

Session 11: Trace Gases

***Chairs: Antonia Gambacorta and Monika Kopacz
NCWCP 2552-53***

Agenda:

8:30 – 12:10 **NUCAPS**

12:10 – 13:20 Lunch

13:20 – 14:45 **Applications (carbon, methane, HCHO, NO₂)**

14:45 – 15:30 Break (no posters)

15:30 – 17:00 **SO₂ presentations**

AC4 Program and JPSS

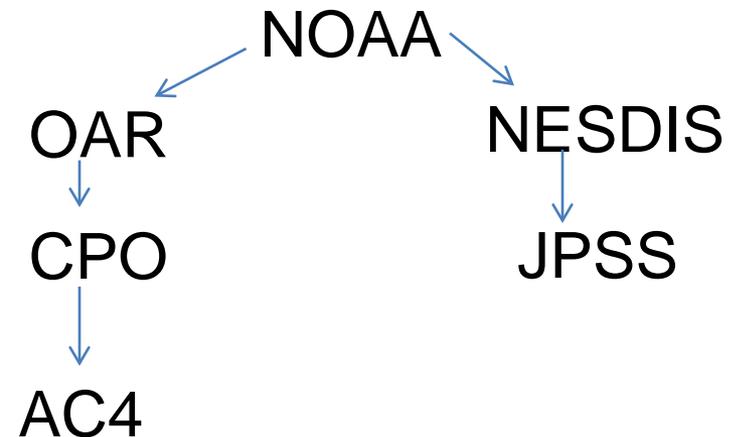
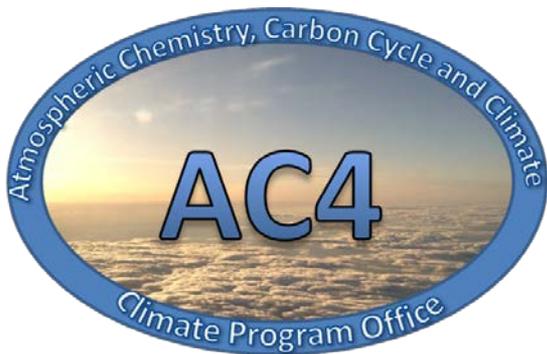
Monika Kopacz, Kenneth Mooney
AC4 Program Managers

August 11, 2016

Atmospheric Chemistry, Carbon Cycle and Climate (AC4) Program

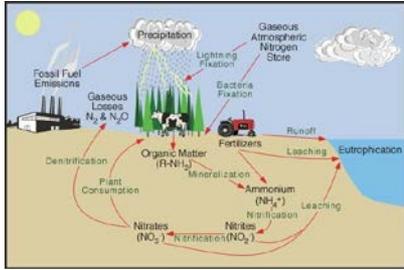
AC4 is a competitive research program which manages a portfolio of multi-year projects

AC4 Goal: Determine the processes governing atmospheric concentrations of greenhouse gases and aerosols in the context of the Earth System and climate



FY13-FY16 Atmospheric Chemistry, Carbon Cycle, and Climate (AC4) Research Portfolio

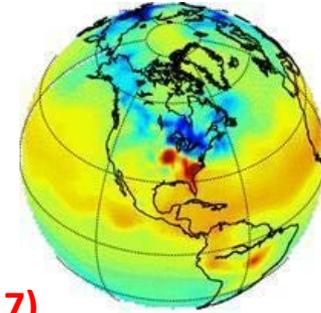
Nitrogen Cycle (FY13,15)



Atmospheric composition from space (FY16)



CarbonTracker (FY13)



Emissions and Chemistry of Wildfires (FY16-17)

Urban Emissions (FY13,14,17)



Oil & Gas Emissions (FY 14,17)



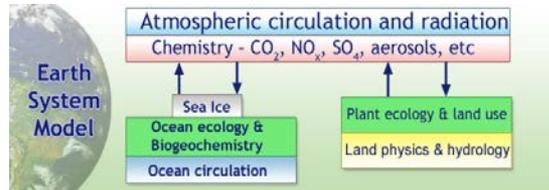
ESRL/CSD, PMEL, ARL Field Campaigns



ESRL/GMD Monitoring



GFDL Nitrogen Modeling



Atmospheric Composition from space

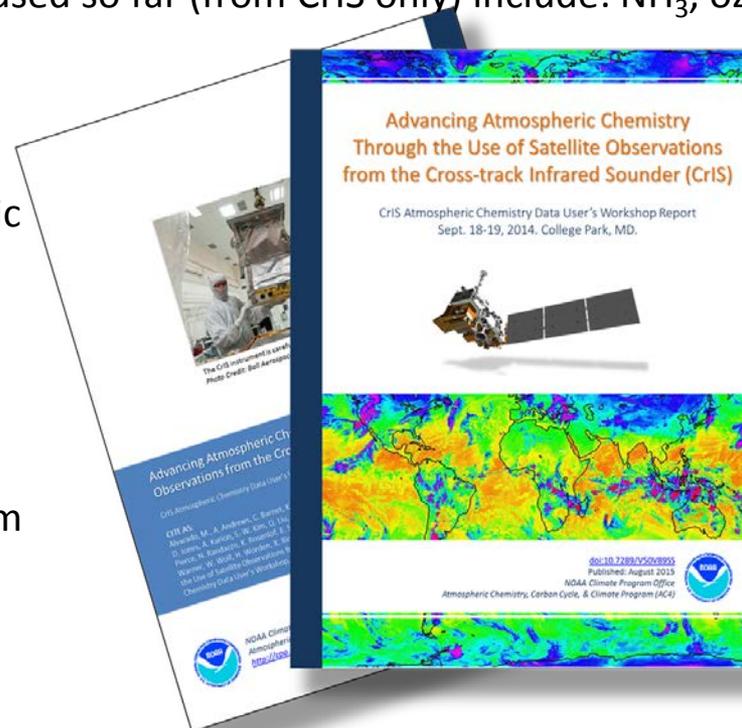


Data from JPSS instruments and AC4 program science:

- AC4 typically supports field and laboratory data, which can be complemented by JPSS data
- CrIS, OMPS and VIIRS composition products (trace gases and aerosols) can all supply relevant products
- Retrievals are used in connection with global and Earth System models
- Data used so far (from CrIS only) include: NH_3 , ozone

AC4 current and future activities:

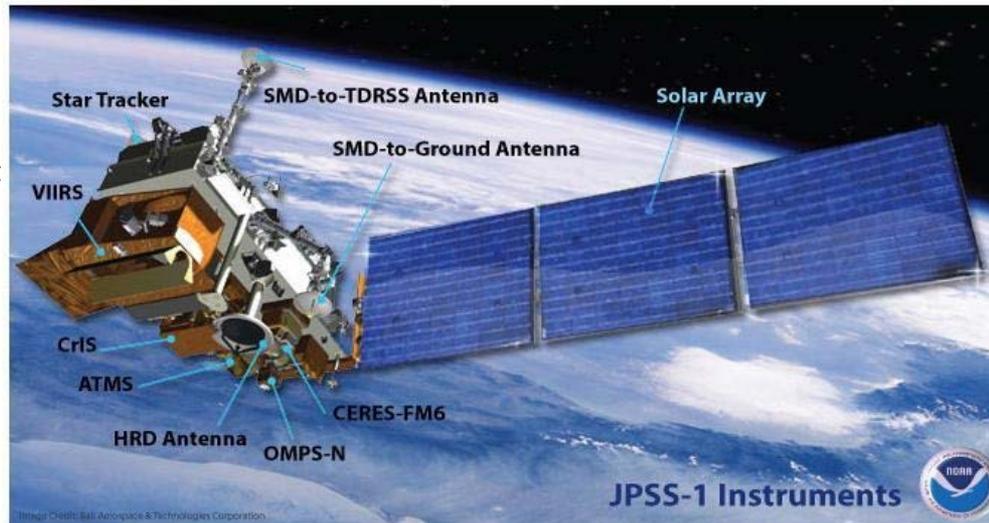
- CrIS data users workshop, focused on atmospheric composition took place September 18-19, 2014; [report published August 2015](#)
- Three projects include NH_3 data product development, validation and application
- Upcoming project on CrIS/OMPS ozone retrieval
- Ongoing interest in atmospheric composition from space, with special emphasis on monitoring and field campaign support/complement



Thank you.

ATMOSPHERIC COMPOSITION FROM SPACE

Useful tropospheric observations have been obtained from space since 1999. In 2011, NOAA-NASA partnership resulted in a launch of SNPP satellite, the first in the JPSS series. Aboard SNPP, and later also JPSS-1 and JPSS-2, there are several instruments relevant to atmospheric chemistry: CrIS, VIIRS, ATMS and OMPS. Together, they can provide data on trace gases (e.g. CO, O₃, CH₄, NH₃, CO₂ etc.) and aerosols.



CrIS instrument focus in AC4:

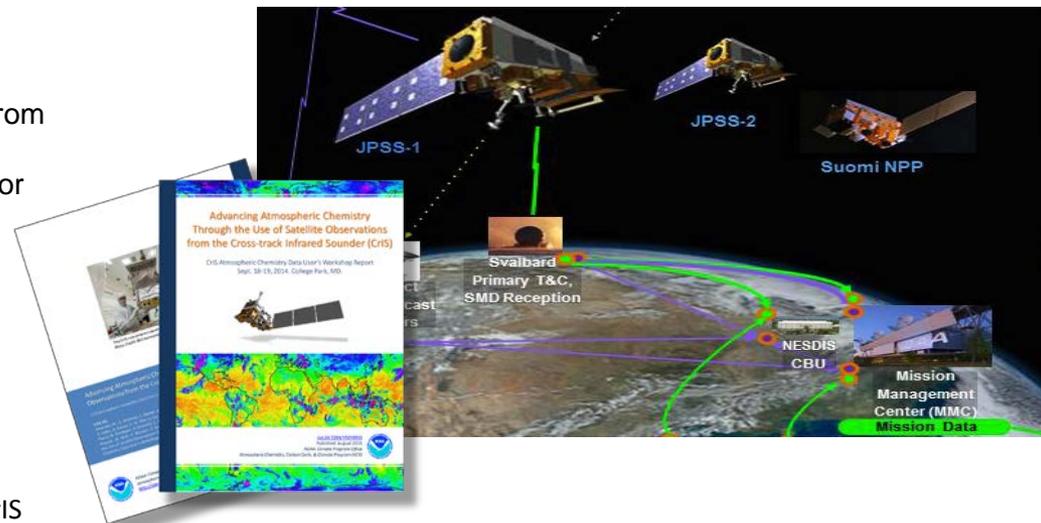
- CrIS is an infrared sounder, similar in observing characteristics to MOPITT, AIRS and TES instruments that have provided data since 1999, 2002 and 2004, respectively
- Mid-tropospheric data from CrIS include: CO, CH₄, O₃, CO₂, NH₃, dust
- Scheduled to be launched on SNPP, JPSS-1 and JPSS-2, CrIS can provide at least 20 years of continuous measurements

NOAA NESDIS activities:

- Development and validation of composition products from CrIS: CO, CO₂ and CH₄ so far
- JPSS call for proposals (LOIs due January 12, 2015) for proving ground included atmospheric chemistry focus

AC4 current and future activities:

- CrIS data users workshop, focused on atmospheric composition took place September 18-19, 2014; [report published August 2015](#)
- Two projects funded include NH₃ data product development, validation and application
- Future plans: inclusion in program announcement(s) CrIS data applications



NOAA Long-term Strategy of trace gases from hyper-spectral thermal sounders

Antonia Gambacorta ⁽¹⁾, Chris Barnet ⁽¹⁾, Nadia Smith (1), Jonathan Smith (1), Walter Wolf (2), Mark Liu (2), Tony Reale (2), Tom King (2), Michael Wilson (2), Letitia Suillard (2), Nick Nalli (2), Bomin San (2), Kexin Zhang (2), Changyi Tan (2), Flavio Iturbide-Sanchez (2), Xiaozhen Xiong (2), Mitch Goldberg ⁽³⁾

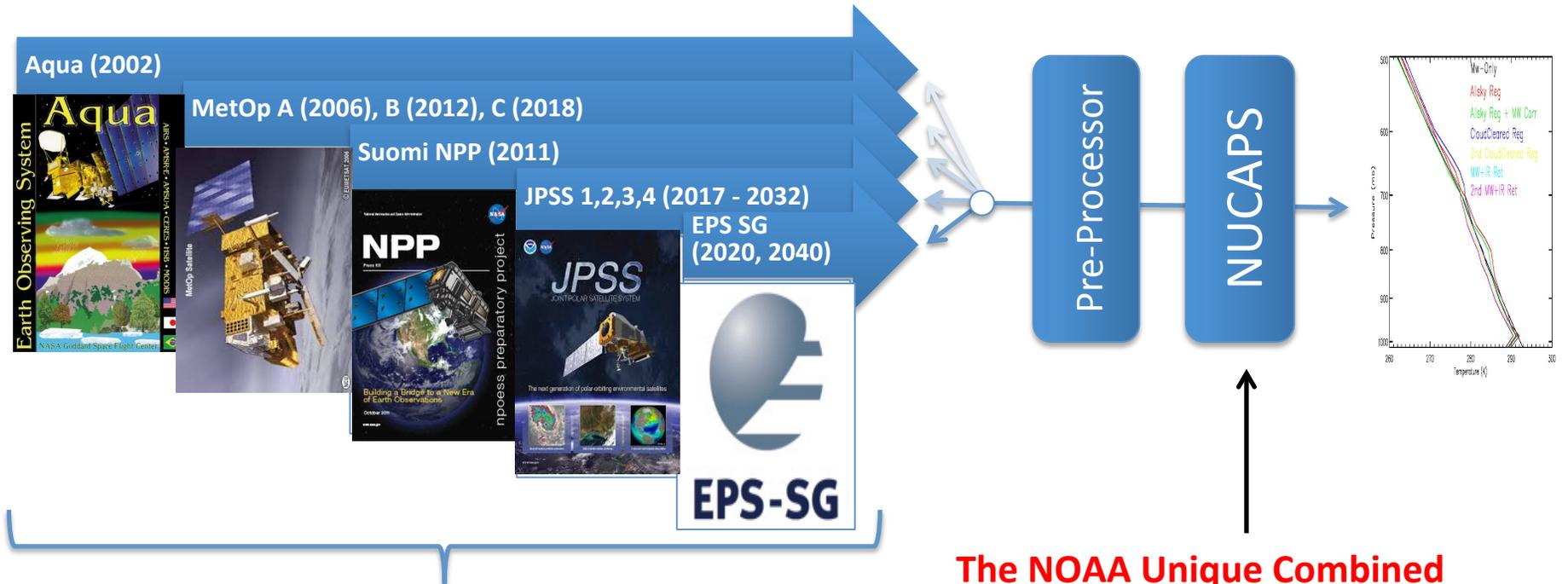
3rd JPSS Annual Meeting
August 11, 2016

1. Science and Technology Corporation, STC
2. NOAA NESDIS STAR
3. NOAA JPSS Project Scientist



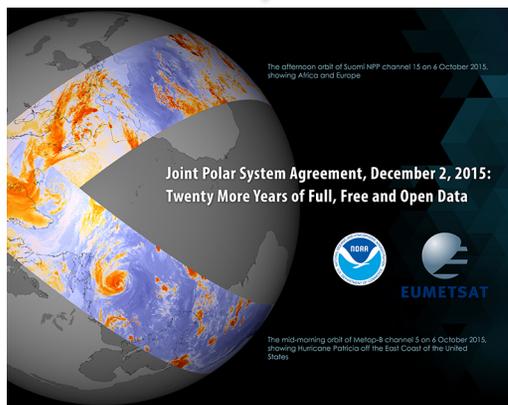


NOAA long-term strategy of trace gases from hyper spectral sounders



The NOAA Unique Combined Atmospheric Processing System (NUCAPS)

- Same exact executable
- Same underlying Spectroscopy
- Same look up table methodology for all platforms





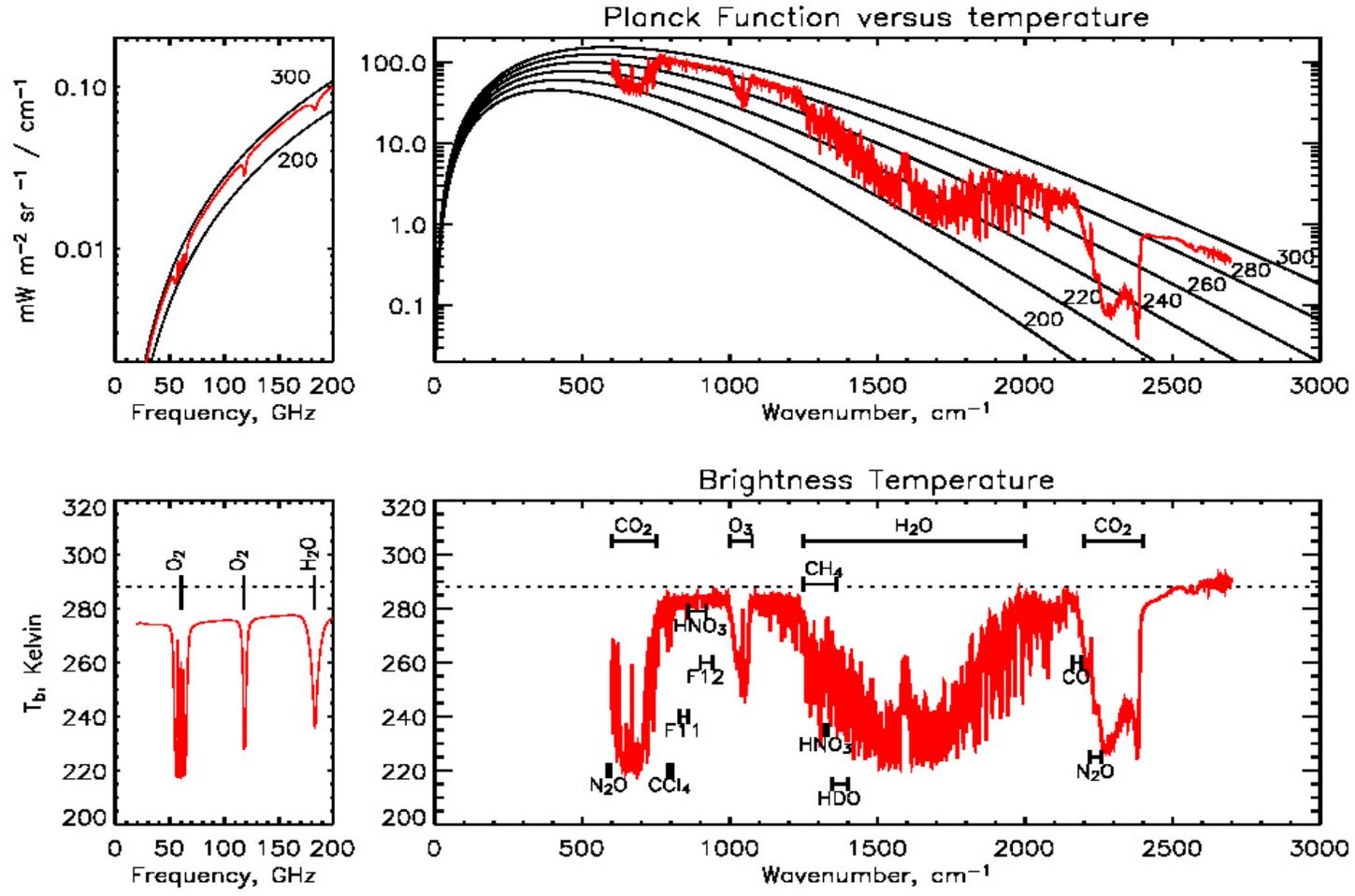
Philosophy of NUCAPS



- **The challenge:** high computational efficiency and sophisticated inversion methods to maximize utilization of large volumes of data for real time weather and long-term climate applications
- **Philosophy of NUCAPS:** developing a mathematically sound and globally applicable (land/ocean, day/night, all season, all sky, TOA-surface) retrieval algorithm that can fully exploit all available satellite assets (infrared, microwave, visible) to retrieve the full suite of surface temperature and vertical profiles of temperature, moisture and trace gases. These are among the essential metrics defining a modern, physical and independent data record of atmospheric variables, suitable for both weather and climate applications.



Hyper spectral sounders sensitivity to trace gases





Summary of products from NUCAPS



gas	Range (cm ⁻¹)	Precision	d.o.f.	Interfering Gases
T	650-800 2375-2395	1K/km	6-10	H2O,O3,N2O emissivity
H₂O	1200-1600	15%	4-6	CH4, HNO3
O₃	1025-1050	10%	1+	H2O,emissivity
CO	2080-2200	15%	≈ 1	H2O,N2O
CH₄	1250-1370	1.5%	≈ 1	H2O,HNO3,N2O
CO₂	680-795 2375-2395	0.5%	≈ 1	H2O,O3 T(p)
<u>Volcanic</u> SO₂	1340-1380	50% ??	< 1	H2O,HNO3
HNO₃	860-920 1320-1330	50% ??	< 1	emissivity H2O,CH4,N2O
N₂O	1250-1315 2180-2250	5% ??	< 1	H2O H2O,CO
CFCl₃ (F11)	830-860	20%	-	emissivity
CF₂Cl (F12)	900-940	20%	-	emissivity
CCl₄	790-805	50%	-	emissivity



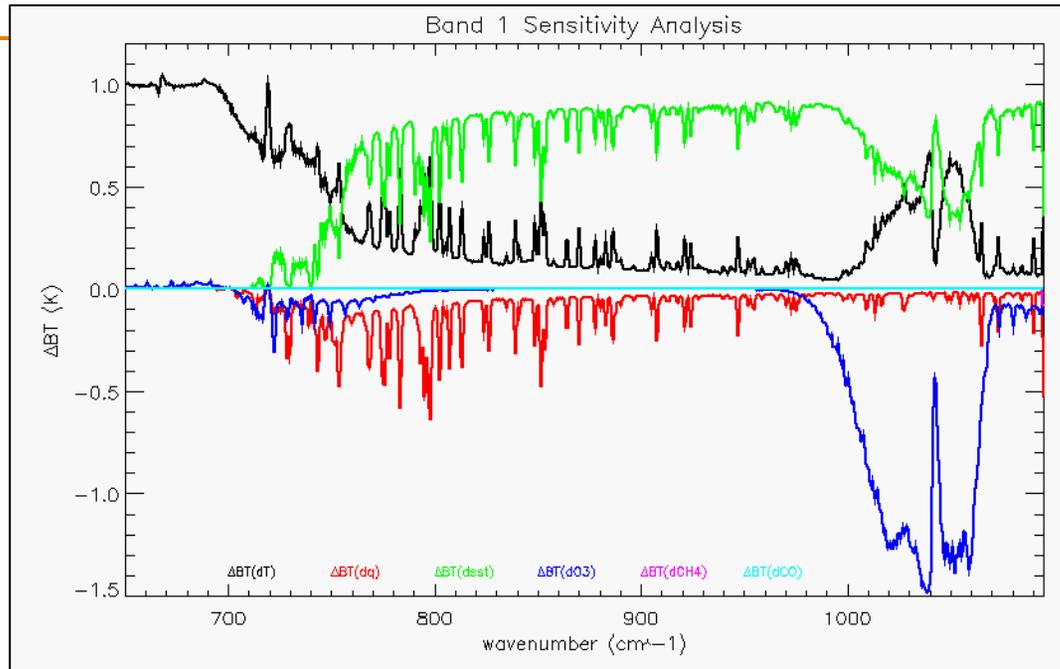
The **challenge** of trace gas retrievals from hyper spectral sounders



- Retrieving trace gases from hyper spectral sounders is a highly non linear and ill-conditioned problem
- Trace gas signals are small and characterized by strong spatial and seasonal variability
- In some cases trace gases are physically correlated with other geophysical variables – for example in respiration of soil CO₂ is correlated with surface temperature; Ts/CH₄; CO/CH₄/O₃;
- Most of geophysical correlations in nature are non-linear.
- With trace gases geophysical *a-priori* information is limited.
- Lack of information content is problematic especially in presence of cloudy, cold, isothermal scenes.
- Trace gases are highly spectrally correlated (CO₂,O₃,H₂O in 15 um band, etc.)
- Errors in spectroscopy and geophysical state.
 - All trace gases dependent on temperature profile.
 - CO₂ and temperature are intimately correlated since CO₂ absorption is used to derive temperature
 - CO₂ can be correlated with clouds both in the retrieval and geophysical sense.
- Stitching satellite instruments together with different
 - Spatial sampling,
 - Spectral sampling, and
 - Noise characteristics
- Ground truth
 - Need full atmospheric state – up to ≥ 30 km.



Spectral Sensitivity Analysis (LW band)



Perturbation Applied

SST	1K
T	1K
H2O	10%
O3	10%
CH4	2%
CO	1%

Brightness temperature difference (ΔBT) terms represent the sensitivity of each channel to a given perturbation species and are indicative of the degree of “spectral purity” of each channel.

