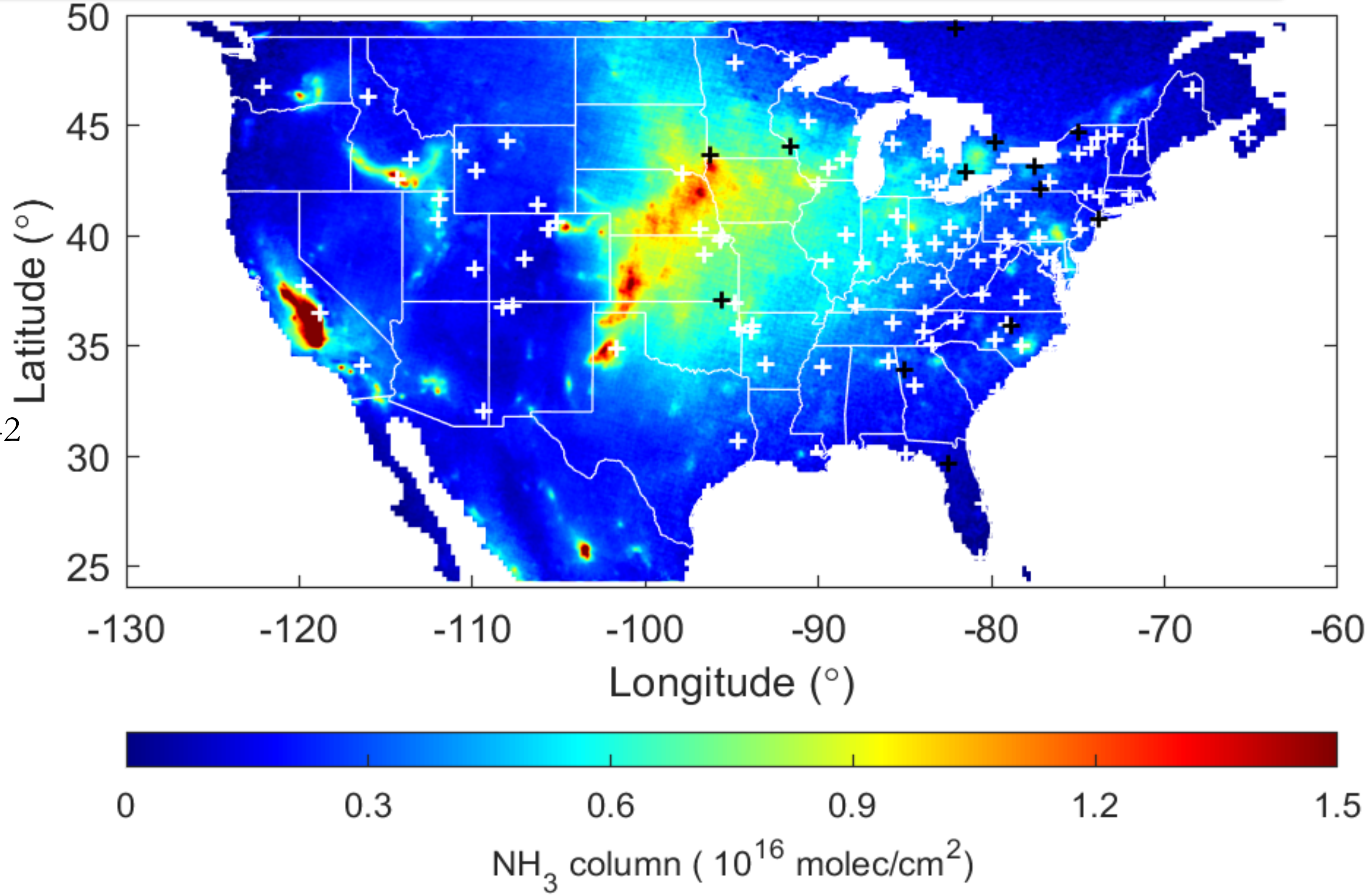
95^{th} percentile = 7.9×10^{15} molec cm^{-2}

N=93

Median area 136 km^2

Lengthscale ~ 30 km

of the top 14 hot spots, only **5** have AMoN sites within 100 km distance, and only **2** have long-term data and similar elevation with the hot spots



Areal-column largest: Central plains, SJV, Texas panhandle, Snake River

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Satellites NH_3 for future site placement

Clean Air Status and Trends Network (CASTNET) site in Beaufort, NC.
Photo courtesy of the U.S. Environmental Protection Agency (EPA).

Need for
Improved Monitoring
of Spatial and Temporal Trends
of Reduced Nitrogen

by Melissa A. Puchalski, John T. Walker, Gregory M. Beachley, Mark A. Zondlo, Katherine B. Benedict, Richard H. Grant, Bret A. Schichtel, Christopher M. Rogers, April B. Leytem, Joann Rice, Kristi Morris, James J. Schauer, and Rui Wang

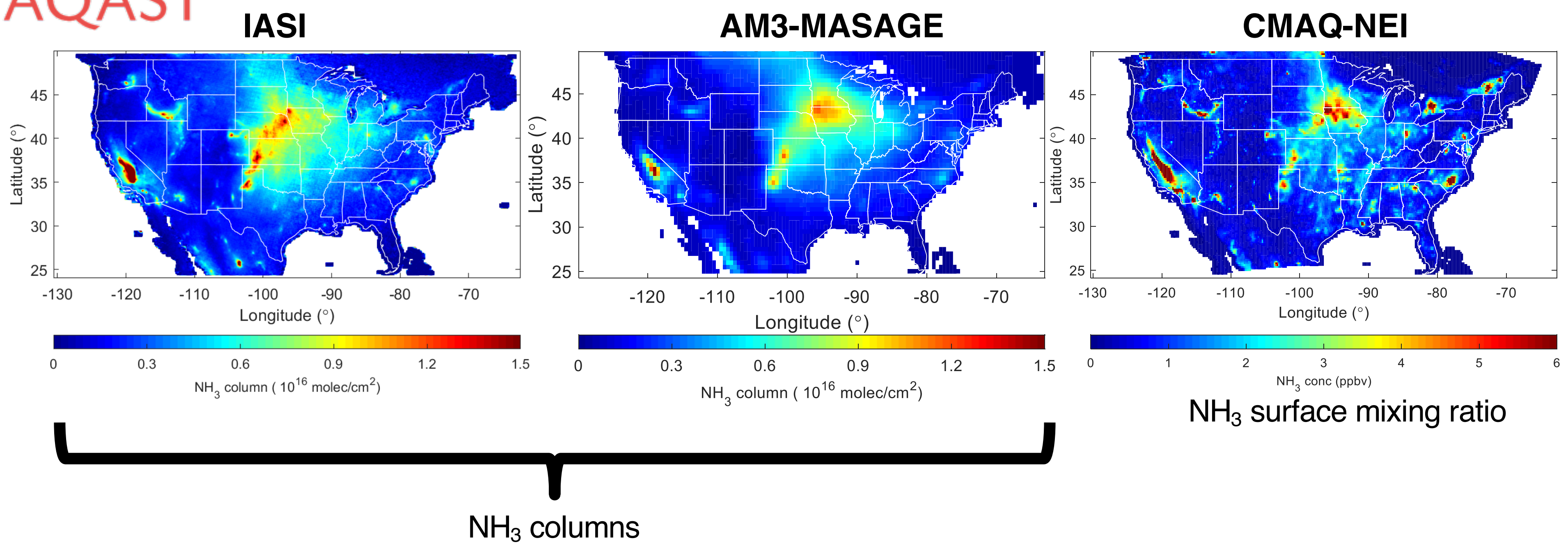
The authors discuss needed improvements in monitoring and characterization of reduced inorganic nitrogen.

See Puchalski *et al.*, *Environmental Monitor* July 2019 issue

How satellites can be used for improving the surface monitoring network:

- representativeness
- hotspots
- capturing spatial gradients

Annual cycle compared to model/inventories



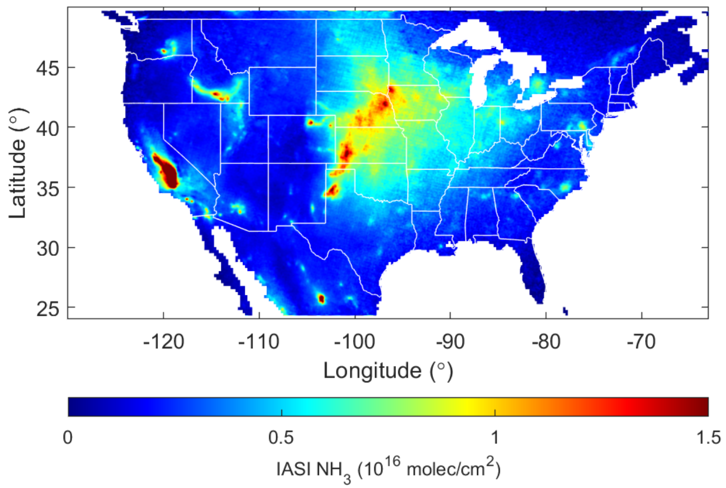
MASAGE: Fabien Paulot, NOAA GFDL

CMAQ: James Kelly, EPA
Jesse Bash, EPA

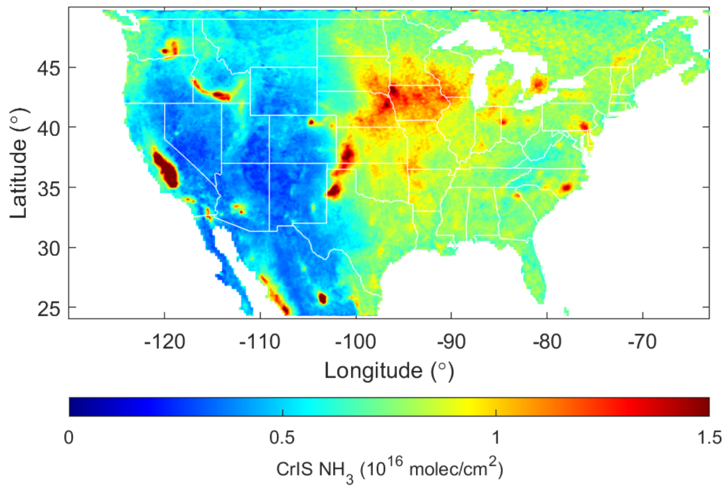
- general patterns well-represented on the continental scale, but significant differences near hotspots
- absolute amplitudes differ between IASI and MASAGE (also CMAQ)
- relative amplitudes also differ regionally and between hotspots

Comparison of IASI vs. CrIS

IASI: v2.2r, 2008 - 2017 Metop-A & Metop-B



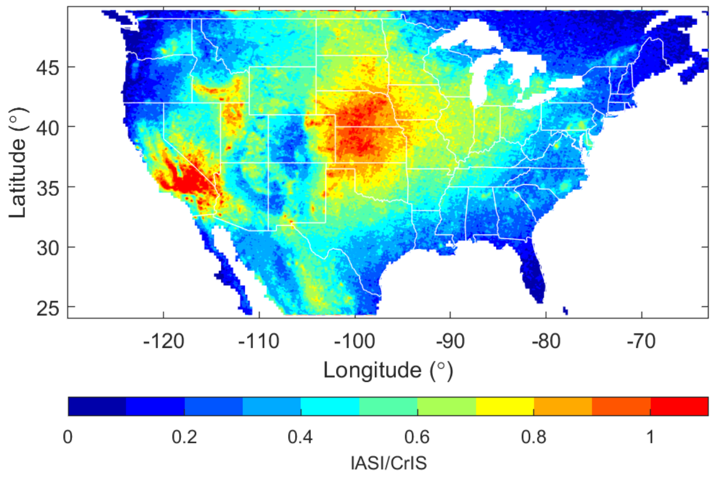
CrIS: v1.5, 2013 - 2017, quality flag = 5



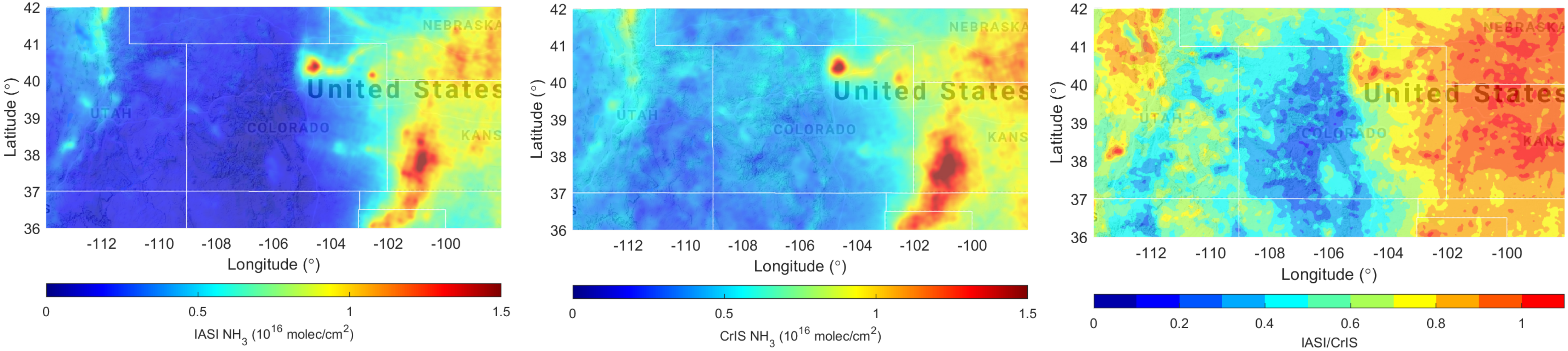
Excellent agreement over hotspots (ratio ~ 1)