• For each atmospheric species, we select channels with:

- the highest degree of spectral purity (the highest sensitivity to the species of interest and the lowest sensitivity to all other interfering species).
- the lowest noise sources (NEDT, calibration & apodization corr., RTA errors. See ahead.)
- unique spectral features (to capture atmospheric variability, maximize vertical resolution)



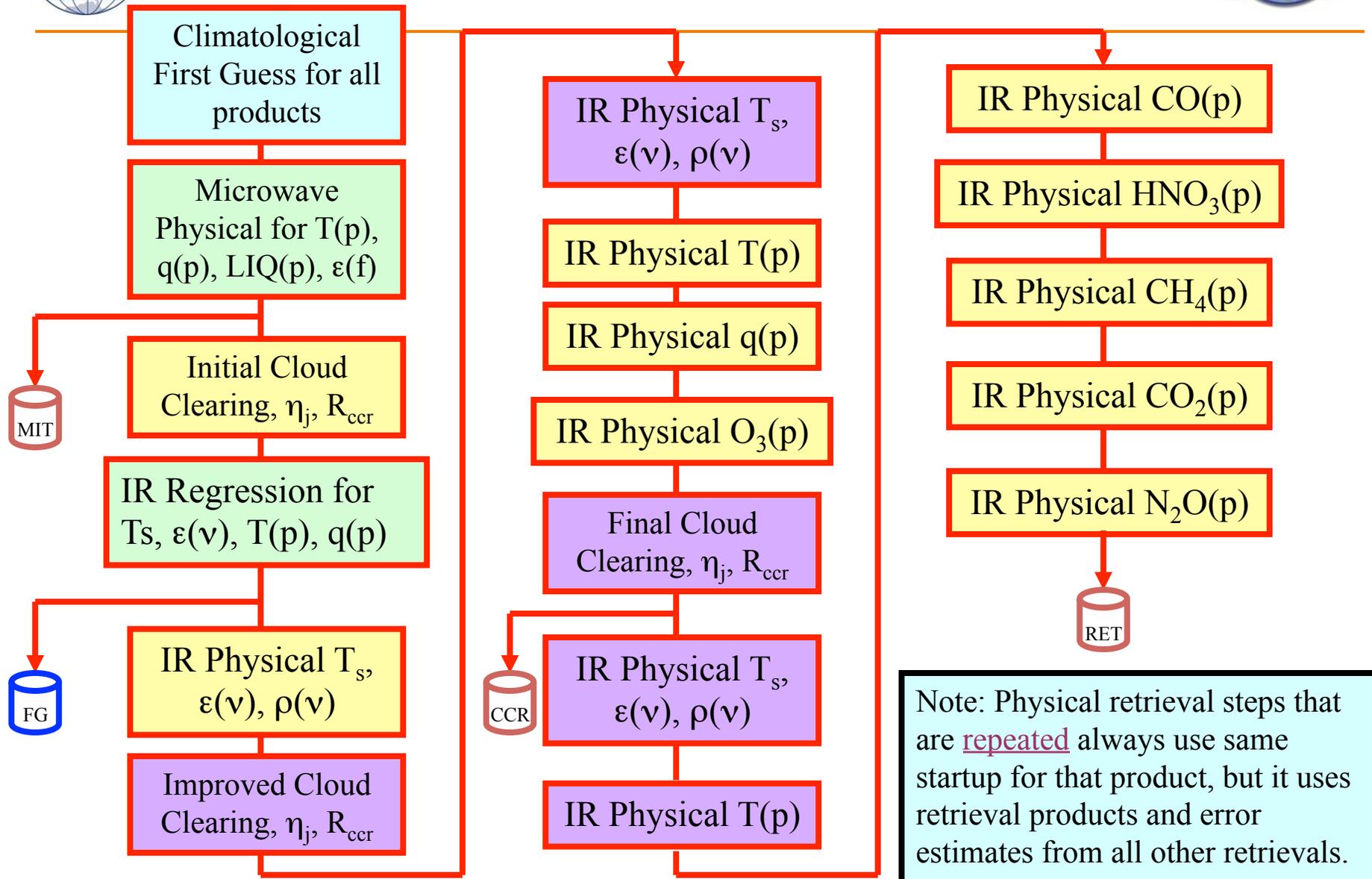
NUCAPS long-term **strategy** of trace gases from hyper spectral sounders



- A minimum dependence on the geophysical a priori and full exploitation of the measurement and knowledge of the physics of radiative transfer.
 - Channel selection aimed at maximizing spectral purity and information content.
 - Spectral correlation, cloud clearing errors and instrument noise used as terms of the measurement error covariance in a weighted least square minimization
- A sequential approach, solving for most linear (including cloud clearing) or high S/N parameters first and a formal error propagation from one step to the next
- A retrieval is a signal averaging process over many channels and only makes changes where we have information content. Vertical averaging kernels, $A_{j,j}$, define where the instrument has skill.
- Users need to know vertical and spatial error covariance and vertical weighting functions.
 - Many of the “signals” we see have seasonal or spatial variability in the information content.
 - Broad vertical weighting functions tend to mix stratospheric and upper tropospheric contributions together.
 - Trace gas retrievals are sensitive to stratospheric-tropospheric exchange.
- Reprocessing capability to study long-term stability of algorithm.
 - All archived data (“granule” processing)
 - Global “gridded” data sub-sets (for rapid evaluation of algorithm modifications)
 - All validation datasets (including radio-sonde, aircraft match up datasets)



NUCAPS Flow Diagram



Note: Physical retrieval steps that are repeated always use same startup for that product, but it uses retrieval products and error estimates from all other retrievals.



The path forward



- We have built a retrieval system aimed at making the best use of hyper spectral data.
- Previous validation efforts have proven that we can meet requirements.
- With temperature and water vapor, users are clearly identifiable.
- What defines the operational need for these trace gas products instead?
 - Just because we can do it, it does not mean that we shall do it.
 - We would like to support any project supported by the NOAA AC4 Program to engage new potential users and gain insights on the applicability of our products. This will ultimately lead to a user requirement to justify the effort of transitioning products into operations.
 - NOAA JPSS is funding an unprecedented list of Proving Ground and Risk Reduction (PGRR) initiatives to demonstrate the operational need of our products. This is not validation in the traditional sense, it is developing new user's applications.
- What defines a trace gas operational user?
 - We need a real time, vetted, institutional user: EPA, National Forest Service, DOA, etc.
 - We need users that need archived consistent products: NUCAPS CO2 might serve as forecast climatology for the National Weather Service.



Main goal of this session



- This session should discuss what trace gases should be explored in a research sense and what trace gases should be distributed operationally.
- NASA and NOAA have different research mandates, goals and intended users.
 - NASA's focus is primarily on new instrument concepts and fundamental research.
 - NOAA leverages on NASA's research to develop a real time, operational and archival product, intended for specific end users applications of societal benefits.
- We are now looking for those user applications that will (1) verify the applicability of our trace gas products, (2) educate us on the need for new or improved products, QCs and formatting, (3) justify new efforts for algorithm improvements and transition to operations.
- The ultimate result is a continued and intelligent use of hyper-spectral trace gas products, both for real time and long-term applications.



Back Up slides



Why are CO₂ averaging functions broad while T(p) functions have profile information?

- Spectroscopy: The CO₂ lines are strong narrow lines. Temperature affects the width (and hence the channel transmittance) while # of CO₂ molecules affects the strength. Once the line is saturated (near the surface, where p is large) we lose sensitivity.

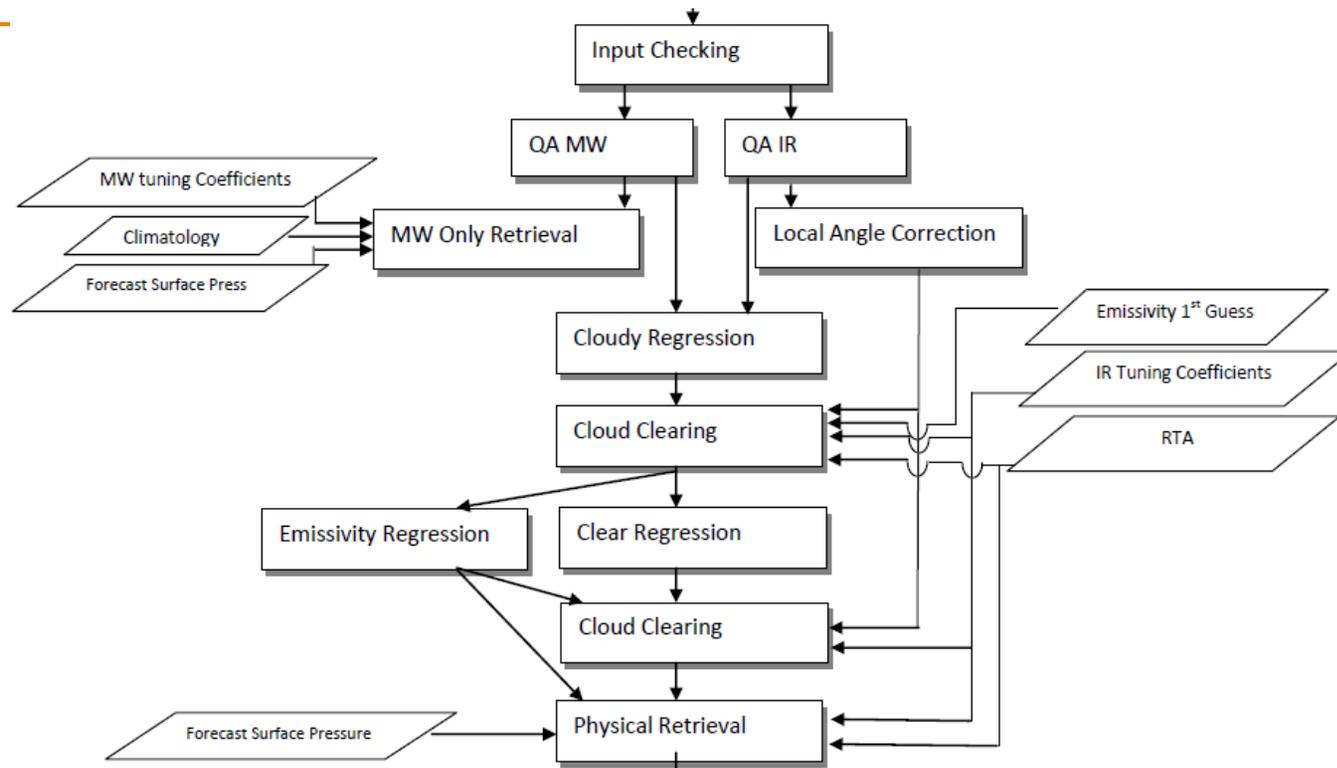
$$\kappa_i(\nu, p, T, \theta) \simeq \sum_{j=1}^J \frac{N_i \cdot S_{ij}}{\pi} \frac{\gamma_{ij}}{(\nu - \nu_{ij})^2 + (\gamma_{ij})^2} \cdot \sec(\theta) \quad \gamma_{ij} \simeq \gamma_{ij}^0 \cdot \frac{p}{P_0} \cdot \sqrt{\frac{T}{T_0}}$$

- Radiative transfer: The temperature enters both in the absorption coefficient and in the Planck function.

$$R_n(\vec{X}) \simeq \int_{\nu} \Phi_n(\nu) \int_p B_{\nu}(T(p)) \cdot \frac{\partial \exp\left(-\int_{z'=\infty}^{z(p)} \sum_i \kappa_i(\vec{X}, p, \dots) dz'\right)}{\partial p} \cdot dp \cdot d\nu$$



NUCAPS Flow Chart



- **I. A microwave retrieval module** which computes Temperature, water vapor and cloud liquid water (Rosenkranz, 2000)
- **II. A fast eigenvector regression** retrieval that is trained against ECMWF and CrIS all sky radiances which computes temperature and water vapor (Goldberg et al., 2003)
- **III. A cloud clearing module** (Chahine, 1974)
- **IV. A second fast eigenvector regression** retrieval that is trained against ECMWF analysis and CrIS cloud cleared radiances
- **V. The final infrared physical retrieval** based on a regularized iterated least square minimization: temperature, water vapor, trace gases (O₃, CO, CH₄, CO₂, SO₂, HNO₃, N₂O) (Suskind, Barnet, Blaisdell, 2003)

Ammonia (NH₃) Distributions and Recent Trends by 13-year AIRS Measurements

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*Published in **ACP: The Global Tropospheric Ammonia Distribution as seen in the 13-year AIRS Measurement Record**

*Ready to Submit: **Increases in Atmospheric Ammonia over Major Agricultural Areas from Space Measurements**

* Funded by NASA's The Science of Terra and Aqua Program (NNX11AG39G), and the Atmospheric Composition Program (NNX07AM45G).

Why Ammonia

- Ammonia (NH_3) plays an increasingly important role in the global biogeochemical cycle of reactive nitrogen as well as in aerosol formation and climate.
- Measurements with daily and large global coverage are challenging and have been lacking partly because the lifetime of NH_3 is relatively short and partly because it requires high sensitivity for the retrievals that can be only obtained from areas with high thermal contrasts near the surface (Clarisse *et al.*, 2010).
- AIRS afternoon overpasses (1:30pm) are best correlated with the daily emission peak time and during the daily period with the highest thermal contrast. Additionally, AIRS large coverage with wide swaths and cloud-clearing provide daily NH_3 maps. The 13-year data records makes AIRS the best sensor for NH_3 trends and variability studies (to date).

Atmospheric Infrared Sounder

Launched May 2002



- A grating spectrometer originally designed to improve weather forecast and now also used for climate and air quality studies.
- Spectral resolution at ≈ 1200 ($\sim 0.5 \text{ cm}^{-1}$)
- Covers 650-2665 in three bands with a total of 2378 channels
- Spatial resolution 13.5 km^2 (with retrievals at $\sim 45 \text{ km}^2$)
- Wide swaths and cloud clearing provide daily global coverage
- Very high Signal-to-Noise accuracies of 1K over 1 km-layer.

AQUA

AMSR-E

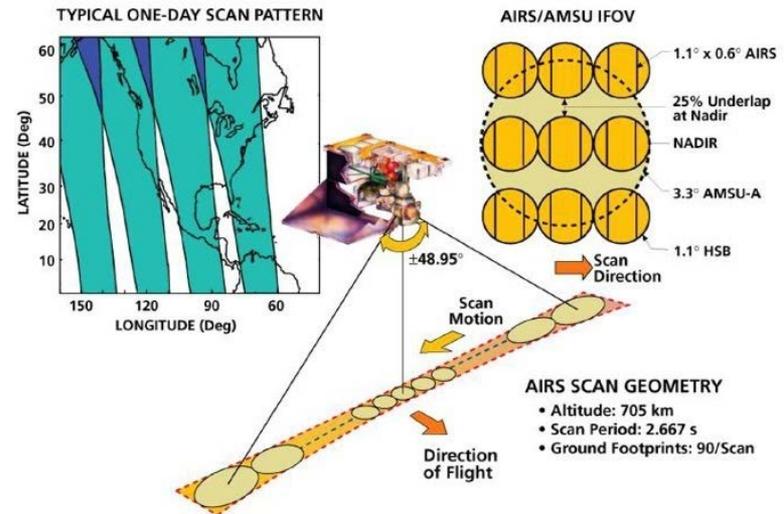
MODIS

AIRS

CERES

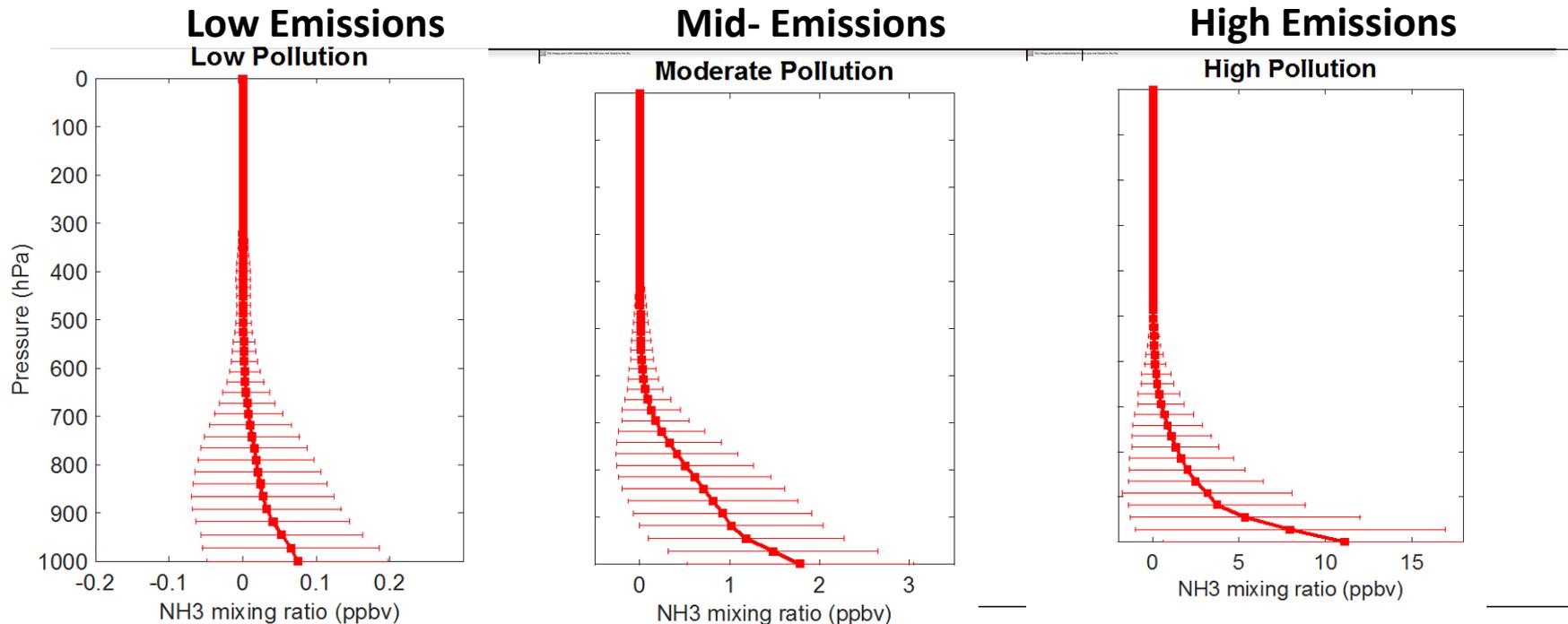
AMSU

HSB



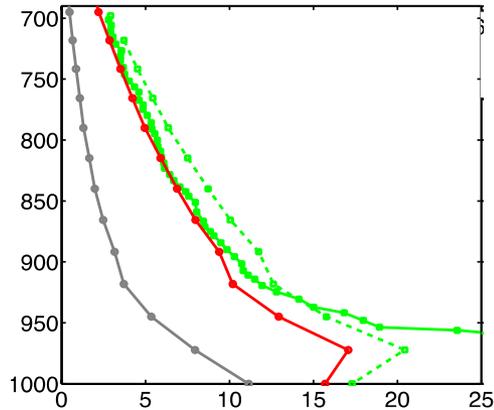
AIRS NH₃ Algorithm

- AIRS NH₃ retrievals use Optimal Estimation (OE) technique (Rodgers, 2000);
- CCRs and SARTA are used as in AIRS algorithm for other species;
- The *a priori* levels are computed from GEOS-chem;
- Globally one set *a priori*.
- Select *a priori* levels based on brightness temperature differences weighted by noise (dbti);



Validation vs CRDS/Picarro in DISCOVER-AQ CA

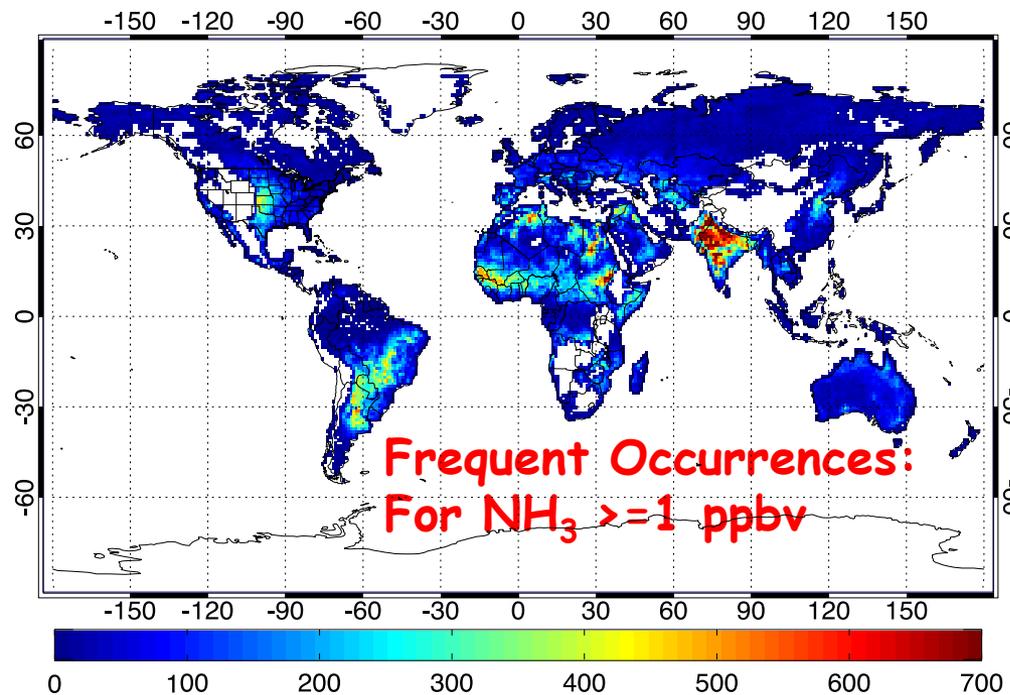
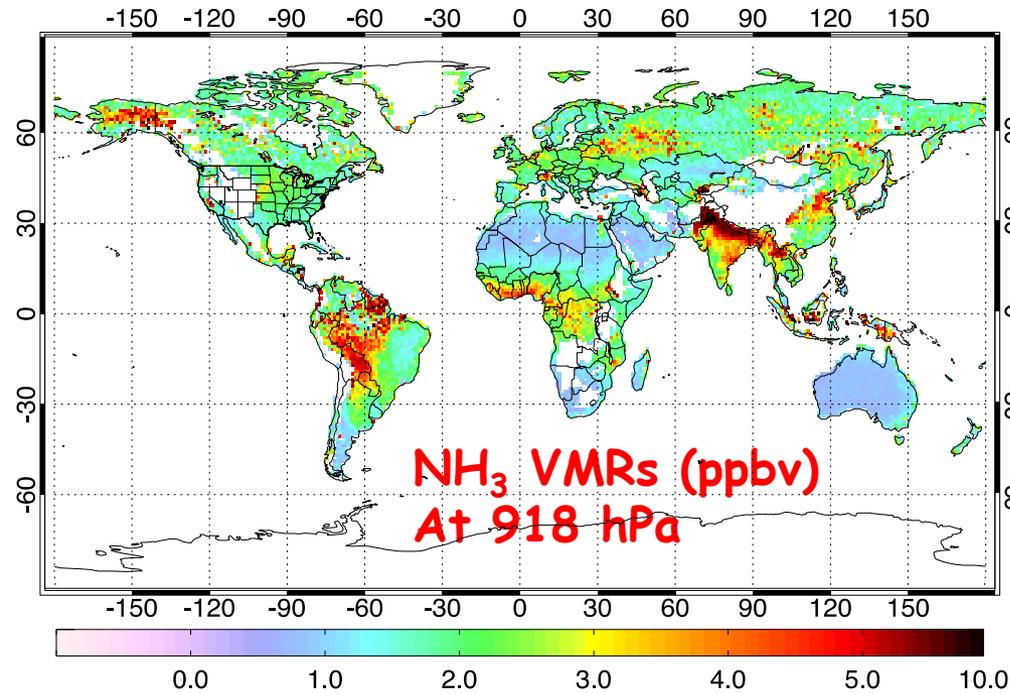
Spiral Profiles Only - 01/16 to 02/06, 2013
CRDS/Picarro data courtesy of Co-author J. Nowak



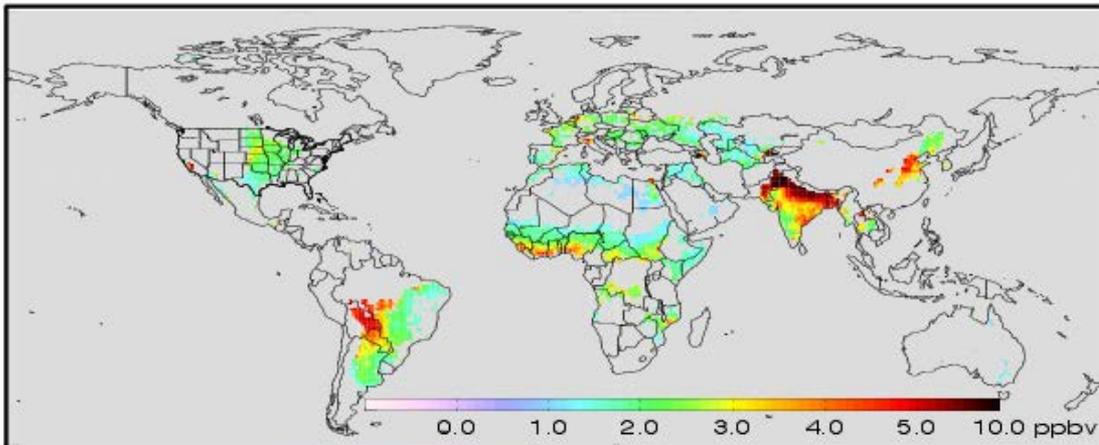
—●— m, -0.469h

- Gray - a priori; Red - retrievals; Green solid - in situ; and Green dashed - convolved in situ.
- AIRS L2 pixel sizes are $\sim 45 \text{ km}^2$, can coincide with multiple in situ profiles.
- AIRS NH_3 measurements are most sensitive at 850-950 hPa layer.