IASI lower than CrIS over moderate/low columns

IASI/CrIS



Comparison of hotspots in Colorado



Hotspot values consistent (ratio=1) around key emission sources

Annual maps don't tell the story, however

2008-2016, Metop/A & Metop/B, oversampling high resolution (0.02°×0.02°) maps

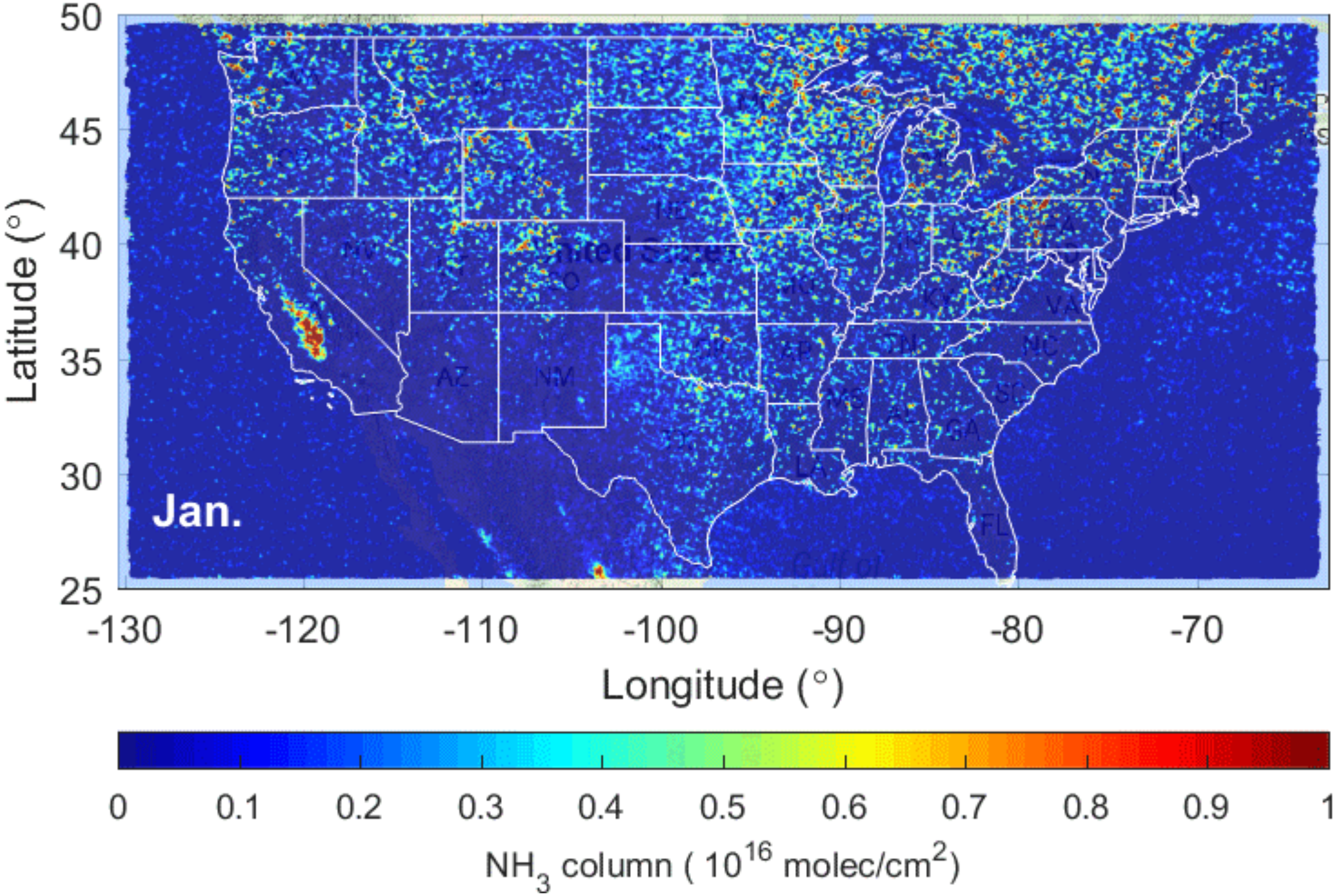
- **Overall seasonality:** low in winter, peak in spring/ summer

- **A high variability of seasonalities:**

  San Joaquin Valley peaks in July

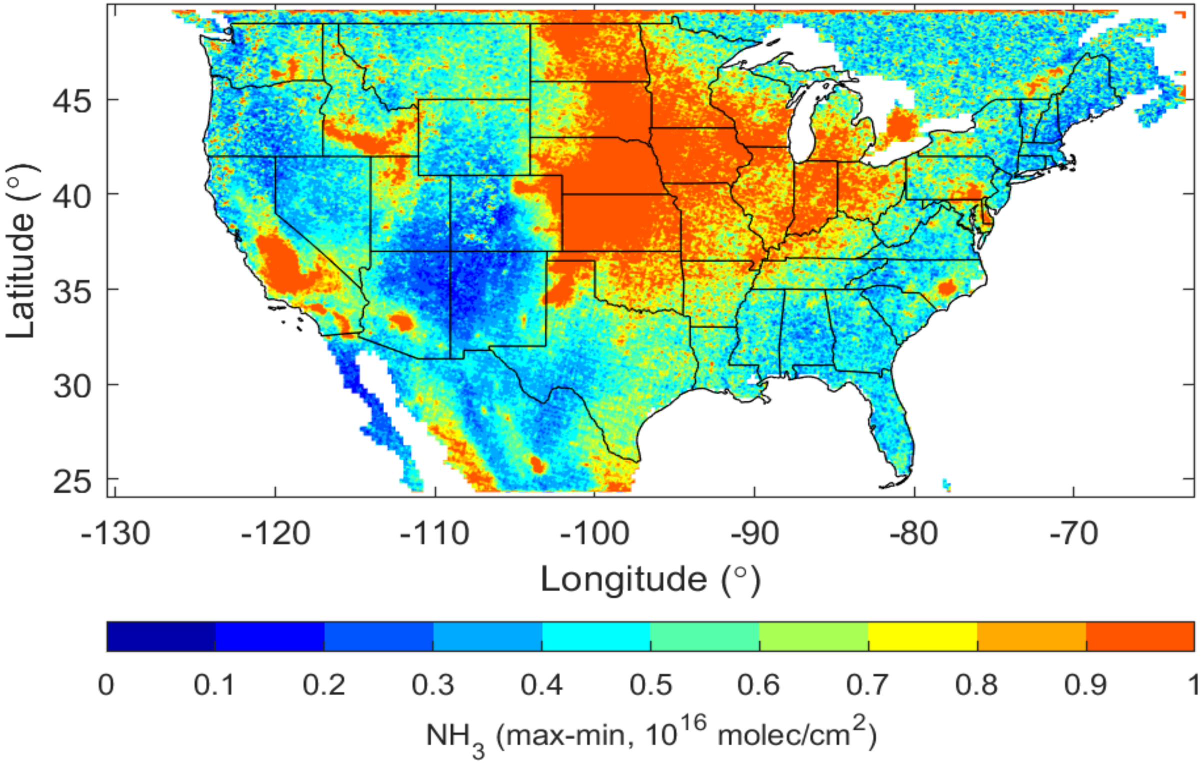
  Midwest in spring in May

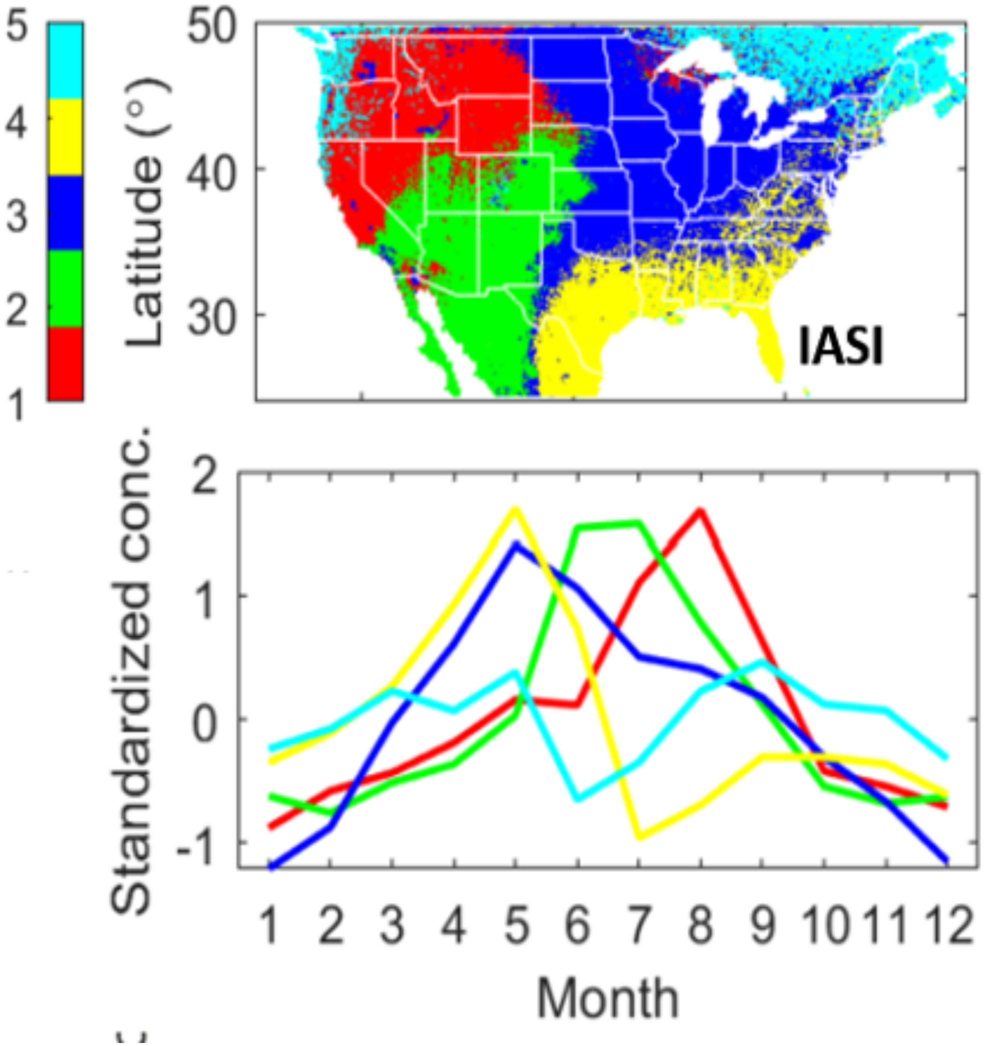