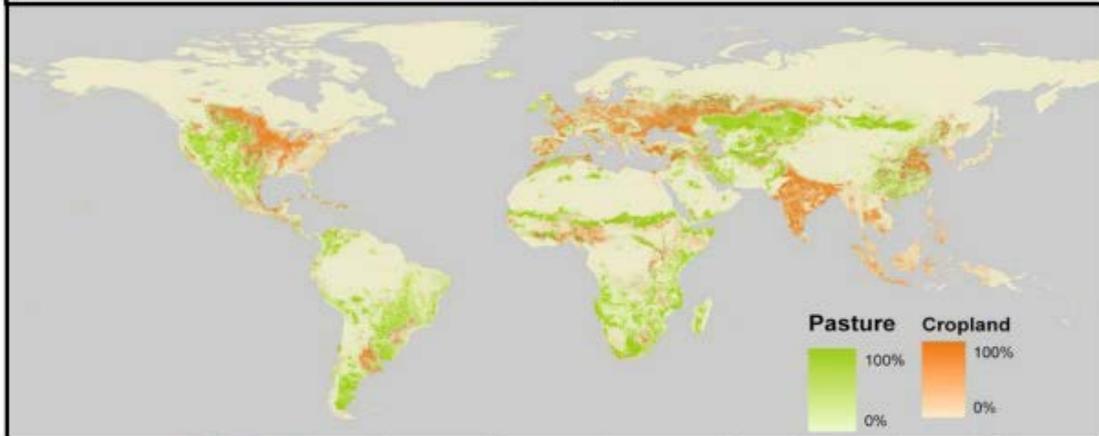
Global NH_3 in 2002-2015



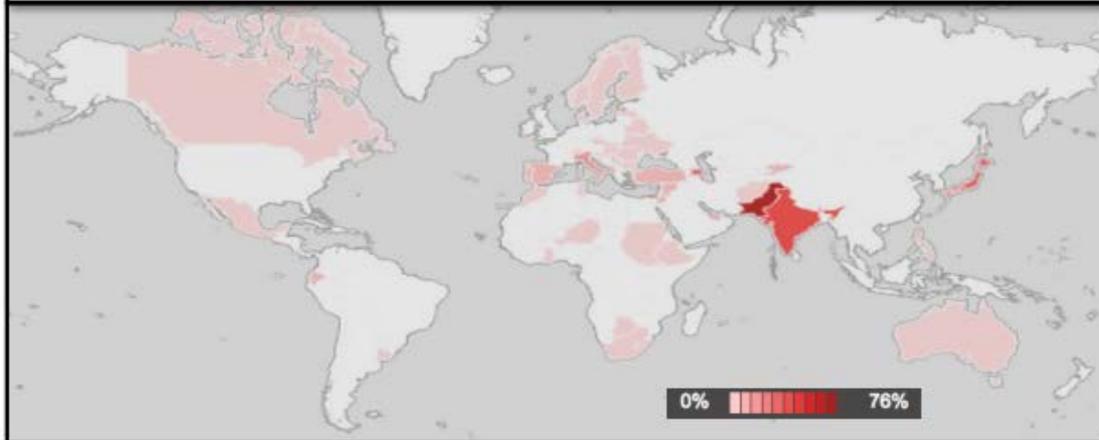
- AIRS NH_3 at 918 hPa for daytime and land only averaged over Sept. 2002 to Aug. 2015;
- Use Q0; DOFS ≥ 0.1 ;
- High concentrations are mainly due to human activities and fires;
- Use occurrences of higher emissions (lower) to distinguish between the two major sources: agricultural (high VMRs & high frequencies); BB emissions (high VMRs & low frequencies);
- Sources are seen in valleys (e.g., San Joaquin Valley, California in the U.S., the Po Valley, Italy, Fergana Valley, Uzbekistan, and the Sichuan Basin in China); Agricultural especially in irrigated lands (e.g., Azerbaijan, Nile Delta and near Nile River in Egypt, the Mid-West U.S., in the Netherlands, in Mozambique and Ethiopia, Africa, and especially the Indo-Gangetic Plain of South Asia).



Top panel: The NH_3 VMRs from the persistent sources filtered with the collocated occurrences of elevated emissions (≥ 1.4 ppbv) using a threshold of 40 days;

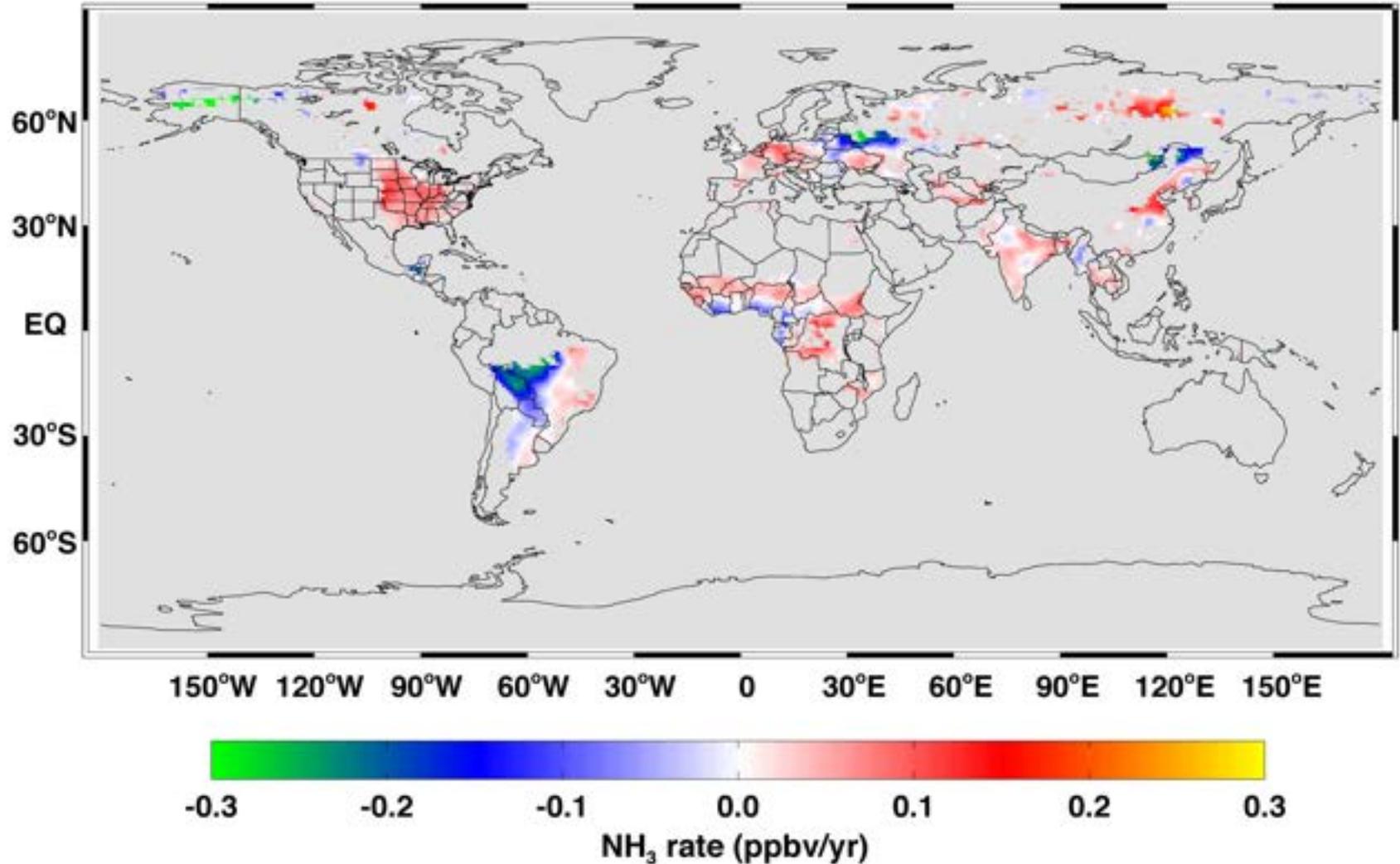


Middle panel: Pasture and Cropland Map



Bottom panel: irrigated agricultural land areas.

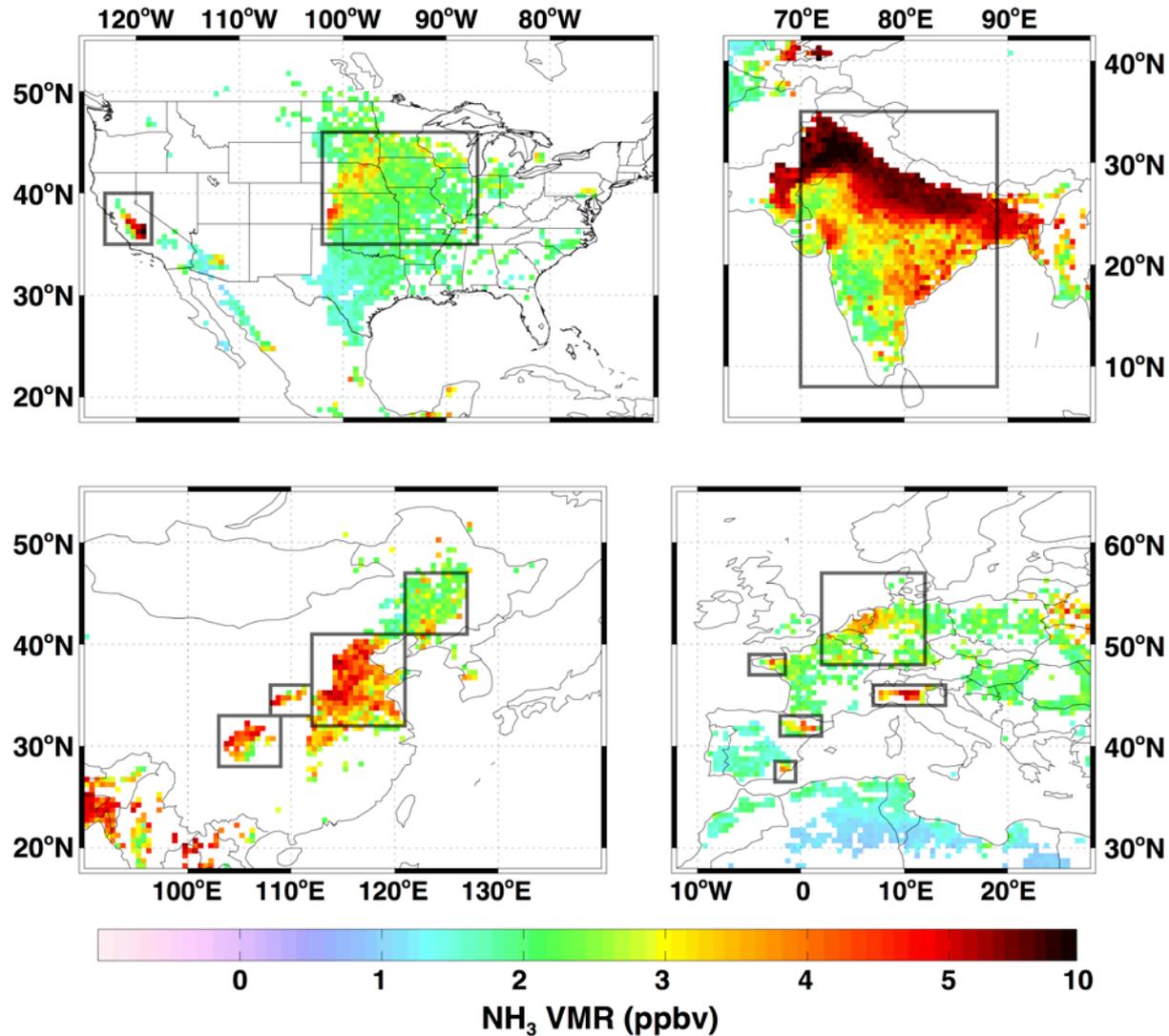
NH₃ Trends - Last 13 years



- Concentrations of anthropogenic emissions increased and BB decreased
- Trends due to BB are not conclusive due to the short record.

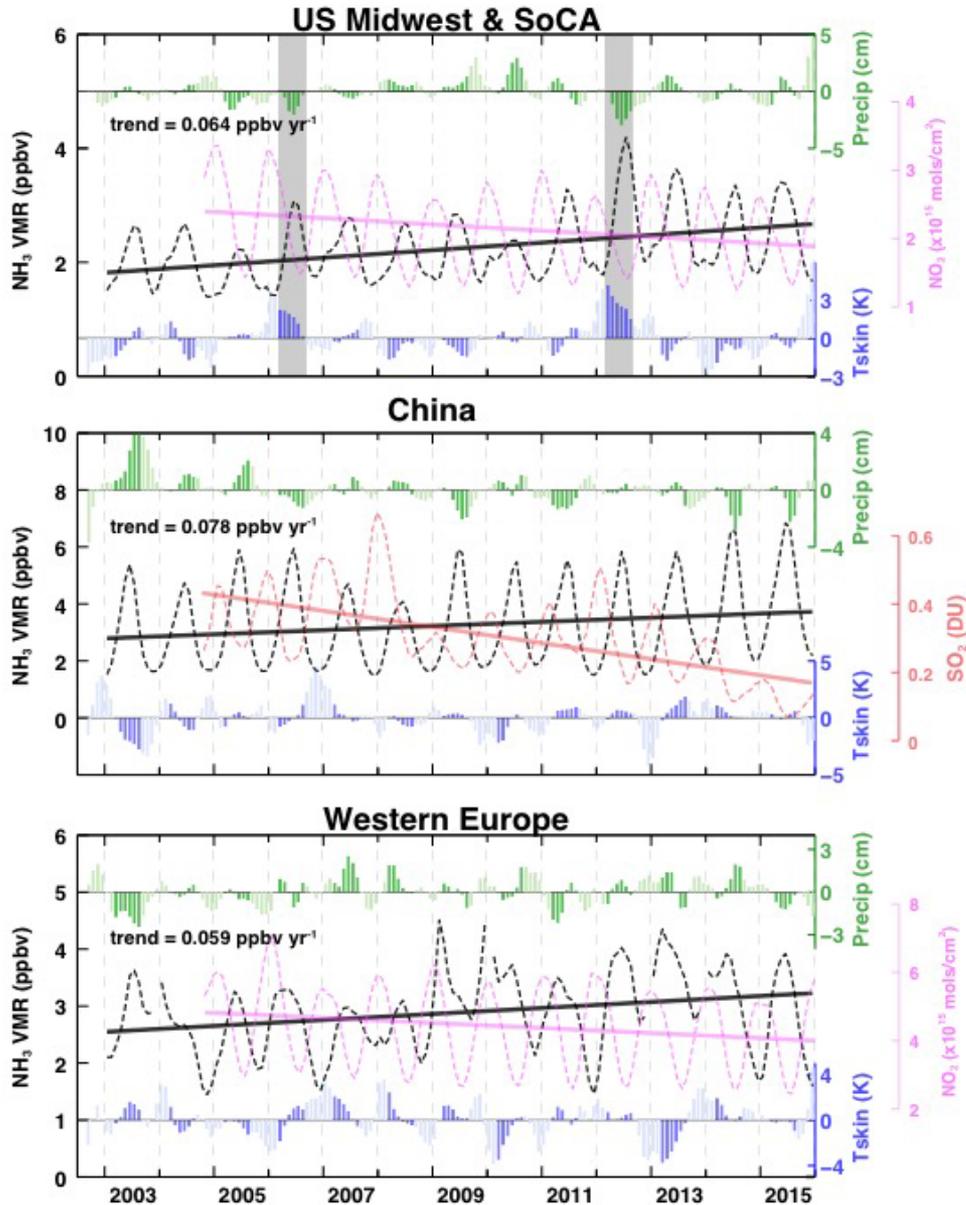
NH₃ over USA, China, India, and Europe

Using high concentration and high frequencies



Black boxes are regions used for follow up trend studies.

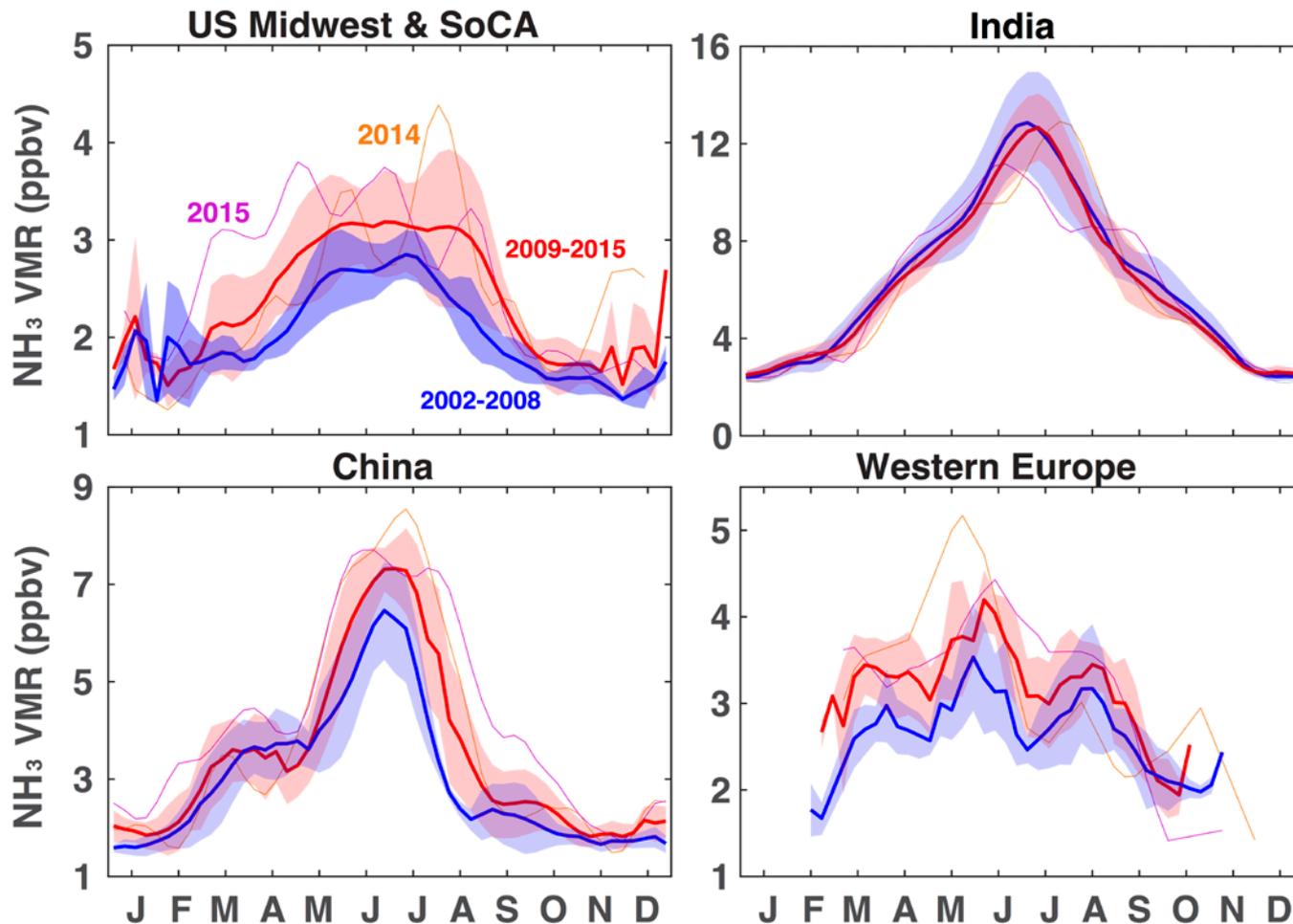
AIRS NH₃ vs OMI NO₂ for US (top), SO₂ for China (middle) and NO₂ for Western Europe (lower)



- All 3 regions show increasing NH₃ trends in the last 13 years, in black.
- Decreased SO₂ from OMI largely explains the reason of NH₃ increases in Midwest U.S. (not shown), China, and Europe (not shown).
- OMI NO₂ decreasing explains winter NH₃ increasing over the US and Europe.
- Meteorological conditions also affect NH₃ concentrations (high surface temperatures and low precipitation), see top panel shaded areas.

AIRS NH₃ Seasonal Variation

- over USA, China, Europe, and India

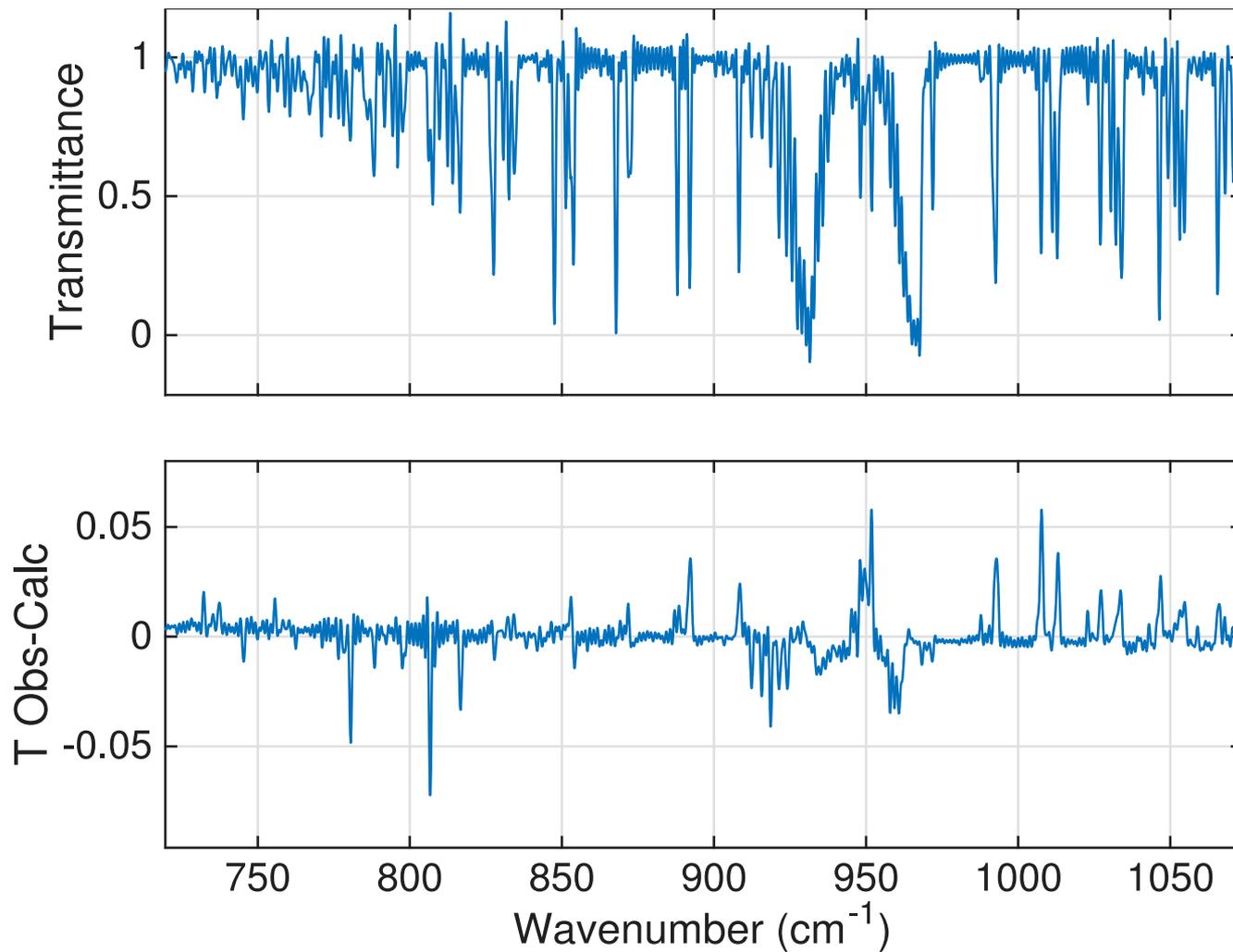


- The highest NH₃ concentrations in average occur in India/Pakistan, and China. Note scales.
- NH₃ in India seasonal variation are broad and no obvious increasing/decreasing trends;
- NH₃ for USA, China and Europe have increased, with peaks in both spring and summer;
- Clear increasing trends over US Midwest, China, and Western Europe.