  High plains in July / August



Seasonality of emissions: regional differences

Absolute differences between maximum-minimum IASI NH_3

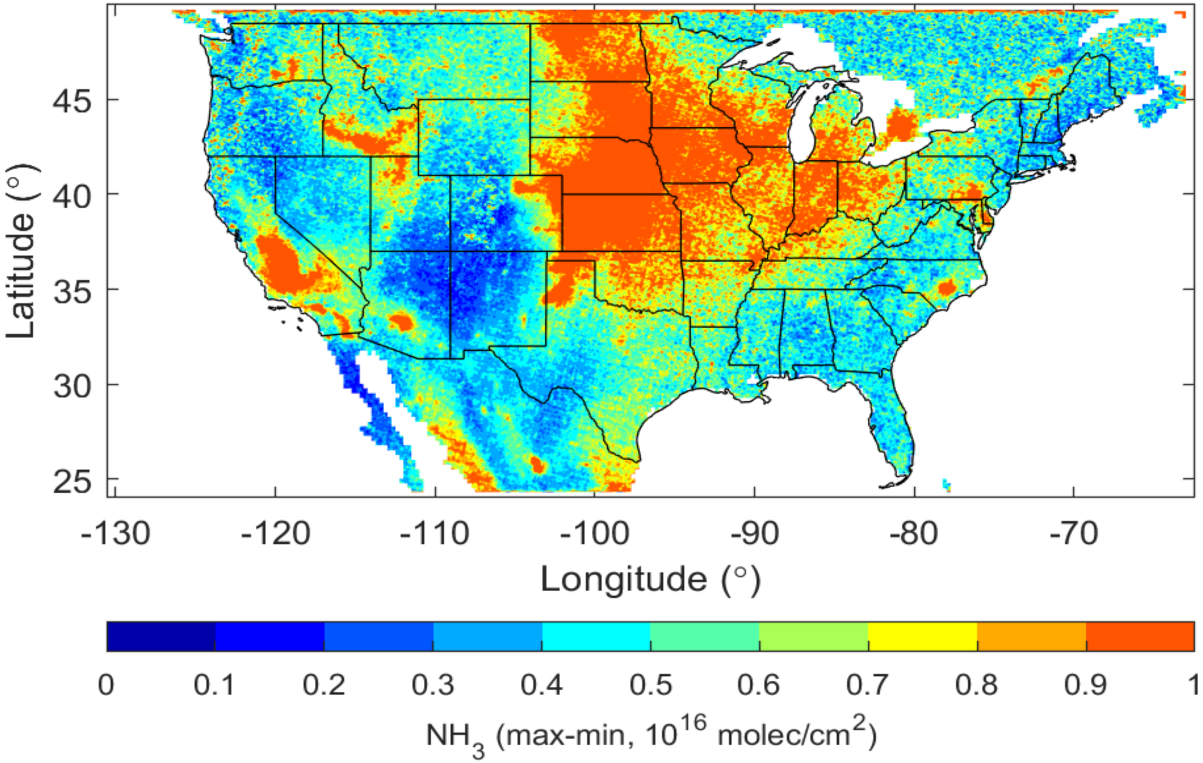


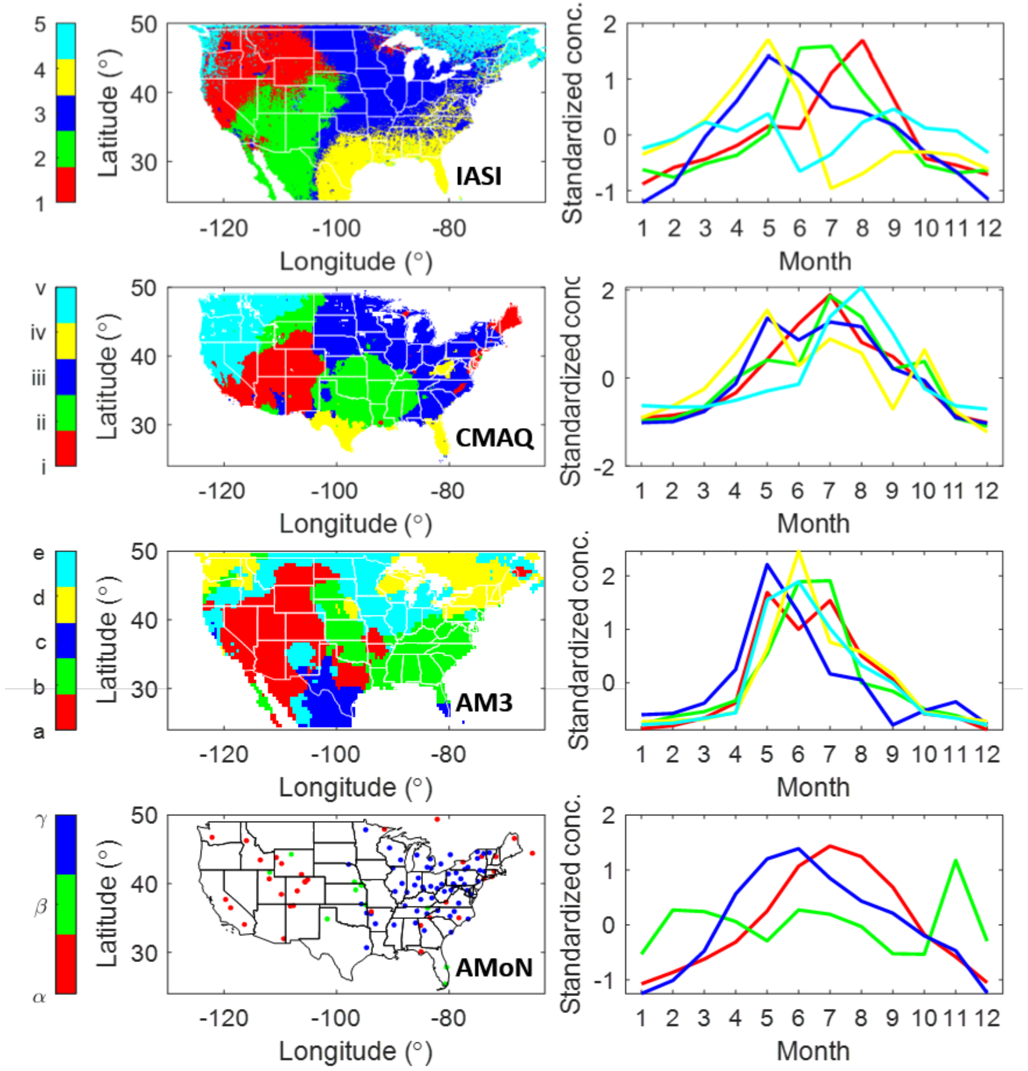


- seasonalities are huge – annual maps misleading
- generally captured by models/inventories but show a much narrower and simplistic monthly pattern