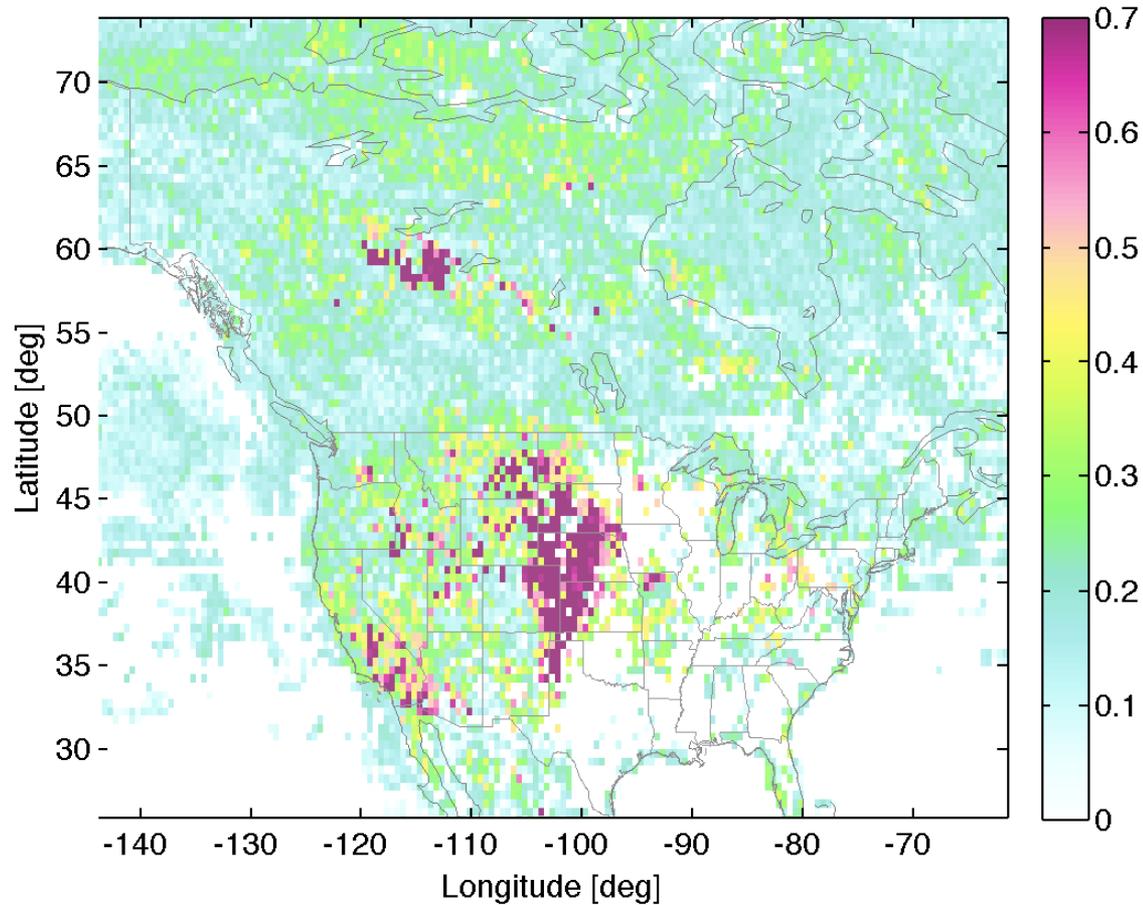
Summary

- AIRS NH_3 products not only include 13 years data record, it also provide daily maps!
- AIRS retrieved vertical profiles show good agreement (~5 - 15%) with in situ profiles from the 2013 DISCOVER-AQ field campaign in central California.
- AIRS daily measurements captures the strong continuous NH_3 emission sources from the anthropogenic (agricultural) source regions, as well as emissions from biomass burning (BB).
- Ammonia trends increase over agriculture regions, where fertilizers are used as routine practice, decrease over BB regions (with insufficient records).
- Ammonia increases resulted primarily from dramatic decreases in concentrations of acidic aerosols (sulfate and nitrate), an unintended consequence of effective controls of NO_x and SO_2 emissions.

CrIS NH3 (TVAC Gas Cell)

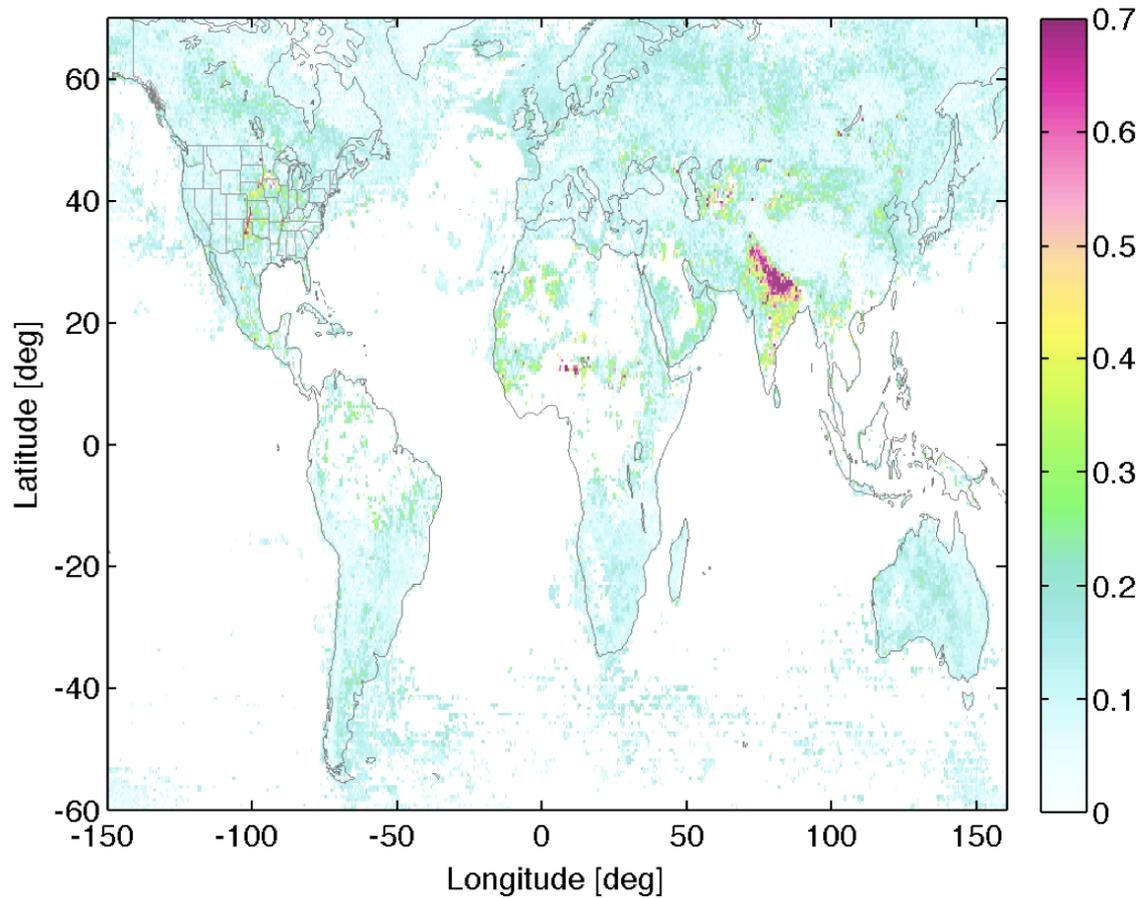


CrIS NH3 B(T) Signals (on/off line)



July 2012

CrIS NH3 B(T) Signals



May 2012



Validation of SNPP NUCAPS trace gas EDRs: O₃, CO, and CO₂

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2016 STAR JPSS Annual Meeting
College Park, Maryland, USA
August 2016

Acknowledgments



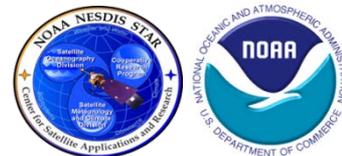
- The **NOAA Joint Polar Satellite System (JPSS-STAR) Office** (M. D. Goldberg, L. Zhou, et al.) and the **NOAA/STAR Satellite Meteorology and Climatology Division** (F. Weng and I. Csiszar).
- **SNPP Sounder EDR Validation Dataset collection**
 - **NOAA AEROSE**: E. Joseph, V. R. Morris, M. Oyola (HU/NCAS); D. Wolfe (NOAA/ESRL)
 - AEROSE works in collaboration with the NOAA PIRATA Northeast Extension (PNE) project (R. Lumpkin, G. Foltz and C. Schmid), and is supported by the NOAA Educational Partnership Program (EPP) grant NA17AE1625, NOAA grant NA17AE1623, JPSS and STAR
 - **CalWater/ACAPEX**: R. Spackman (STC); R. Leung (PNL); C. Fairall, J. Intrieri (NOAA); N. Hickmon, M. Ritsche, A. Haruta, and the ARM Mobile Facility 2 (AMF2)
 - **NASA Sounder Science Team**: E. Olsen (for his expertise and assistance with the AIRS v6 EDR products), T. Pagano, E. Fetzer (NASA/JPL)
 - **World Ozone and Ultraviolet Radiation Data Centre (WOUDC)** data contributors (DWD-GRUAN, & INPE, & KNMI, & NASA-WFF, & SMNA. <http://www.woudc.org>)
 - **SHADOZ: Southern Hemisphere Additional Ozonesondes** (A. Thompson et al.)
- **NUCAPS validation effort (past and present)**: M. Wilson, T. King, W. W. Wolf, A.K. Sharma (STAR)

- **JPSS Sounder Trace Gas EDR Cal/Val Overview**
 - JPSS Level 1 Requirements
 - Validation Hierarchy
 - NUCAPS Algorithm
 - v1.5 (operational, CrIS nominal res)
 - v1.8.1. (CrIS full-res)
- **NUCAPS IR Ozone Profile EDR Product Evaluation**
 - v1.5 (operational)
 - Global Focus Day
 - Ozone sonde ensemble
 - v1.8.1 (CrIS full-res)
 - Global Focus Day

- **NUCAPS Trace Gas EDR Product Evaluation Versus AIRS v6 (Preliminary)**
 - Basic Methodology
 - Carbon Monoxide (CO)
 - v1.5 (operational)
 - v1.8.1 (full-res CrIS)
 - Carbon Dioxide (CO₂)
 - v1.5 (operational)
 - v1.8.1 (full-res CrIS)
- **Summary and Future Work**

JPSS Specification Performance Requirements

CrIS Trace Gas EDR Uncertainty (O₃, CO, CO₂, CH₄)



CrIS Infrared Trace Gases Specification Performance Requirements		
PARAMETER	THRESHOLD	OBJECTIVE
O ₃ (Ozone) Profile Precision, 4–260 hPa (6 statistic layers)	20%	10%
O ₃ (Ozone) Profile Precision, 260 hPa to sfc (1 statistic layer)	20%	10%
O ₃ (Ozone) Profile Accuracy, 4–260 hPa (6 statistic layers)	±10%	±5%
O ₃ (Ozone) Profile Accuracy, 260 hPa to sfc (1 statistic layer)	±10%	±5%
O ₃ (Ozone) Profile Uncertainty, 4–260 hPa (6 statistic layers)	25%	15%
O ₃ (Ozone) Profile Uncertainty, 260 hPa to sfc (1 statistic layer)	25%	15%
CO (Carbon Monoxide) Total Column Precision	35%, or full res mode 15%	3%
CO (Carbon Monoxide) Total Column Accuracy	±25%, or full res mode ±5%	±5%
CO ₂ (Carbon Dioxide) Total Column Precision	0.5% (2 ppmv)	1.05 to 1.4 ppmv
CO ₂ (Carbon Dioxide) Total Column Accuracy	±1% (4 ppmv)	NS
CH ₄ (Methane) Total Column Precision	1% (≈20 ppbv)	NS
CH ₄ (Methane) Total Column Accuracy	±4% (≈80 ppmv)	NS

Source:
(L1RD, 2014, pp. 45-49)

Validation Methodology Hierarchy

(e.g., Nalli et al., JGR Special Section, 2013)



1. Numerical Model (e.g., ECMWF, NCEP/GFS) Global Comparisons

- Large, truly global samples acquired from Focus Days
- Useful for sanity checks, bias tuning and regression
- Limitation: *Not* independent truth data

2. Satellite Sounder EDR (e.g., AIRS, ATOVS, COSMIC) Intercomparisons

- Global samples acquired from Focus Days (e.g., AIRS)
- Consistency checks; merits of different retrieval algorithms
- Limitation: Similar error characteristics; must take rigorous account of averaging kernels of both systems (e.g., Rodgers and Connor, 2003)

3. Conventional RAOB Matchup Assessments

- WMO/GTS operational sondes launched ~2/day for NWP
- Representation of global zones, long-term monitoring
- Large samples after a couple months (e.g., Divakarla et al., 2006; Reale et al. 2012)
- Limitations:
 - Skewed distribution toward NH-continent
 - Mismatch errors, potentially systematic at individual sites
 - Non-uniform, less-accurate and poorly characterized radiosondes
 - RAOBs assimilated, by definition, into numerical models

4. Dedicated/Reference RAOB Matchup Assessments

- *Dedicated* for the purpose of satellite validation
 - Known measurement uncertainty and optimal accuracy
 - Minimal mismatch errors
 - Atmospheric state “best estimates” or “merged soundings”
- Reference sondes: CFH, **GRUAN** corrected RS92/RS41
 - Traceable measurement
 - Uncertainty estimates
- Limitation: Small sample sizes and limited geographic coverage
- E.g., **ARM sites** (e.g., Tobin et al., 2006), **AEROSE**, **CalWater/ACAPEX**, **BCCSO**, **PMRF**

5. Intensive Field Campaign Dissections

- Include dedicated RAOBs, some *not* assimilated into NWP models
- Include ancillary datasets (e.g., ozonesondes, lidar, M-AERI, MWR, sunphotometer, etc.)
- Ideally include funded aircraft campaign using IR sounder (e.g., NAST-I, S-HIS)
- Detailed performance specification; state specification; SDR cal/val; case studies
- E.g., **SNAP**, **SNPP-1,-2**, **AEROSE**, **CalWater/ACAPEX**, **JAIVEX**, **WAVES**, **AWEX-G**, **EAQUATE**

NOAA Unique Combined Atmospheric Processing System (NUCAPS) Algorithm (1/2)

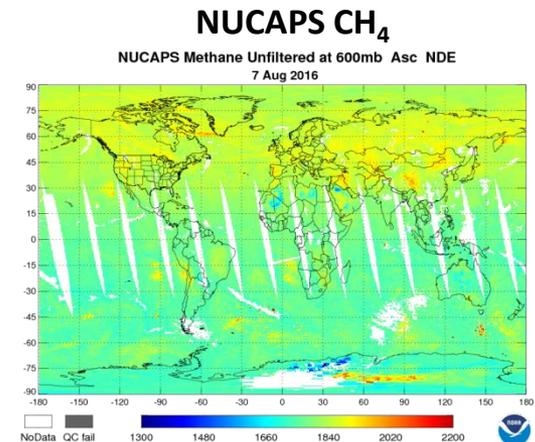
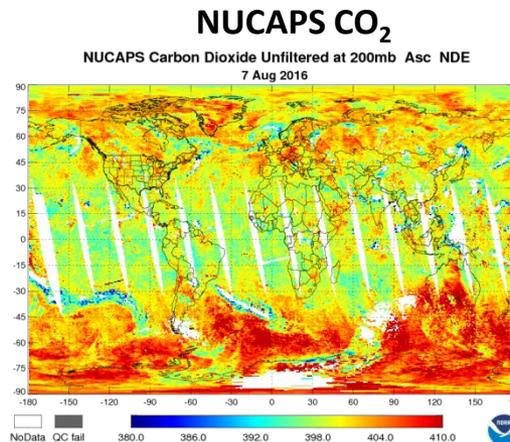
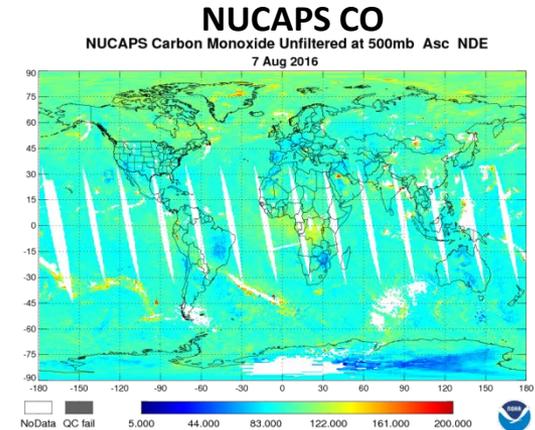
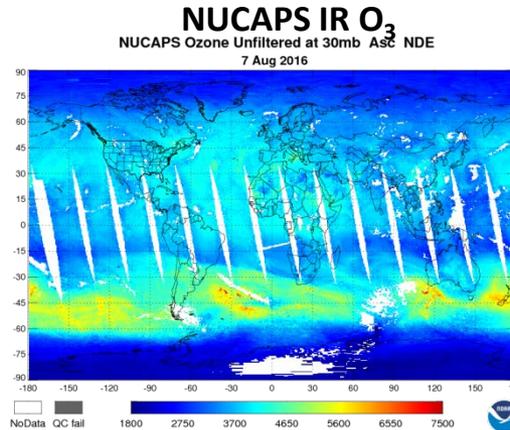


Operational algorithm

- Unified Sounder Science Team (AIRS/IASI/Cris) retrieval algorithm (*Susskind, Barnet and Blaisdell, IEEE 2003; Gambacorta et al., 2014*)
- Global non-precipitating conditions
- Atmospheric Vertical Temperature, Moisture Profiles (AVTP, AVMP) and trace gas (O_3 , CO , CO_2 , CH_4)
- Validated Maturity for AVTP/AVMP, Sep 2014

Users

- **Weather Forecast Offices (AWIPS)**
 - Nowcasting / severe weather
 - Alaska (cold core)
- NOAA/CPC (OLR)
- NOAA/ARL (IR ozone, trace gases)
- TOAST (IR ozone)
- Basic and applied science research (e.g., *Pagano et al., 2014*)
 - Via NOAA Data Centers (e.g., CLASS)
 - Universities, peer-reviewed pubs



Long Term Monitoring

http://www.star.nesdis.noaa.gov/jpss/EDRs/products_Soundings.php

<http://www.ospo.noaa.gov/Products/atmosphere/soundings/nucaps/index.html>

NOAA Unique Combined Atmospheric Processing System (NUCAPS) Algorithm (2/2)



- **NUCAPS Offline Code Versioning**
 - **Version 1.5**
 - **Current operational system**
 - **Runs on nominal CrIS spectral resolution data**
 - **Version 1.8.1**
 - **Offline experimental algorithm**
 - **Runs on CrIS full spectral resolution data**
 - **Uses conventional regression algorithm for the IR/MW first guess (as opposed to MW retrieval as in v1.7 full-res)**
 - **Upgrades**
 - Updated IR radiative transfer algorithm (RTA) bias correction coefficients (based on the best combination resulted after testing the use of several atmospheric states and trace gaseous profiles)
 - IR emissivity threshold decreased from 1.05 to 1.0 in the `temp_cris.n1` namelist.
 - Replaced the Taylor expansion to the Exponential formula in the `fasttau_co2.F` program.
 - Updated MW bias correction (as in v1.6)
 - Updated MW RTA model error coefficients (as in v1.6)
 - Removal of MW channel 16 (as in v1.6)



Validation of Products NUCAPS EDR: Trace Gases (1/2)

- **Satellite Intercomparisons (Hierarchy Method #2)**

- » **Aqua AIRS (NASA A-Train)**

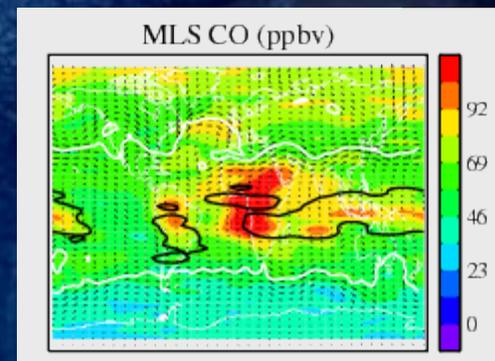
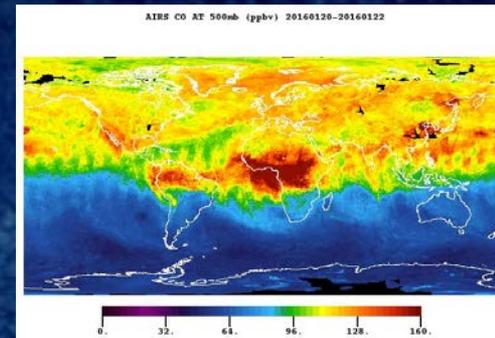
- Launched in 2002, the satellite sounder community has the experience of 13+ years of AIRS processing and AIRS has been well tested and validated
- The Aqua satellite is in the same orbit as SNPP, thereby facilitating collocations with SNPP CrIS/ATMS
- AIRS produces the same trace gas products as NUCAPS: O_3 , CO , CO_2 , CH_4

- » **Orbiting Carbon Observatory (OCO)-2 (NASA A-Train)**

- Launched in July 2014
- Provides CO_2 observations

- » **Microwave Limb Sounder (MLS) (NASA A-Train)**

- Launched in July 2004
- Provides CO observations





Validation of SNPP NUCAPS trace gas EDRs

IR OZONE PROFILE EDR

IR Ozone Profile EDR Validation (1/8)

In Situ Truth Datasets



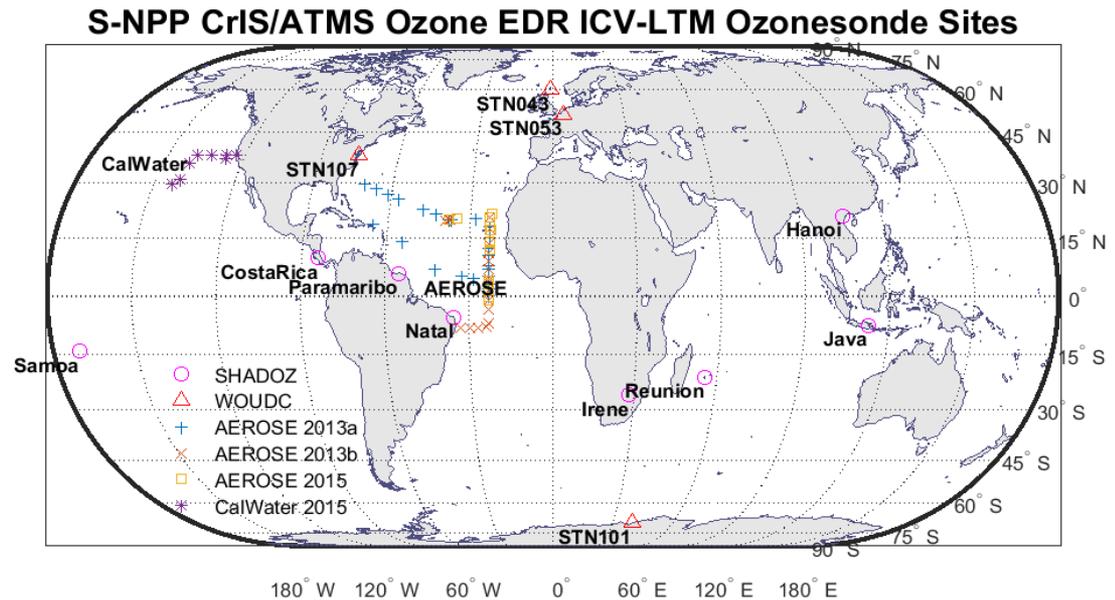
- Collocated ozonesondes for O₃ (ozone) profile EDR

- Dedicated Ozonesondes

- NOAA AEROSE (Nalli et al. 2011)
- CalWater/ACAPEX 2015

- Sites of Opportunity

- SHADOZ (Thompson et al. 2007)
 - Costa Rica
 - Hanoi
 - Irene
 - Java
 - Natal
 - Paramaribo
 - Reunion
 - American Samoa
- WOUDC
 - STN043
 - STN053
 - STN107
 - STN101



IR Ozone Profile EDR Validation (2/8)

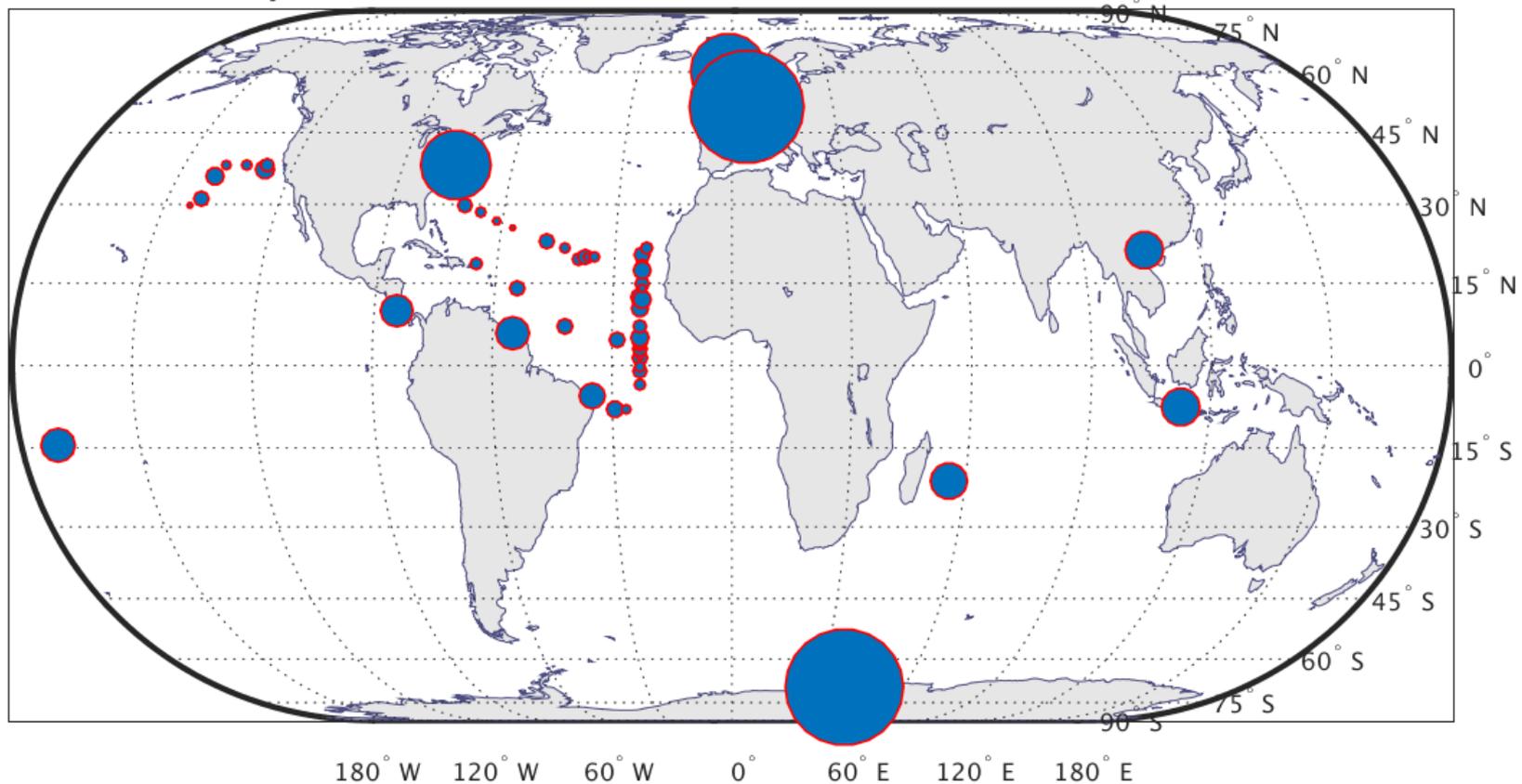
VALAR Ozonesonde-FOR Collocation Sample ($n = 6024$)



Geographic Histogram (Equal Area)

FOR Collocation Criteria: $\delta x \leq 125$ km, $-240 < \delta t < +120$ min

valar_nucaps_offline_v15_collocation_file_o3_shadoz-raob_20160805.mat



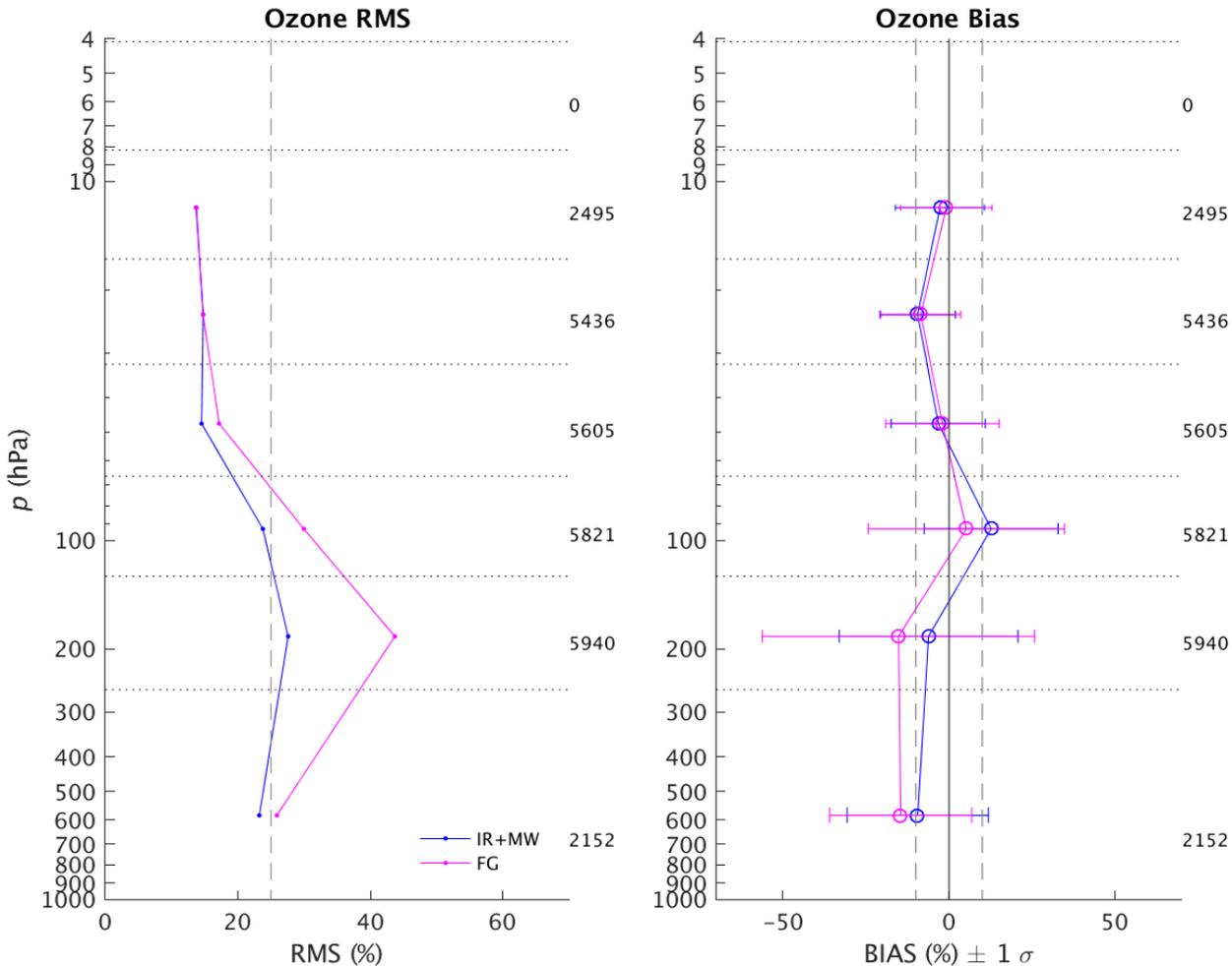
IR Ozone Profile EDR Validation (3/8)

NUCAPS Offline (v1.5) versus Global Ozonesondes



Retrieval and *A Priori* First Guess

IR+MW Yield
= 62.2%



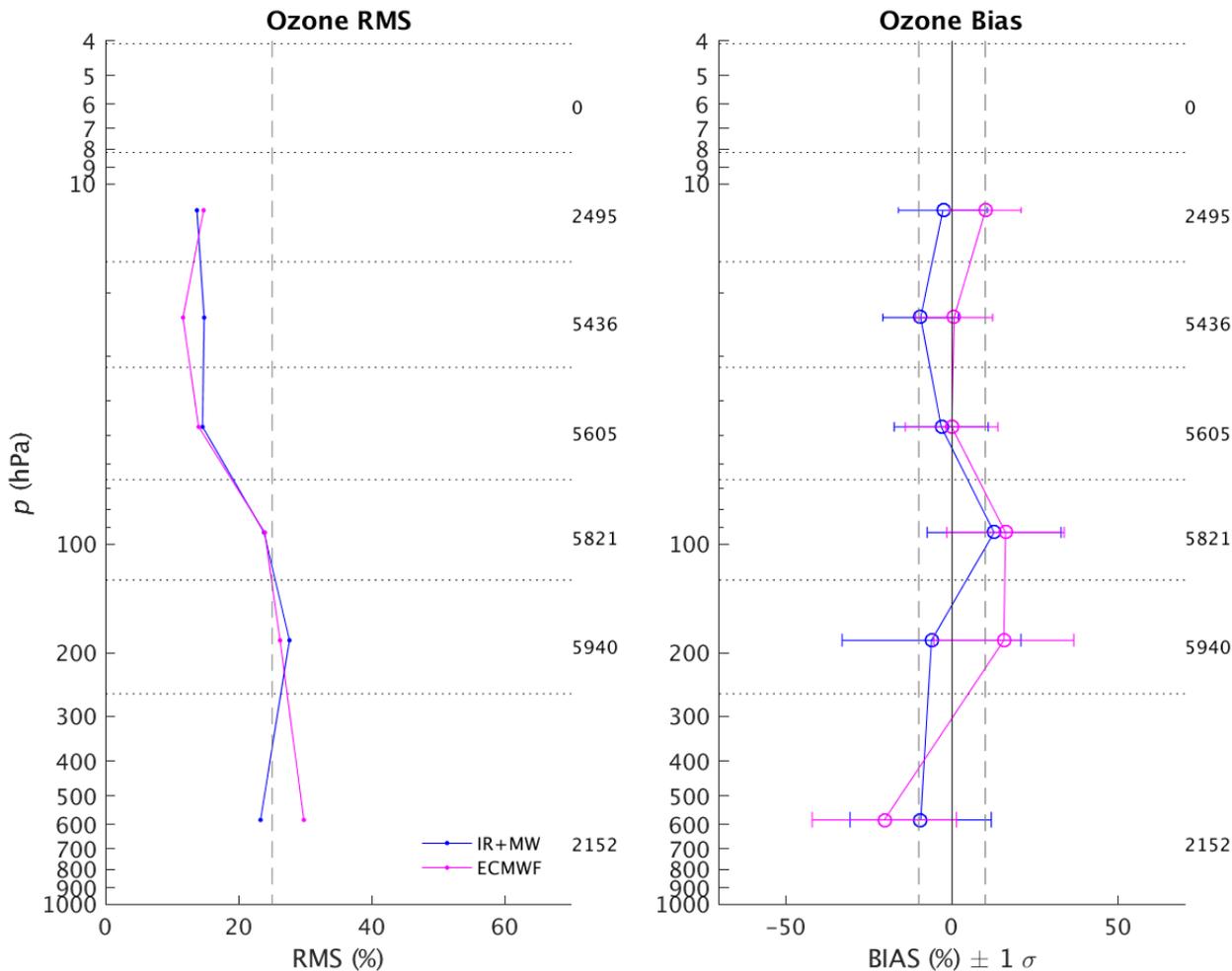
IR Ozone Profile EDR Validation (4/8)

NUCAPS Offline (v1.5) versus Global Ozonesondes



Retrieval and ECMWF

IR+MW Yield
= 62.2%



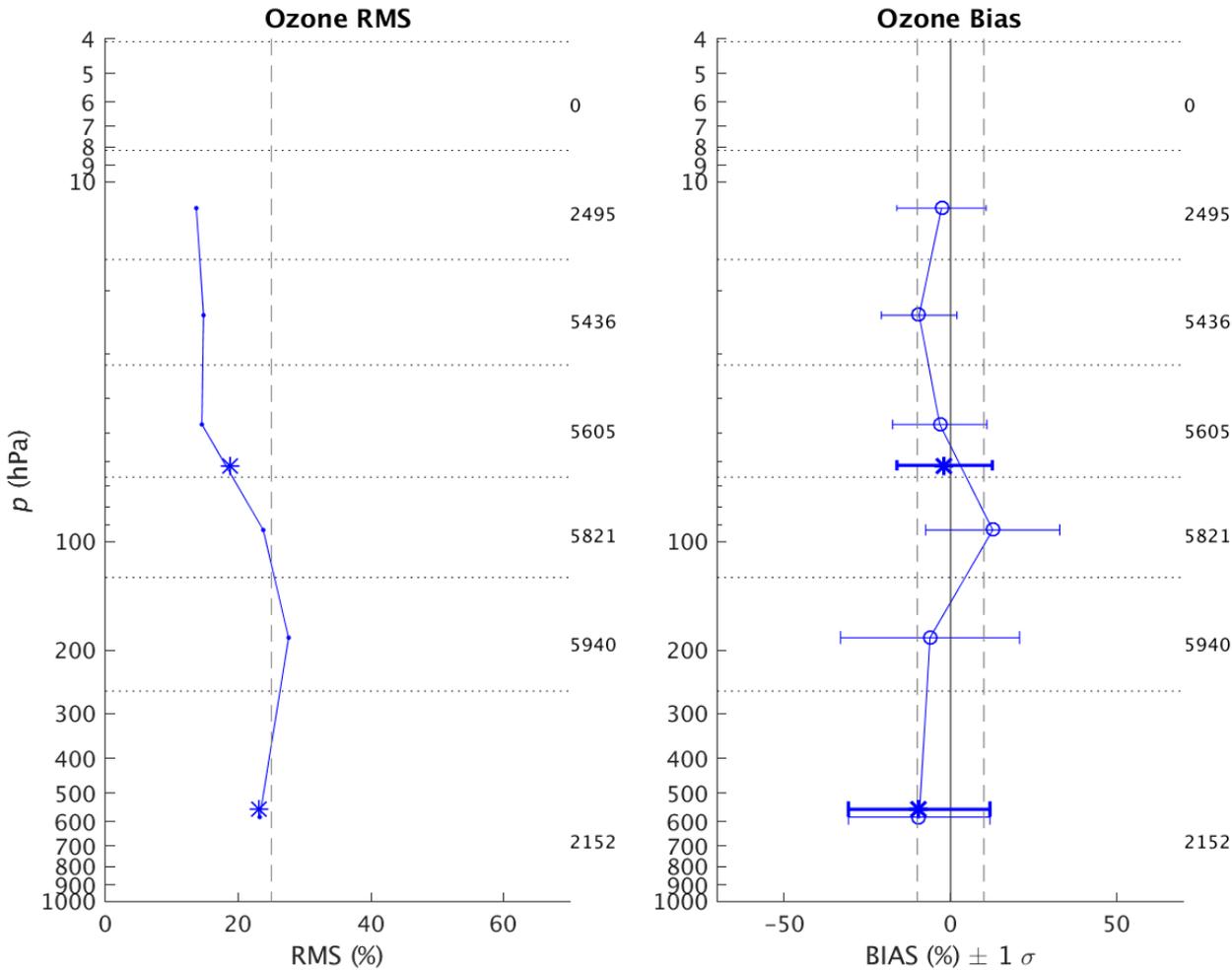
IR Ozone Profile EDR Validation (5/8)

NUCAPS Offline (v1.5) versus Global Ozonesondes



* Broad-Layer Statistics (Per JPSS Level 1 Requirements)

IR+MW Yield
= 62.2%



IR Ozone Profile EDR Validation (6/8)

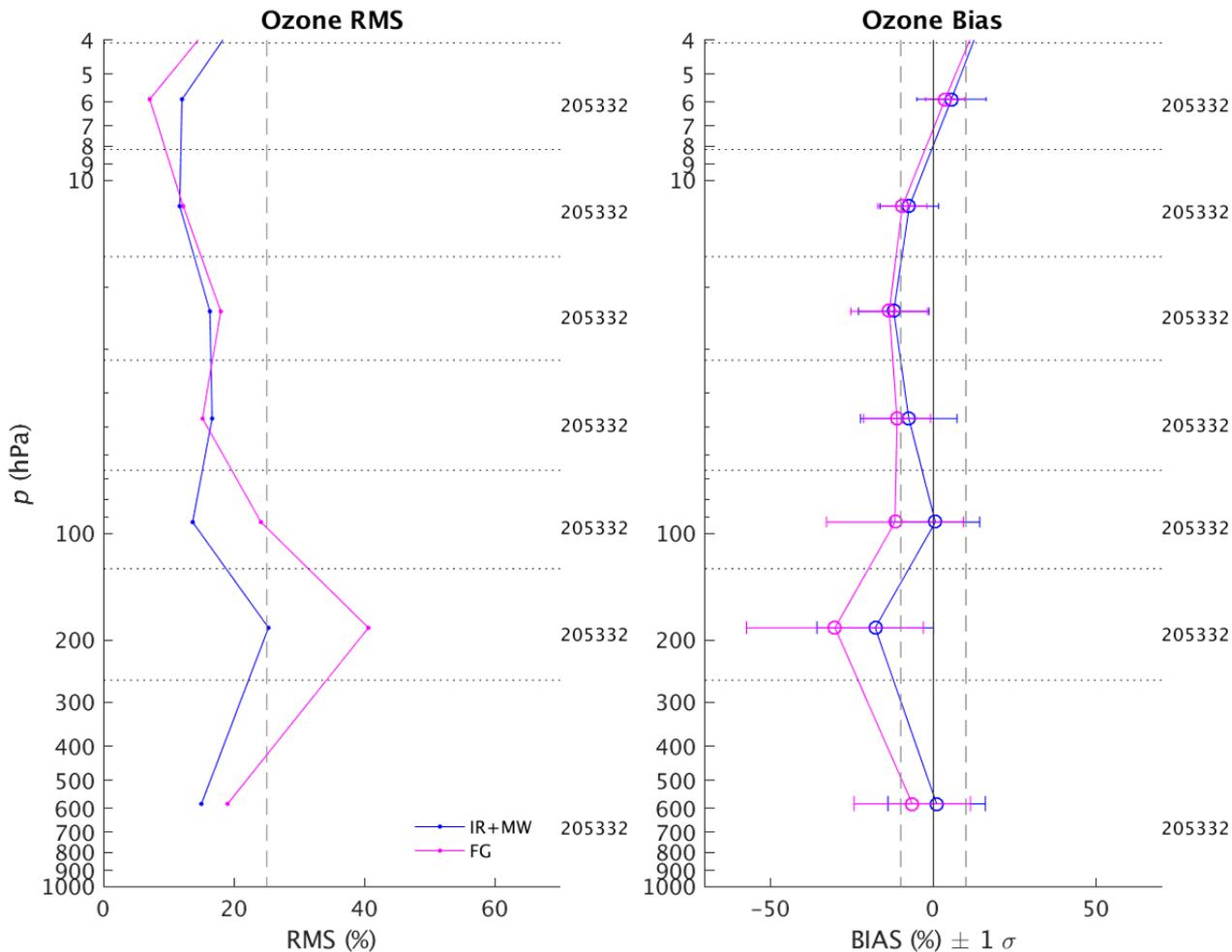
NUCAPS Offline (v1.5) versus Global Focus Day 17-Feb-2015



O₃ Versus ECMWF

IR+MW
First Guess

NUCAPS v1.5
Yield = 63.4%



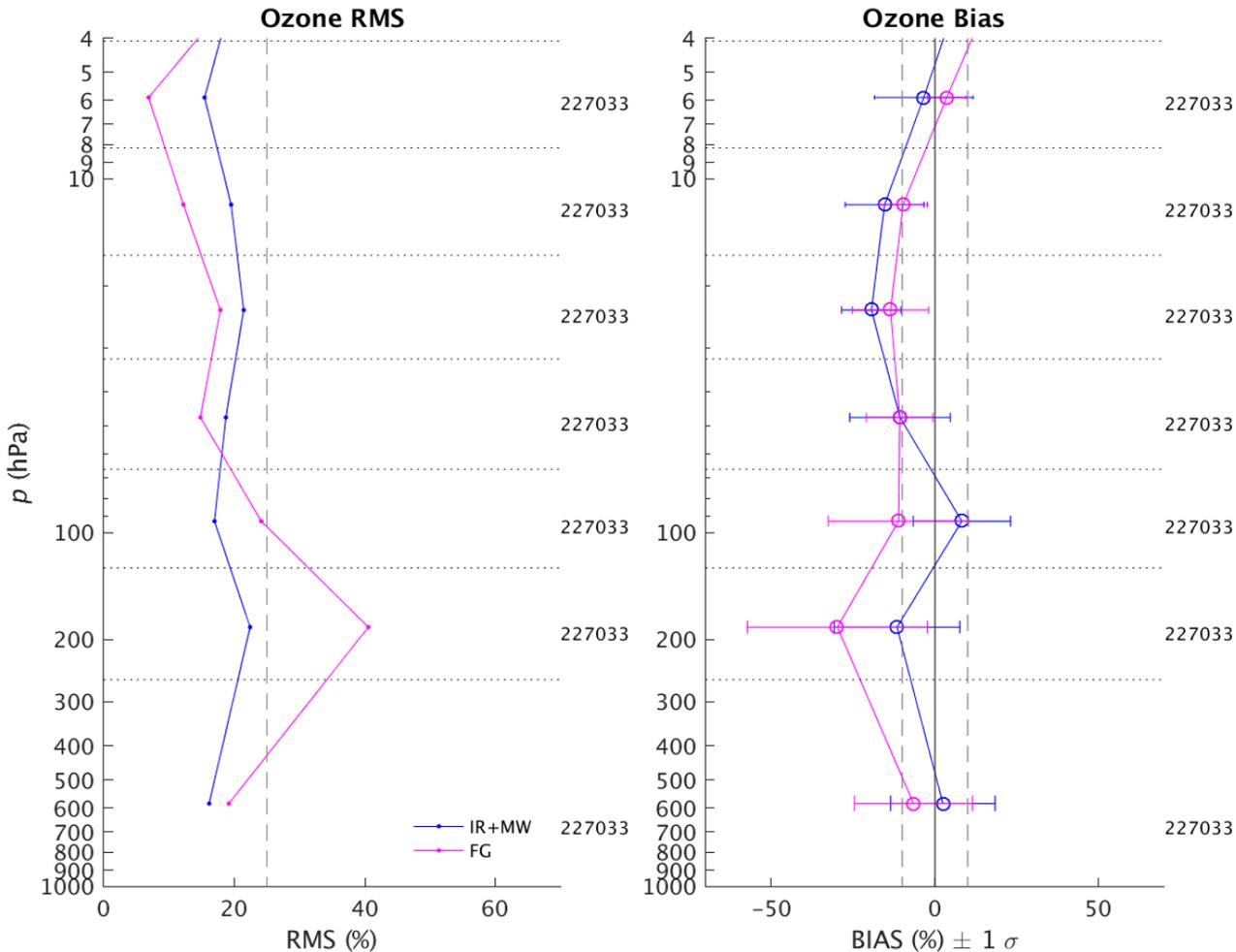
IR Ozone Profile EDR Validation (7/8)

NUCAPS Offline (v1.8.1) versus Global Focus Day 17-Feb-2015



O₃ Versus ECMWF

IR+MW
First Guess
NUCAPS v1.8.1
Yield = 70.1%



IR Ozone Profile EDR Validation (8/8)

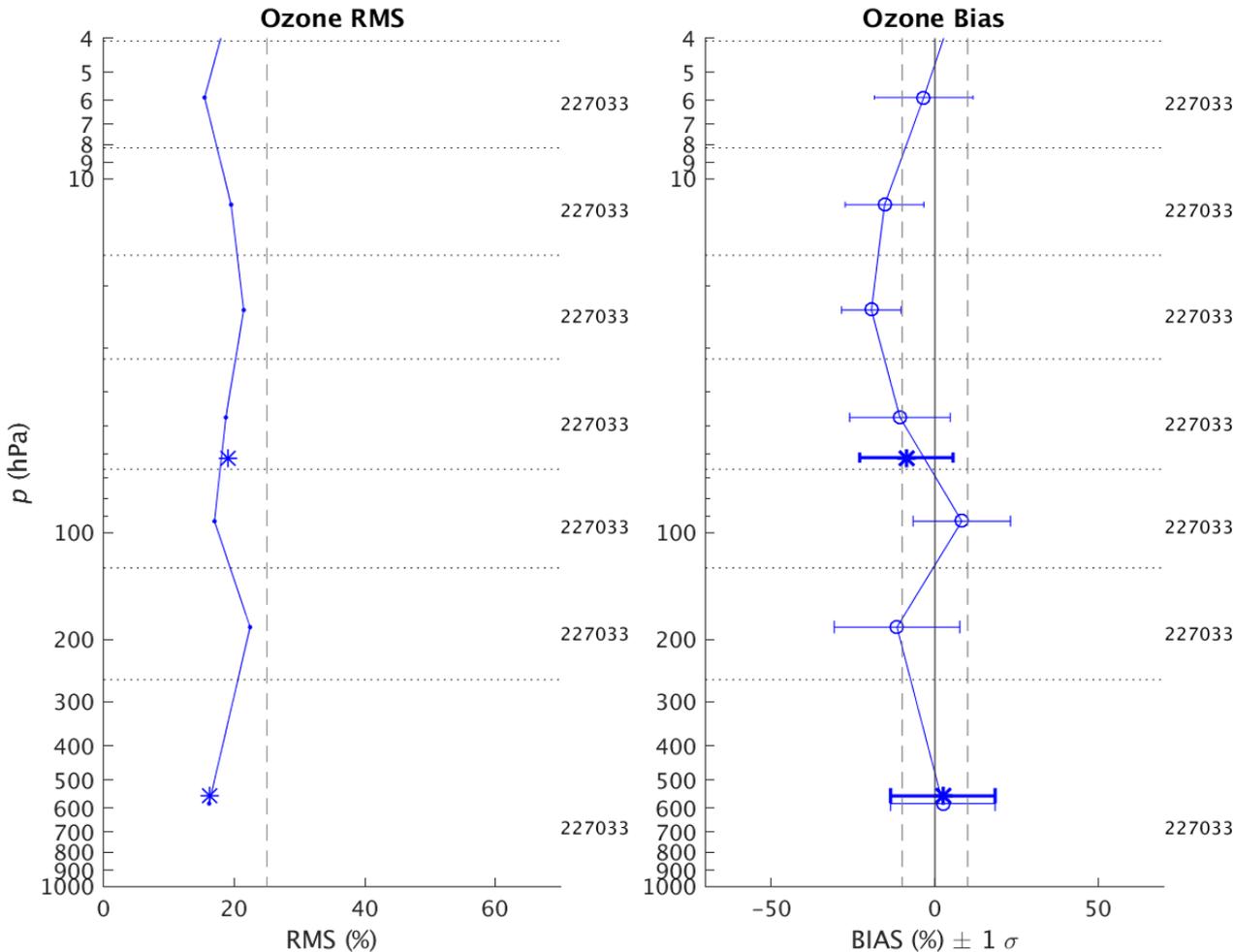
NUCAPS Offline (v1.8.1) versus Global Focus Day 17-Feb-2015