Seasonality of emissions: regional differences

Absolute differences between maximum-minimum IASI NH_3





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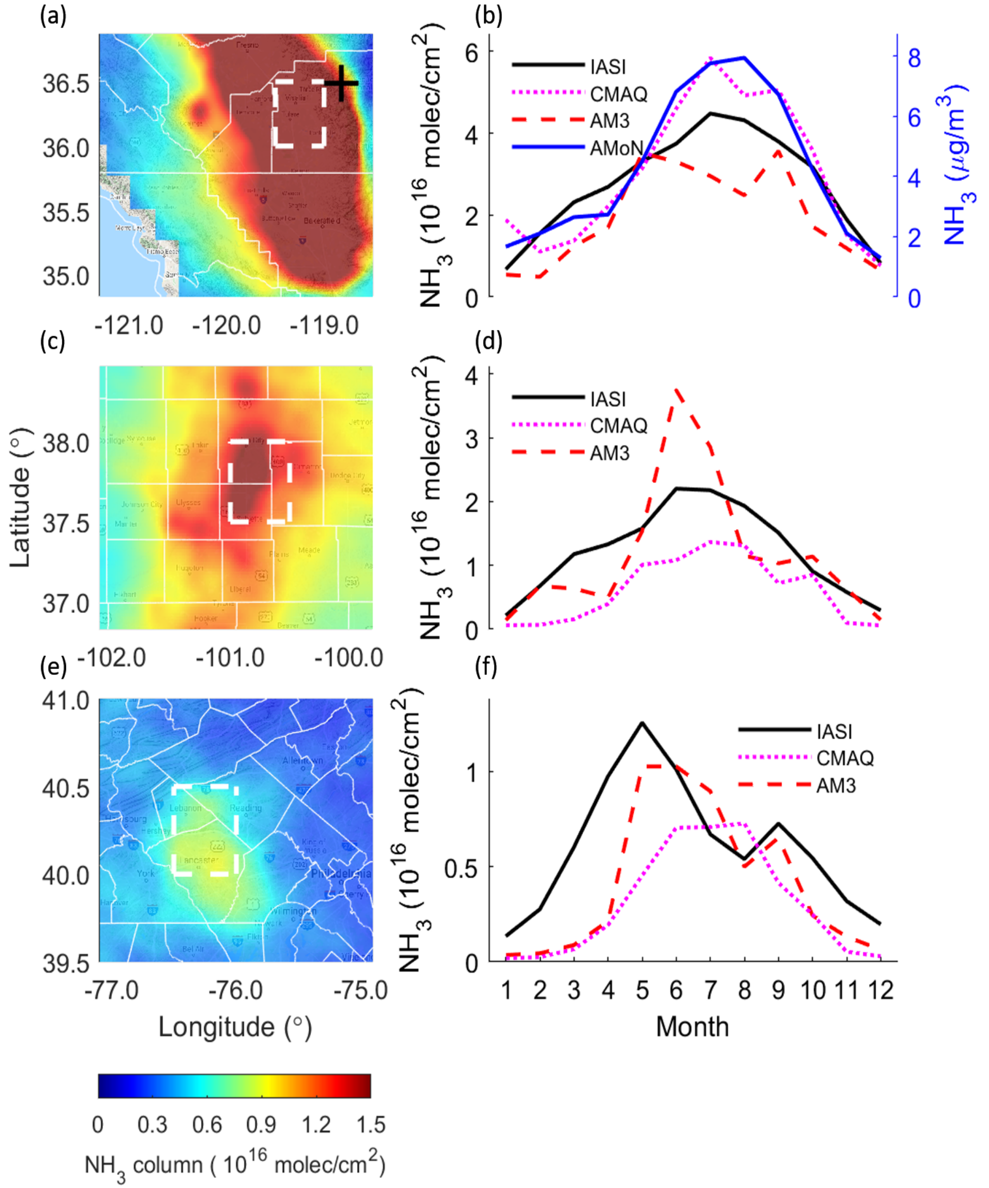
A look at individual hotspots

- San Joaquin Valley (Tulare County):
  seasonality of IASI/CMAQ/AMoN agree well

- Western Kansas
  AM3 more strongly peaked than IASI/CMAQ due to feedlot emissions vs. croplands

- Lancaster County, PA
  earlier springtime peak of IASI/AM3 consistent with spring fertilization of croplands



Ammonia from space: summary

- Great for understanding spatiotemporal trends:
  - inventory improvements (currently done at county level, differences in data sources)
- Great reat for determining next generation of ground-based satellite measurements
- Use with caution in areas with strong inversions (winter, valleys)
- Satellite ammonia measurements, taken once per day, should be corrected for diurnal patterns
- Absolute concentrations for the ground should be used with caution (spatial scales, validation)
  (temperature profiles, thermal contrast, NH_3 vertical profiles all matter!)
- On average validation looks promising, but more validation datasets are critically needed
  (especially over hotspots where conditions may not reflect "average")