* Broad-Layer Statistics

(Per JPSS Level 1 Requirements)

NUCAPS v1.8.1
Yield = 70.1%



Validation of SNPP NUCAPS trace gas EDRs

CARBON MONOXIDE (PRELIMINARY)

Basic Methodology for CO and CO₂



- The **AIRS v6 standard products** were obtained for the global Focus day 17 February 2015
 - Total column integrated CO and CH₄
 - The AIRS Team provided us offline runs for CO₂
- AIRS and NUCAPS were divided into ascending (ASC) and descending (DES) orbits
- Linear interpolations of FOR (lat/lon) were then performed for each orbit (ASC and DES) to create a one-to-one correspondence of collocation data points
 - AIRS CO was interpolated to NUCAPS
 - NUCAPS CO₂ was interpolated to the more sparse AIRS

- **NUCAPS offline runs for global Focus Day 17 February 2015**
 - v1.5 (nominal CrIS res)
 - v1.8.1 (full CrIS res)

- **For NUCAPS CO**, profile EDRs on 100 RTA layers are integrated to obtain total column abundances (molecules/cm²) according to *Nalli et al. (2013)*

$$\Sigma_x(z) \equiv \int_{z_t}^z N_x(z') dz'$$
$$\implies \Sigma_x(z) \approx \Sigma_{x,\mathcal{L}} \equiv \sum_{\mathcal{L}}^n \bar{N}_{x,\mathcal{L}} \delta z_{\mathcal{L}}$$

with stats being computed relative to the AIRS v6 total column product

- **For NUCAPS CO₂**, stats are performed simply for atmospheric column averages (in PPMV)

Total Column Carbon Monoxide (CO) EDR (1/2)

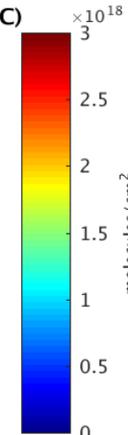
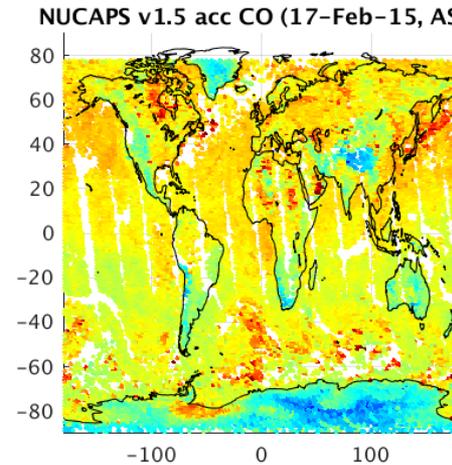
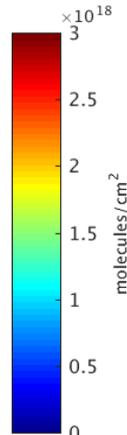
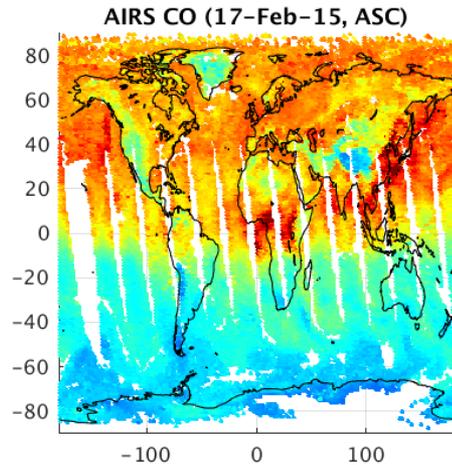
17 Feb 2015 Focus Day, NUCAPS v1.5 and AIRS v6 Accepted Cases



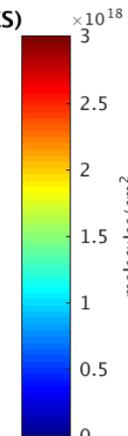
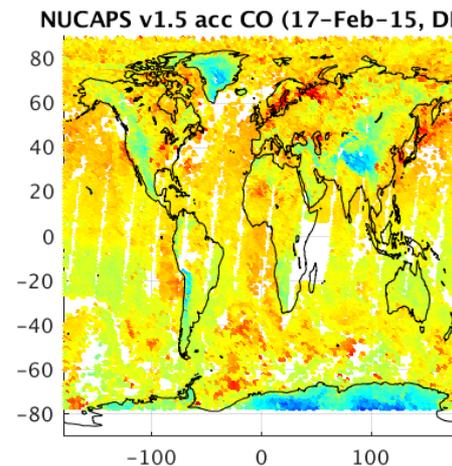
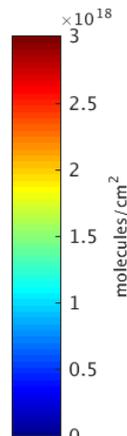
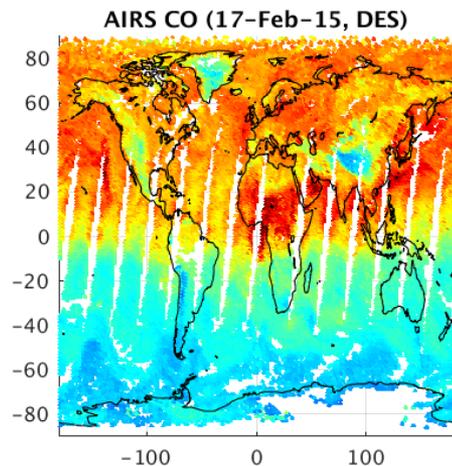
Preliminary

AIRS v6

NUCAPS v1.5



**NUCAPS v1.5
Yield = 63.4%**



Total Column Carbon Monoxide (CO) EDR (2/2)

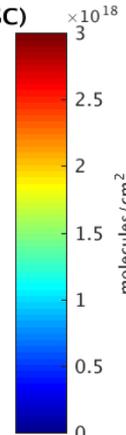
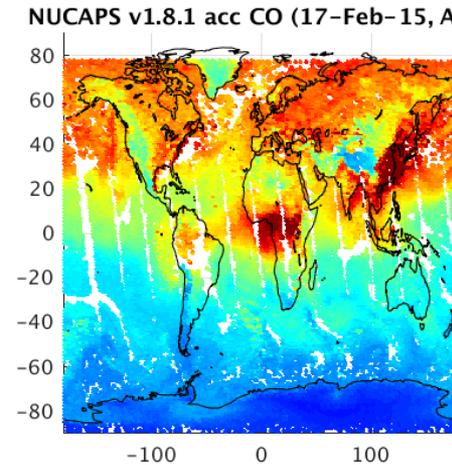
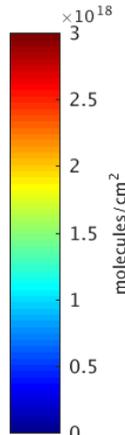
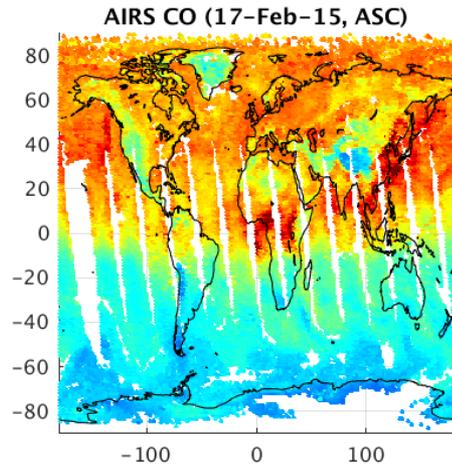
17 Feb 2015 Focus Day, NUCAPS v1.8.1 and AIRS v6 Accepted Cases



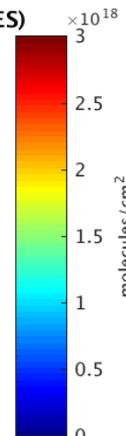
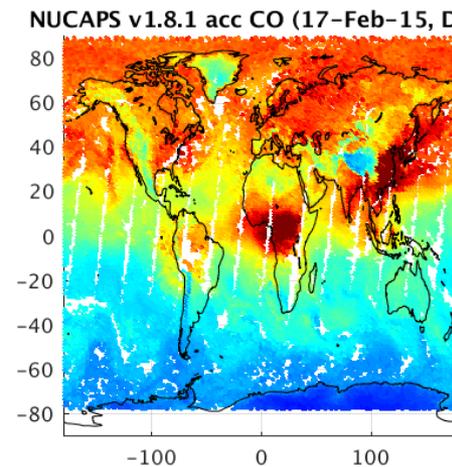
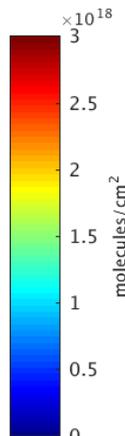
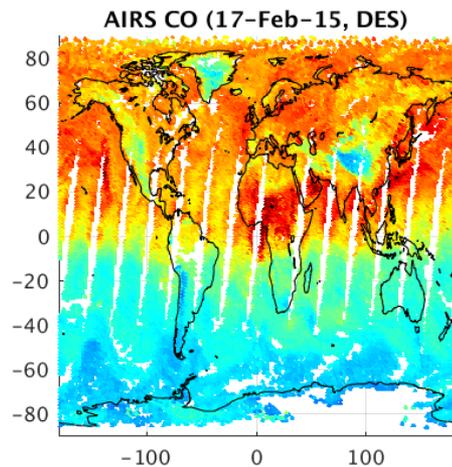
Preliminary

AIRS v6

NUCAPS v1.8.1



**NUCAPS v1.8.1
Yield = 70.1%**



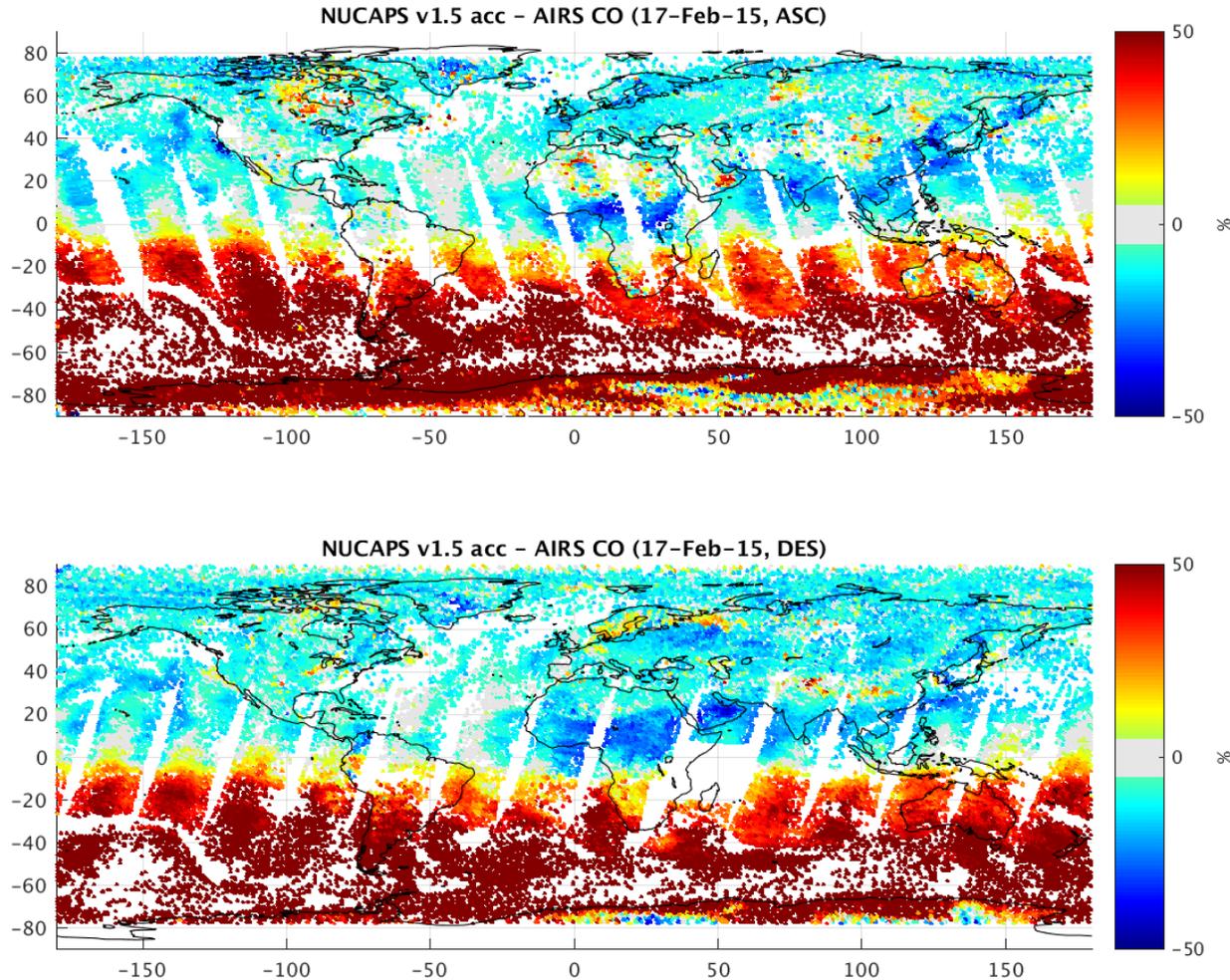
NUCAPS v1.5 CO – AIRS v6 CO

17 Feb 2015 Focus Day, Accepted Cases



Preliminary

NUCAPS v1.5 (Nominal CrIS Resolution)



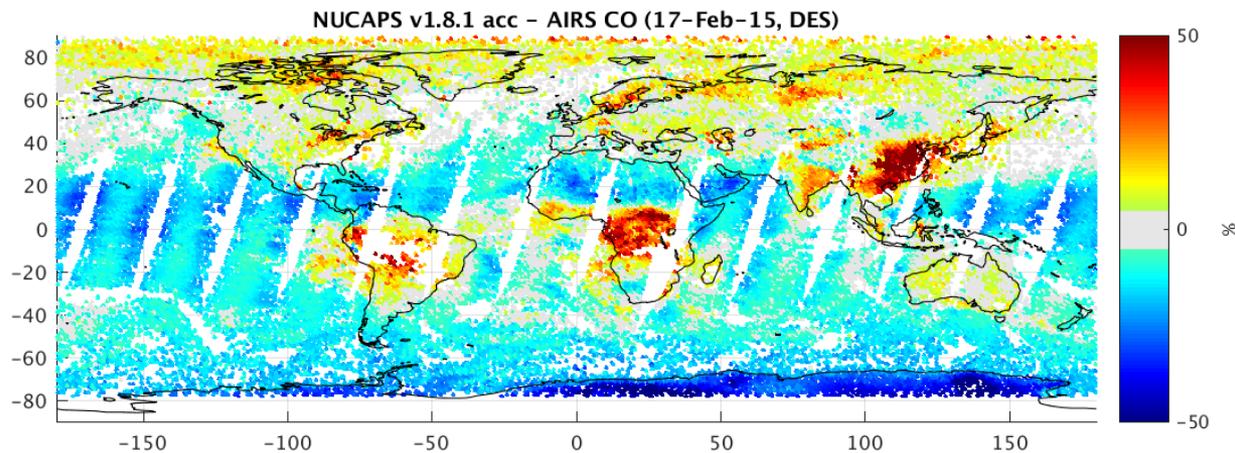
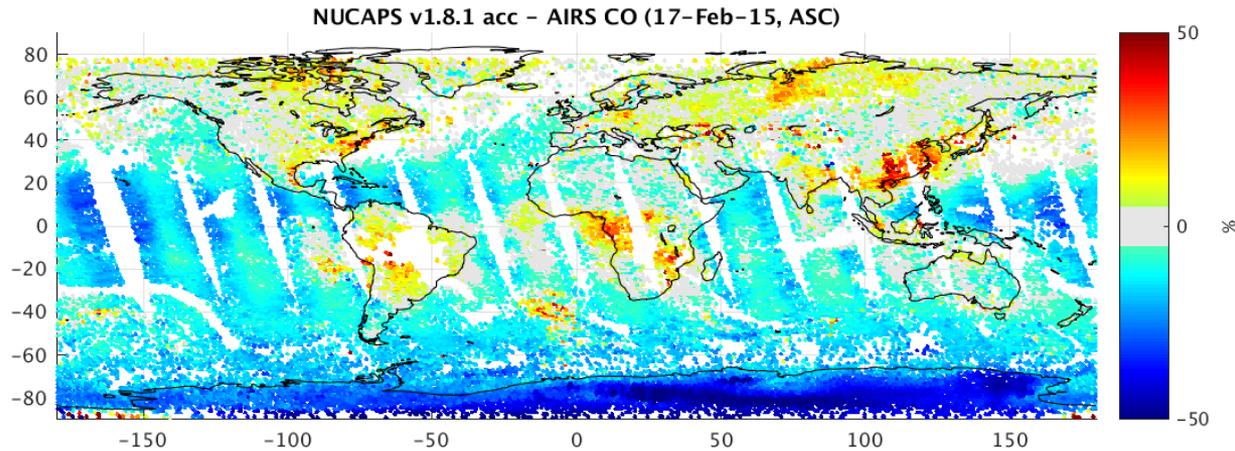
NUCAPS v1.8.1 CO – AIRS v6 CO

17 Feb 2015 Focus Day, Accepted Cases



Preliminary

NUCAPS v1.8.1 (Full CrIS Resolution)





Validation of SNPP NUCAPS trace gas EDRs

CARBON DIOXIDE (PRELIMINARY)

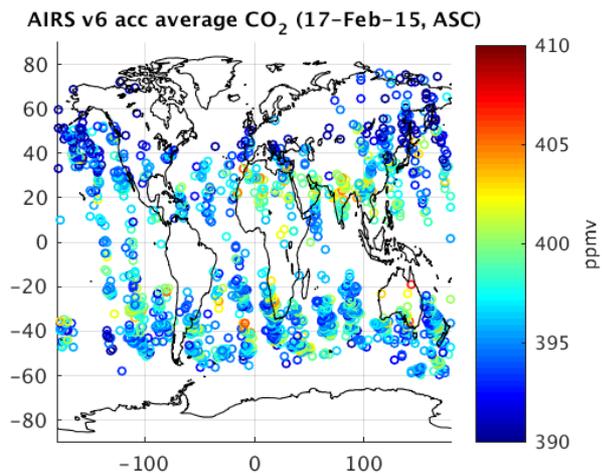
Mean Column Carbon Dioxide (CO₂) EDR (1/2)

17 Feb 2015 Focus Day, NUCAPS v1.5 and AIRS v6 Accepted Cases

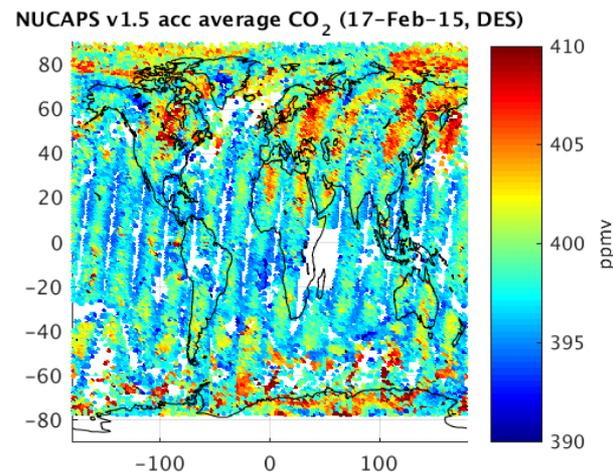
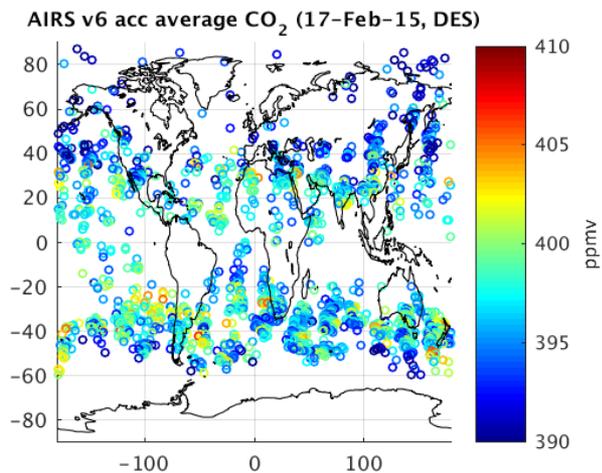
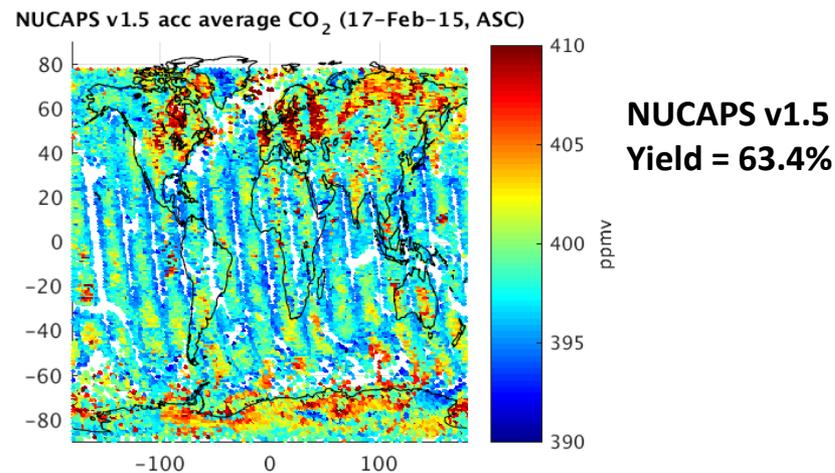


Preliminary

AIRS v6



NUCAPS v1.5



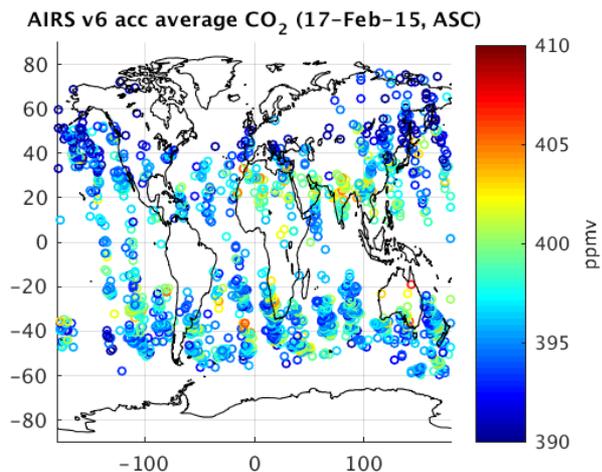
Mean Column Carbon Dioxide (CO₂) EDR (1/2)

17 Feb 2015 Focus Day, NUCAPS v1.8.1 and AIRS v6 Accepted Cases

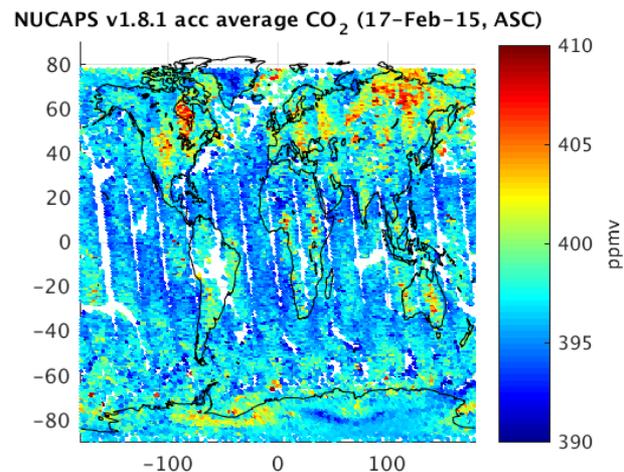


Preliminary

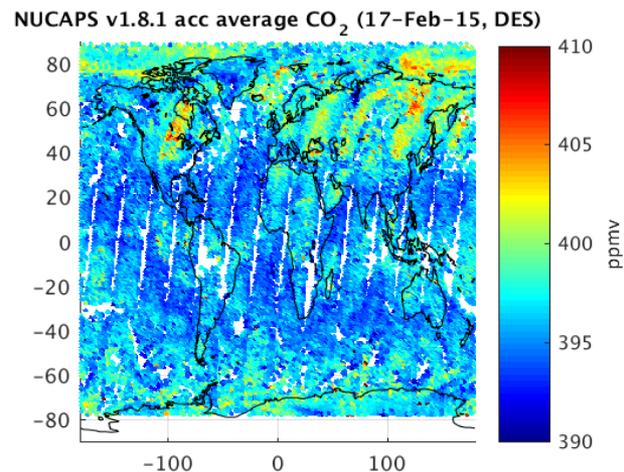
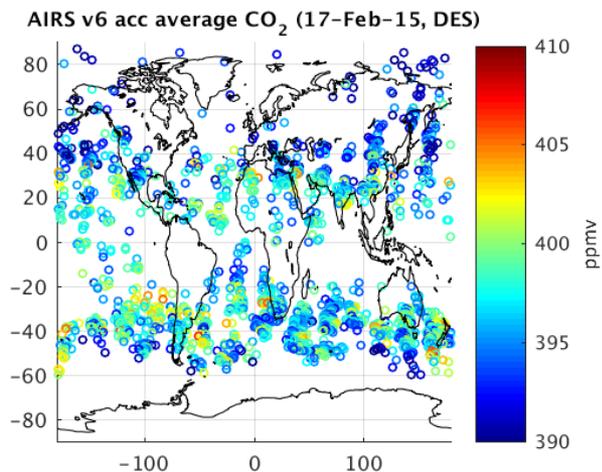
AIRS v6



NUCAPS v1.8.1



**NUCAPS v1.8.1
Yield = 70.1%**



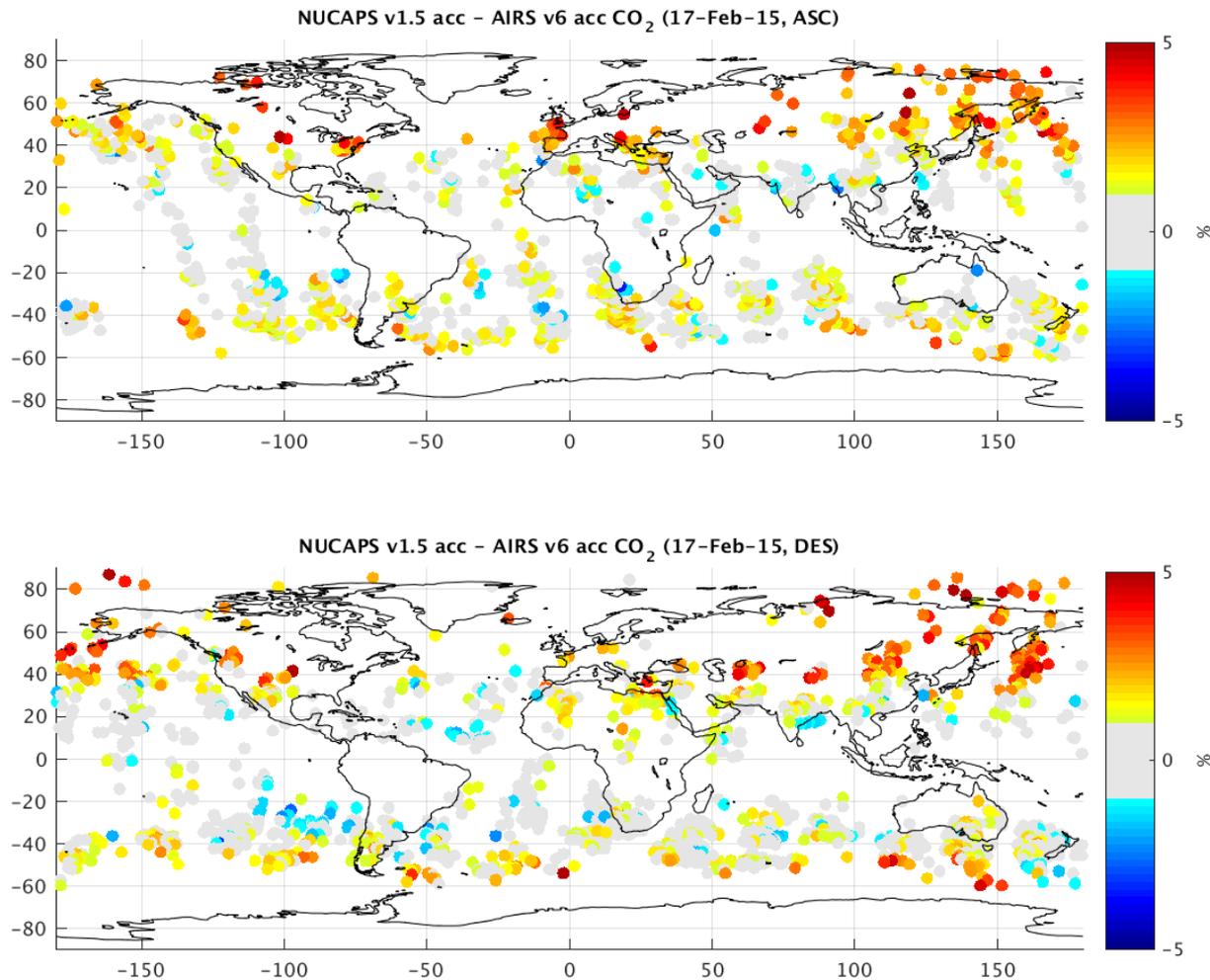
NUCAPS v1.5 CO₂ – AIRS v6 CO₂

17 Feb 2015 Focus Day, NUCAPS and AIRS Accepted Cases



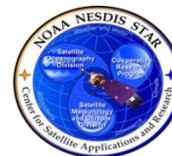
Preliminary

NUCAPS v1.5 (Nominal CrIS Resolution)



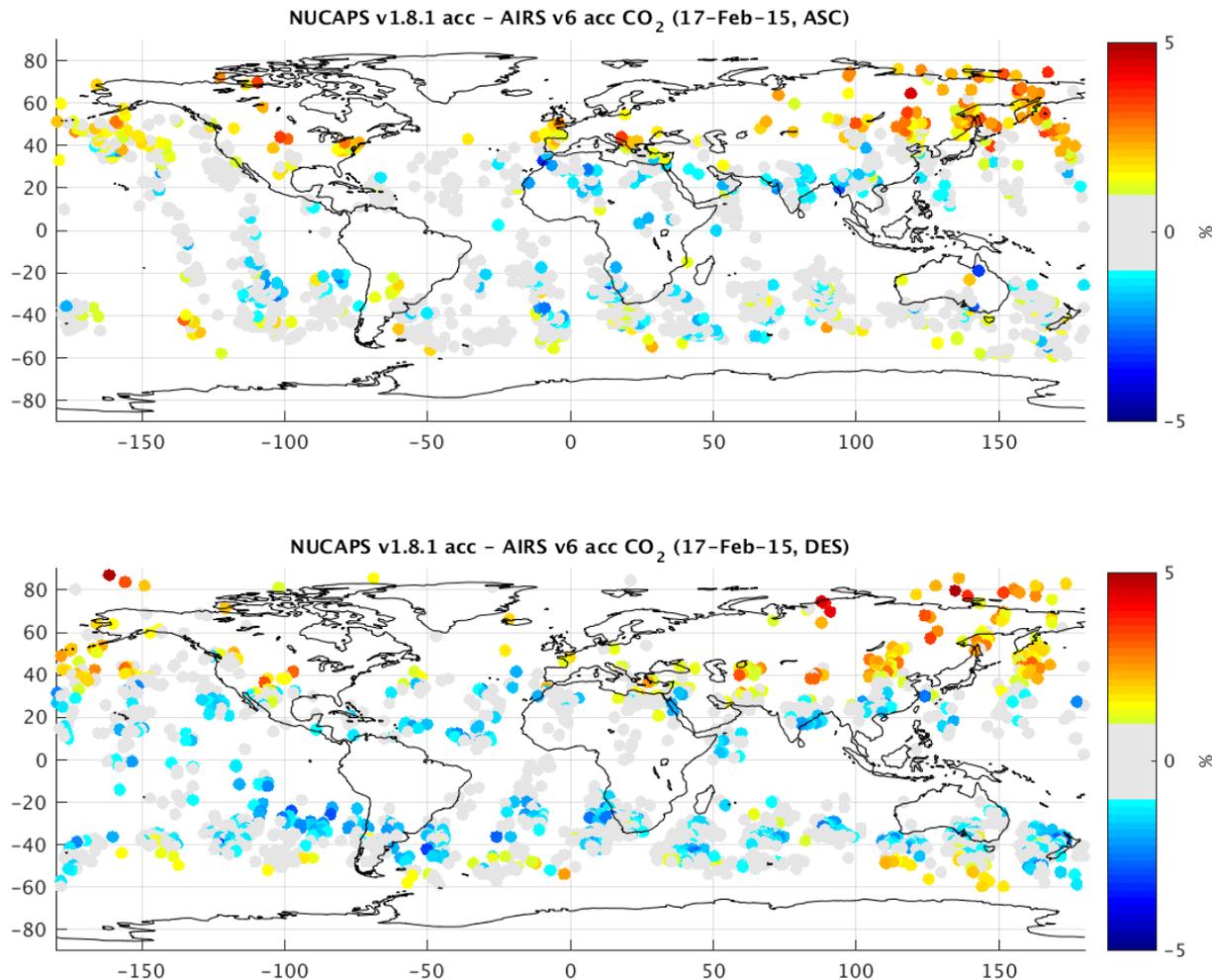
NUCAPS v1.8.1 CO₂ – AIRS v6 CO₂

17 Feb 2015 Focus Day, NUCAPS and AIRS Accepted Cases



Preliminary

NUCAPS v1.8.1 (Full CrIS Resolution)



Preliminary Global Statistics NUCAPS versus AIRS (accepted cases)



	V1.5 CrIS Nom Res			V1.8.1 CrIS Full Res		
Trace Gas EDR	BIAS (%)	STD (%)	RMS (%)	BIAS (%)	STD (%)	RMS (%)
CO (asc)	+21.7 (±25.0)	41.5 (35.0)	46.8	-10.3 (±5.0)	28.1 (15.0)	17.8
CO (des)	+11.0 (±25.0)	33.4 (35.0)	35.1	-3.2 (±5.0)	14.8 (15.0)	15.7
CO ₂ (asc)	+0.9 (±1.0)	1.1 (0.5)	1.4	+0.2 (±1.0)	1.1 (0.5)	1.4
CO ₂ (des)	+0.8 (±1.0)	1.2 (0.5)	1.5	-0.2 (±1.0)	1.2 (0.5)	1.4

O₃, CO, CO₂ Trace Gas Summary



- The **NUCAPS IR ozone (O₃) profile EDR products are shown to meet JPSS Level 1 requirements**
 - The **offline v1.5 (nominal CrIS resolution) ozone EDR** has reached **“Validated Maturity”** based upon coarse/broad layer statistical analyses versus
 - Collocated **global ozonesondes**, including **dedicated ozonesondes** (Validation Hierarchy Method #4)
 - **Global Focus Day** (17 February 2015) **ECMWF** output (Validation Hierarchy Method #1)
 - The **offline v1.8.1 (full CrIS resolution) also meets Level 1 requirements** based upon coarse/broad layer statistical analyses versus
 - **Global Focus Day ECMWF** output
 - **Statistics are comparable to the ozonesonde-validated NUCAPS v1.5**
- For validation of **NUCAPS carbon monoxide (CO)** and **carbon dioxide (CO₂) EDRs**, we rely on satellite EDR Intercomparisons (Validation Hierarchy Method #2) versus **collocated AIRS v6**
 - **AIRS flown on Aqua is in the same orbit as SNPP** and is thus ideal for collocations with SNPP
 - **NUCAPS v1.5 CO and CO₂ retrievals meet the relaxed JPSS Level 1 requirements for BIAS**
 - **NUCAPS v1.5 and v1.8.1 CO descending orbit currently meet JPSS Level 1 requirements**
- **Future Work**
 - **Perform “spot-checks” of AIRS and NUCAPS EDRs using *in situ* datasets of opportunity**
 - Utilize a larger data sample (e.g., month) for the CO₂ validation, apply other techniques for QA (e.g., considering DOF, applying AKs, etc.)
 - Further optimization of NUCAPS full-resolution algorithm
 - Investigate improvements in the ozone *a priori*



SNPP NUCAPS Validation

THANK YOU! QUESTIONS?



Retrieval of Trace Gases using CrIS Full Spectrum Data

**Xiaozhen (Shawn) Xiong^{1,2}, Q. Liu²,
A. Gambacorta³, C. Tan^{1,2},
and other NUCAPS Team members**

¹IMSG Inc.

²NOAA/NESDIS/STAR

³Science and Technology Corporation



Outline

■ **Part I: Lessons Learned from AIRS and IASI Trace Gases Retrievals**

- AIRS and IASI provide measurements of trace Gases (O_3 , CO_2 , CO , CH_4 , N_2O since 2002);
- Valuable information of gases distribution in Mid-Upper troposphere can be observed (examples) :
 - 1) Enhancement of upper troposphere CH_4 over south Asia during Monsoon season;
 - 2) Stratospheric Intrusion and its impact to CH_4 and O_3 ;
- One more study to examine the possibility to combine AIRS and IASI data to make a long-term product;

■ **Part II: Preliminary Assessment to CrIS Trace Gases Retrievals and Improvements**

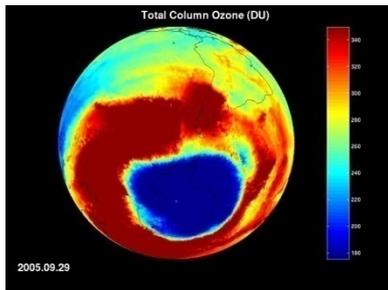
- 1) Preliminary assessment to current trace gases retrieval in NUCAPS (DOF, Averaging Kernels) and Improvements;
- 2) Monitoring the leakage of CH_4 from California **Aliso Canyon Oil Field and Gas Storage Facility**;

■ **Summary and Future Works**

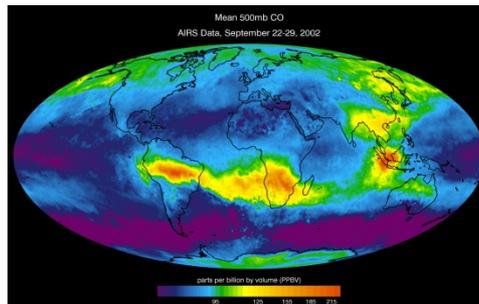


Trace Gases Products

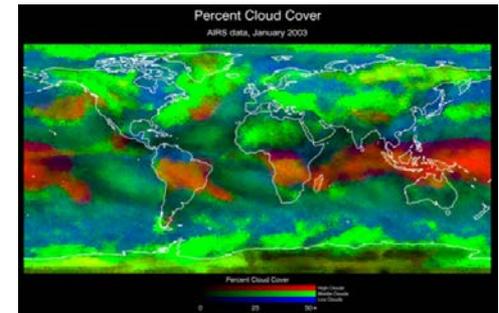
Ozone



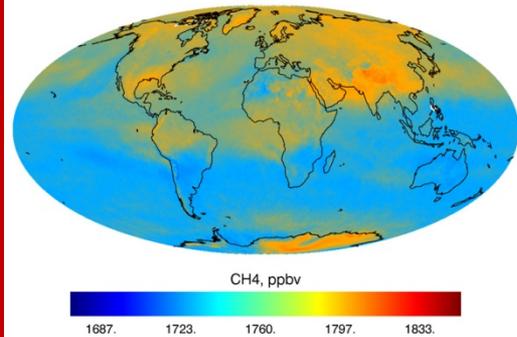
CO



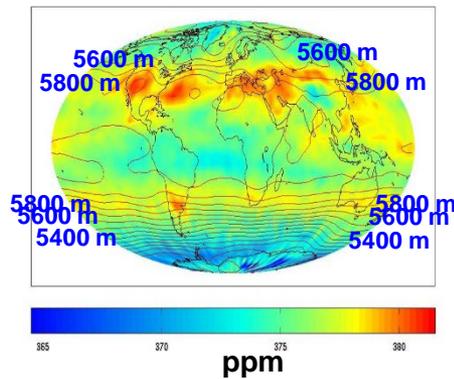
Clouds



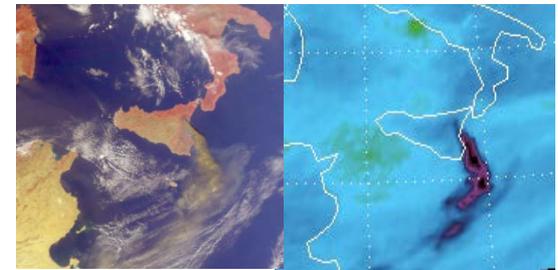
Methane



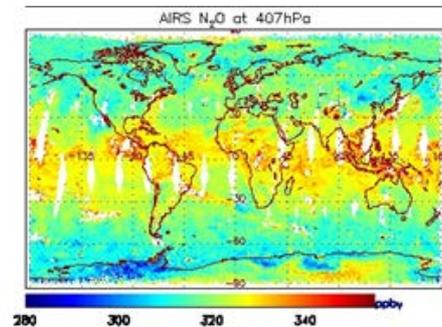
CO₂



SO₂

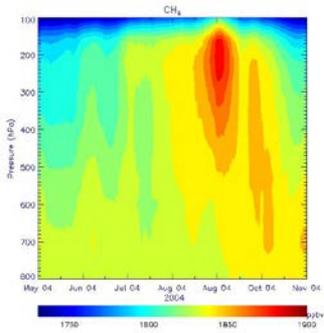


N₂O



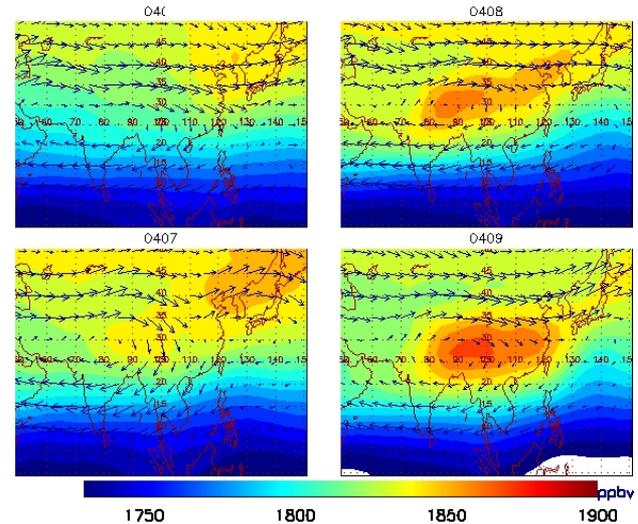
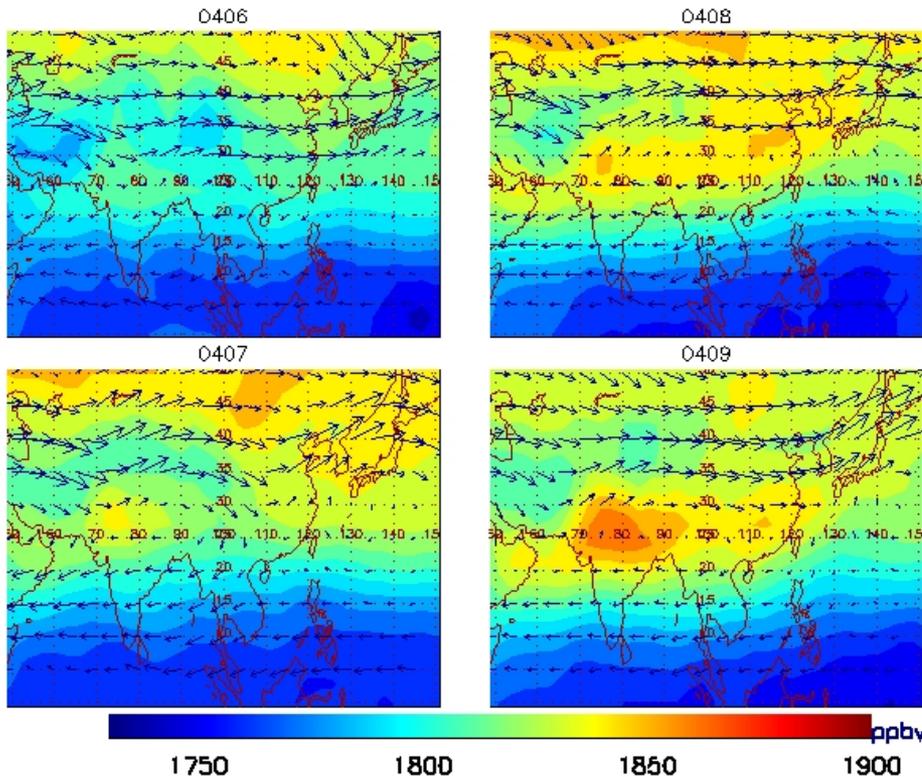
CO₂, CO and CH₄ are listed as Level-1 requirement of products of JPSS

1. AIRS Observed CH₄ Enhancement over South Asia During Monsoon Season (JJAS)

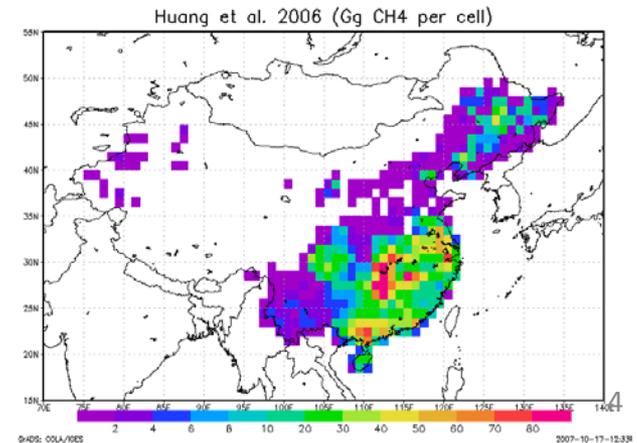


AIRS

Model



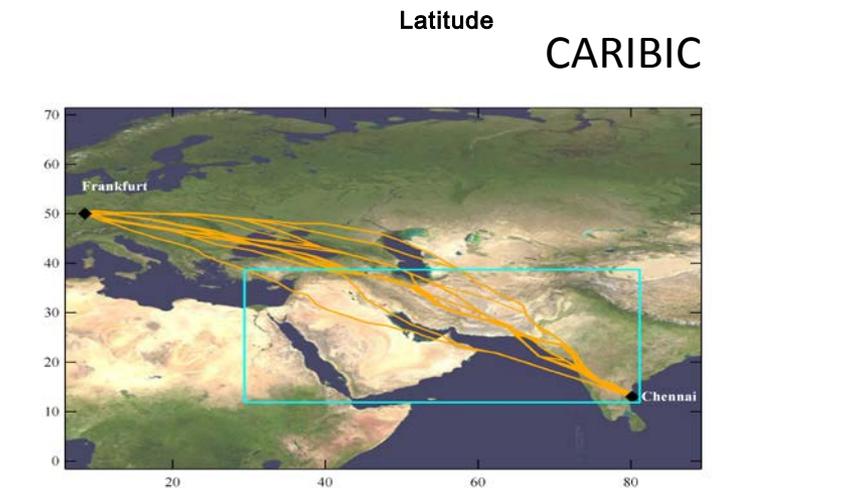
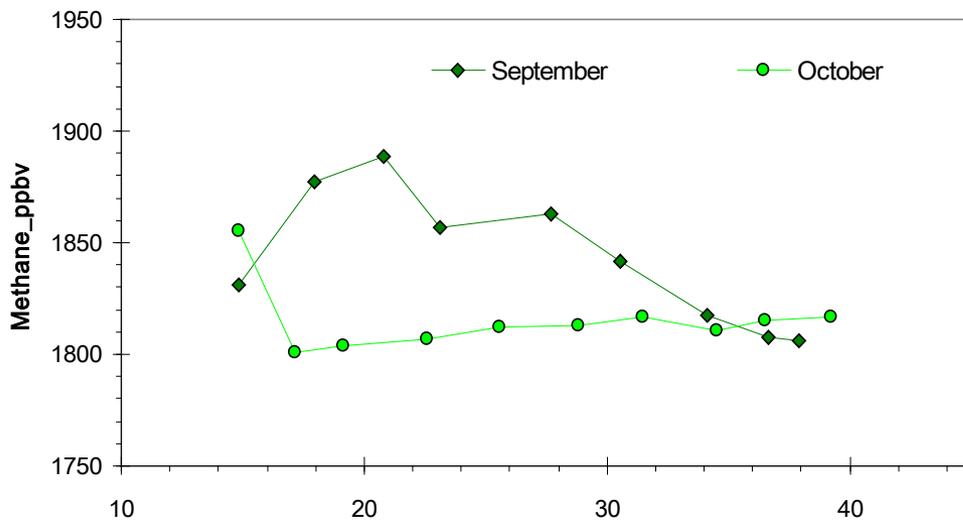
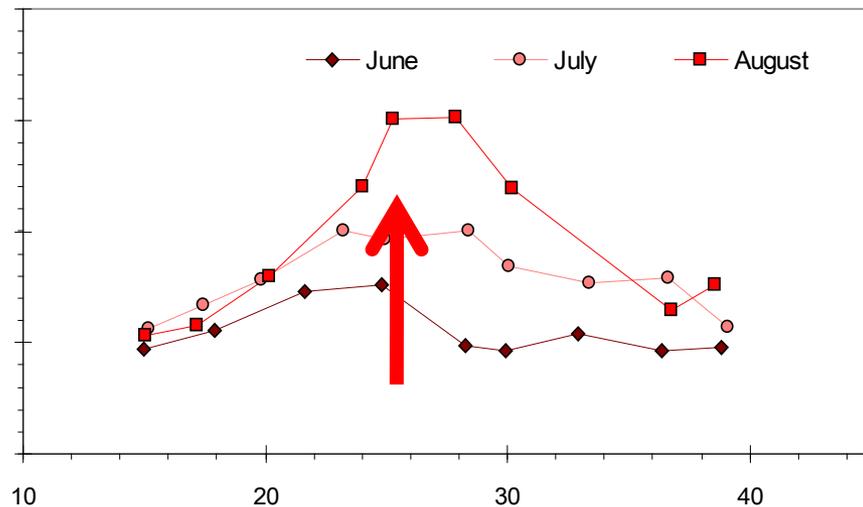
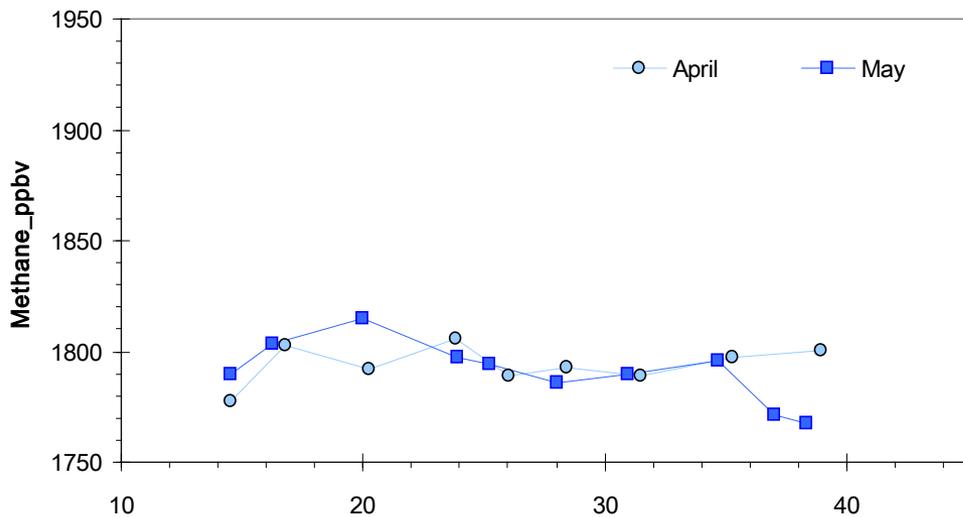
CH₄ emission from rice paddies



Xiong et al., Methane Plume over South Asia during the Monsoon Season: Satellite Observation and Model Simulation, *ACP*, 9, 783-794, 2009.



CARIBIC aircraft measurements proved significant increase of CH₄ as AIRS observed in the same time over South Asia

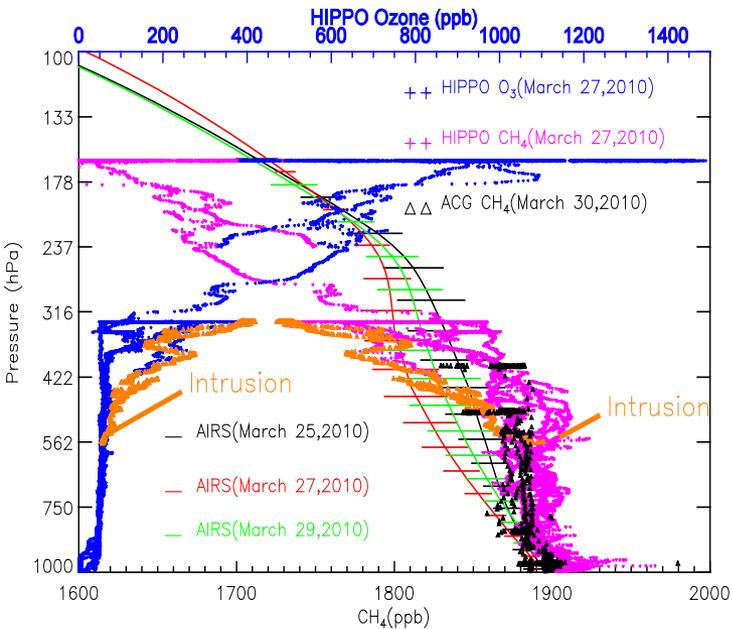


Latitude

Courtesy of Angela Baker and Tanja Schuck (Schuck et al., 2010, ACP)

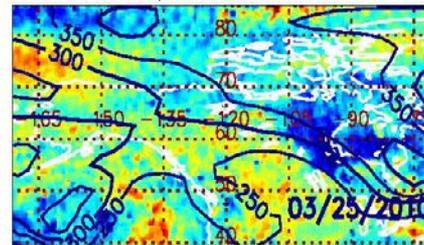
2. AIRS Observed the Impact of Stratospheric Intrusion to CH₄ and O₃

Aircraft Measurements

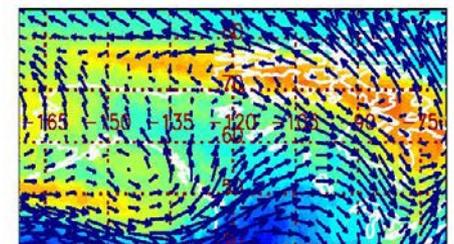
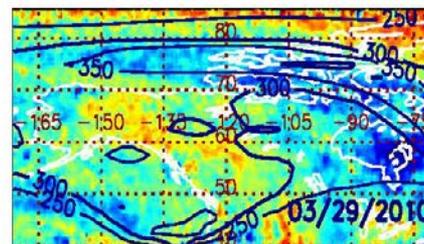
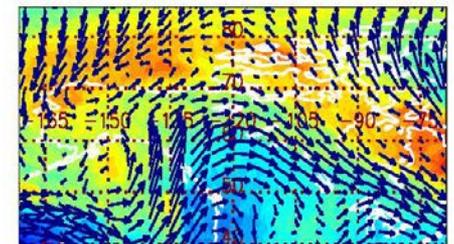
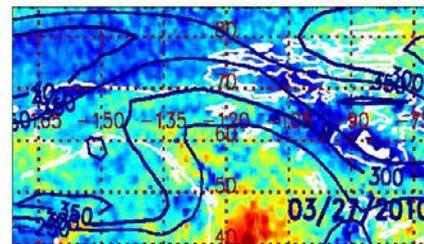
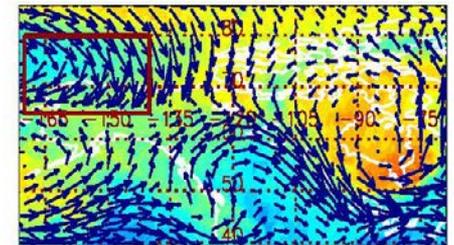


3/25, 3/27, 3/29/2010, Alaska

CH₄ at 407 hPa



Total Ozone



1760 1780 1800 1820 1840 1860 1880 1900 ppbv

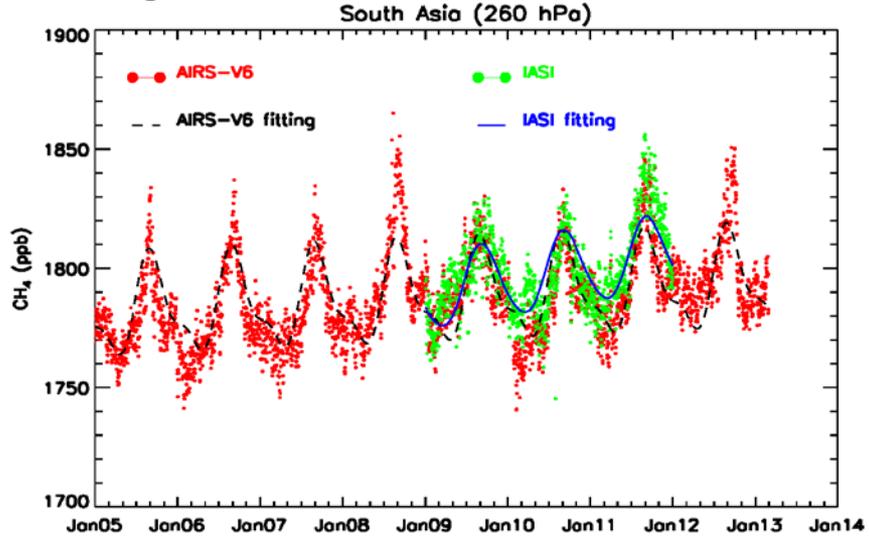
6 8 10 12 14 16 18 1.e+18

Xiong, X. , Barnet, C. D., Maddy, E., et al., 2013, Detection of Methane Depletion Associated with Stratospheric Intrusion by Atmospheric Infrared Sounder (AIRS), *GEOPHYSICAL RESEARCH LETTERS*, VOL. 40, Issue 10, Pages: 2455–2459, doi:10.1002/grl.50476, 2013.



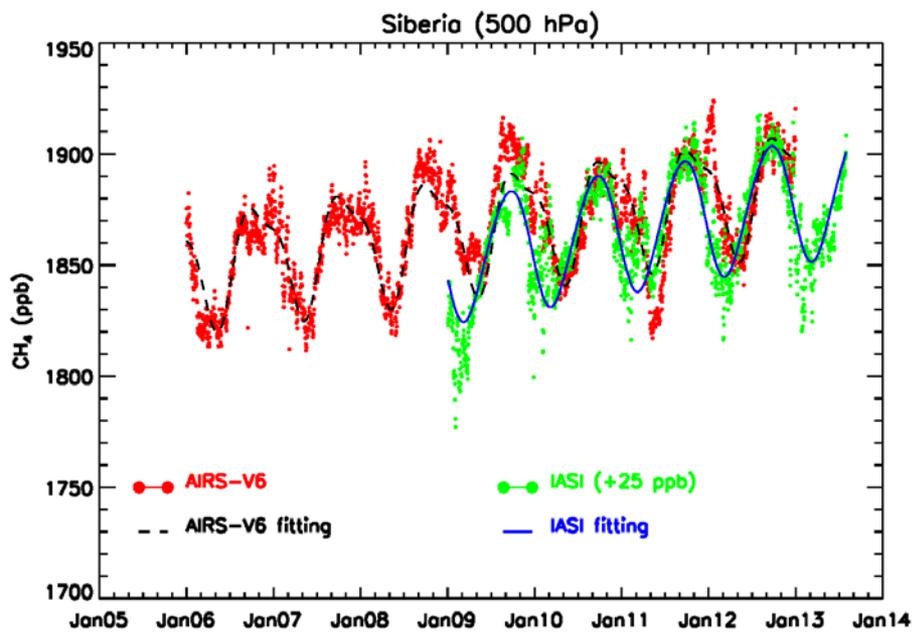
One more study: to make a long-term product by combining AIRS and IASI CH₄ Products

South Asia: repeatable increase of CH₄ during Monsoon Season



Xiong et al., 2016, Comparison of Atmospheric Methane Retrievals from AIRS and IASI, IEEE JSTARS, 10.1109/JSTAR.2016.2588279

Arctic: similar seasonal cycles from AIRS and IASI but has large difference in the cold season





-
- The above examples shows that AIRS and IASI can be used to observe gases distribution in Mid-Upper troposphere, and it is likely to combine AIRS and IASI data to make a long-term product;

 - **CrIS started to operate in the full spectral resolution (FSR) mode since Dec.4, 2014 → making it possible to retrieve trace gases .**

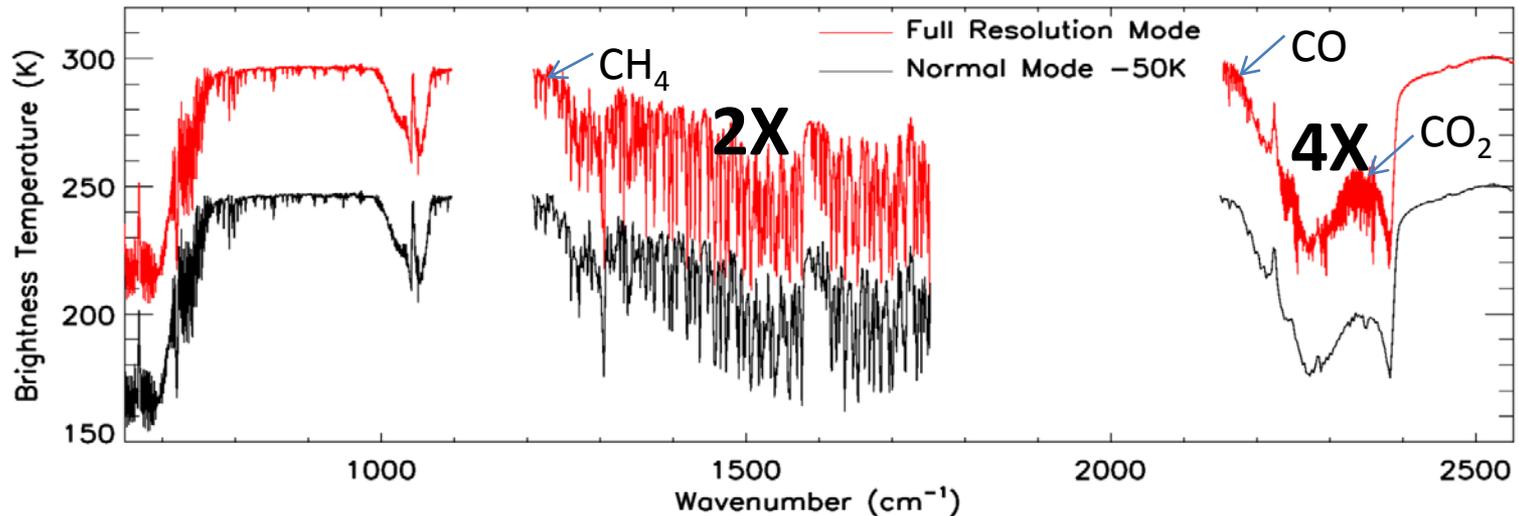


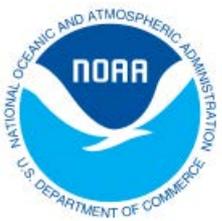
CrIS Normal Resolution and Full Resolution SDR

- CrIS FSR data are available from NOAA/NESDIS/STAR, and it has 2211 channels as compared to 1305 channels in normal mode

<ftp://ftp2.star.nesdis.noaa.gov/smcd/xxiong/> Red: Full resolution

Frequency Band	Spectral Range (cm ⁻¹)	Number of Channel (unapodized)	Spectral Resolution (cm ⁻¹)	Effective MPD (cm)
LWIR	650 to 1095	713* (717)	0.625	0.8
MWIR	1210 to 1750	433* (437)	1.25	0.4
		865* (869)	0.625	0.8
SWIR	2155 to 2550	159* (163)	2.5	0.2
		633* (637)	0.625	0.8



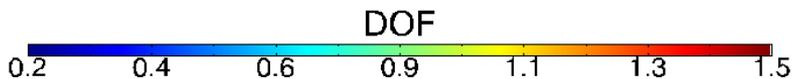
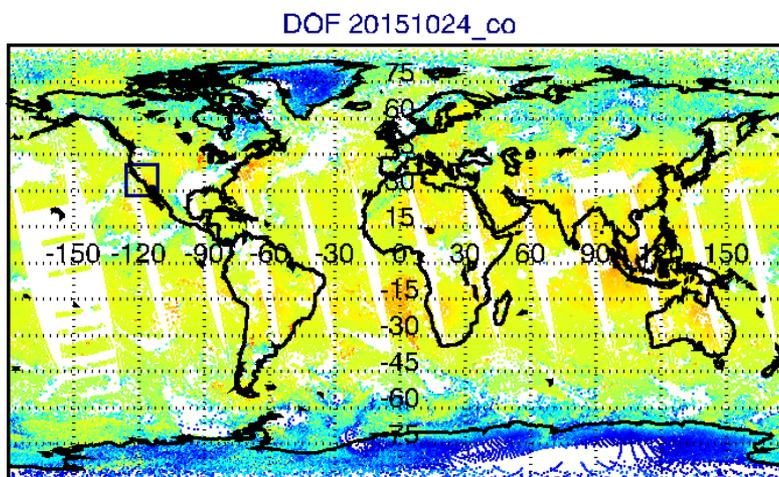
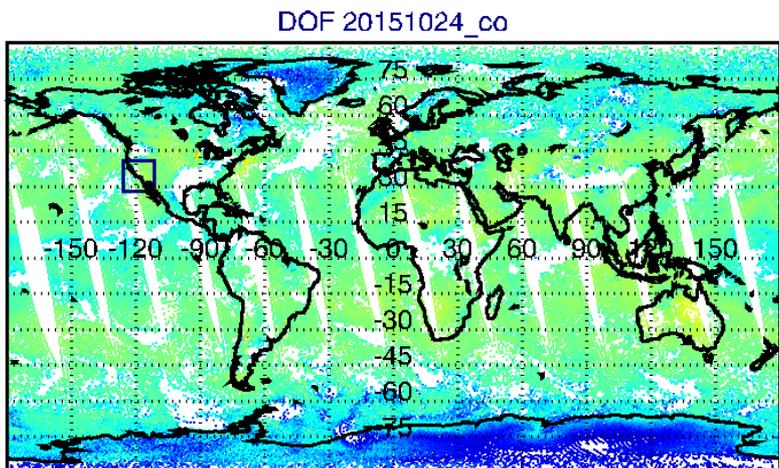


Part 2: Preliminary Assessment to CrIS Trace Gases Retrievals and Improvements

- **First check to NUCAPS trace gases retrieval averaging kernels and DOFs indicated the DOFs are much lower than AIRS and IASI;**
- **Improvements can be made after re-selection of channels, as well as the update to QC;**
- **Historically largest gas leakage in California provides a good case to test if NUCAPS can capture this leakage;**

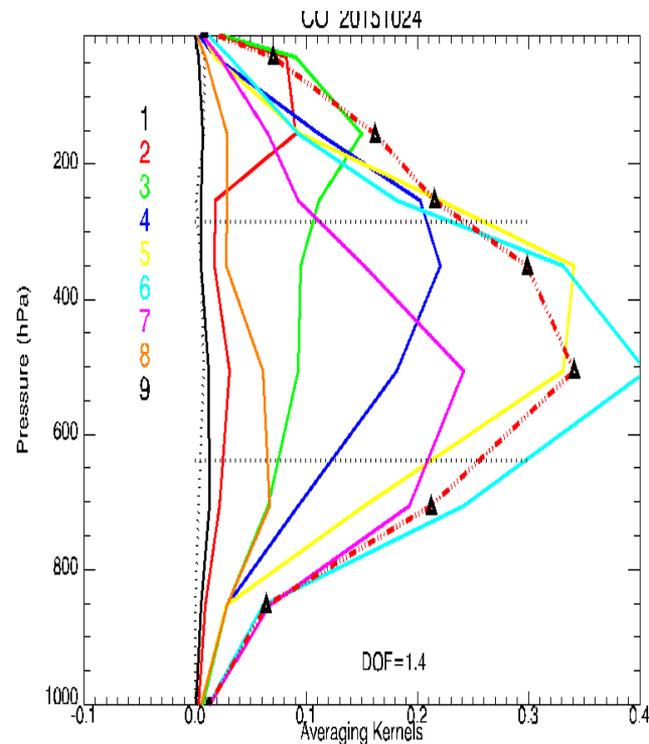
Averaging Kernels and Degree of Freedoms (DOFs) before and after Improvement for CO

Major Sensitivity: 300-650 hPa



current

after

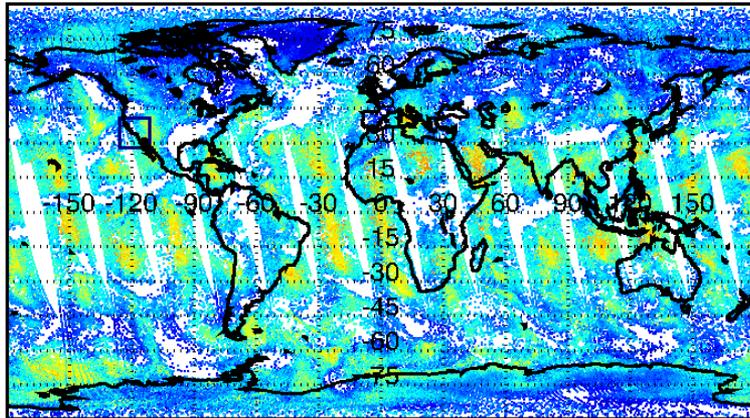


DOFs increase after the re-selection of channels

Averaging Kernels and DOFs Changes for CH₄

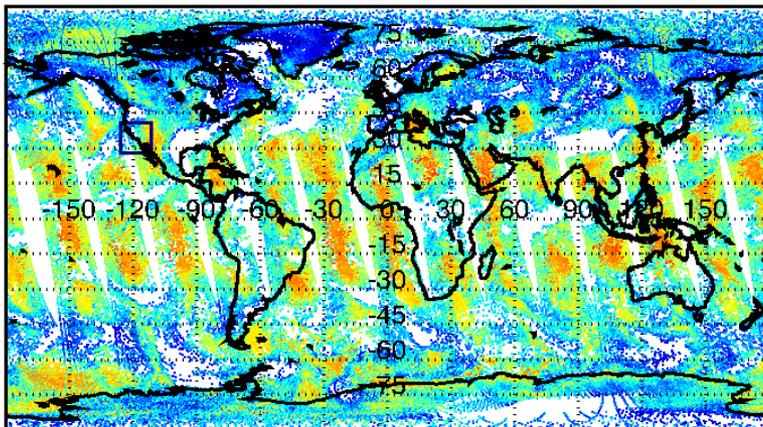
Major sensitivity: 200-550 hPa

DOF 20151024



DOF

DOF 20151024

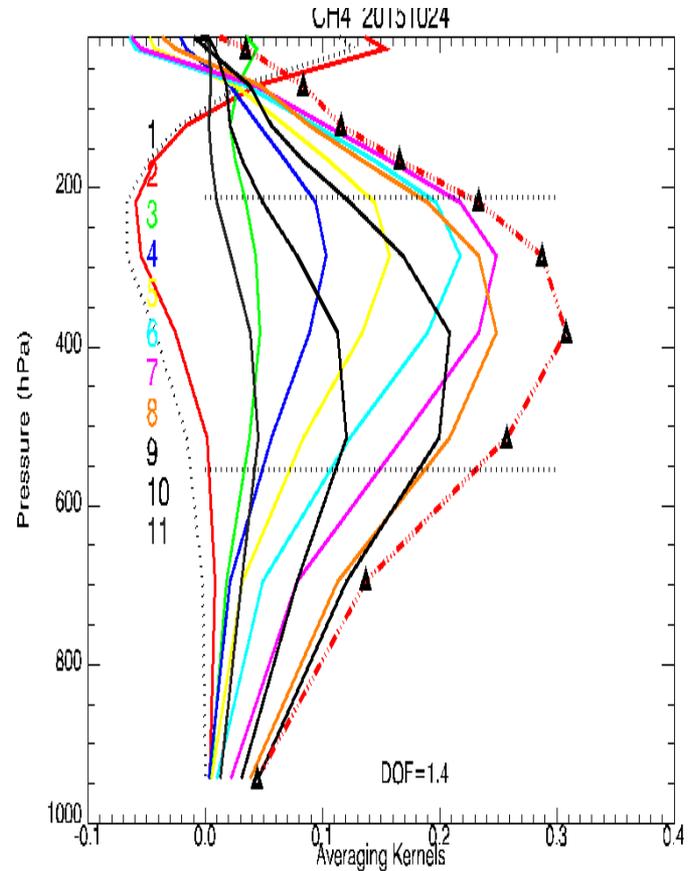


DOF

0.4 0.6 0.8 1.0 1.1 1.3 1.5

current

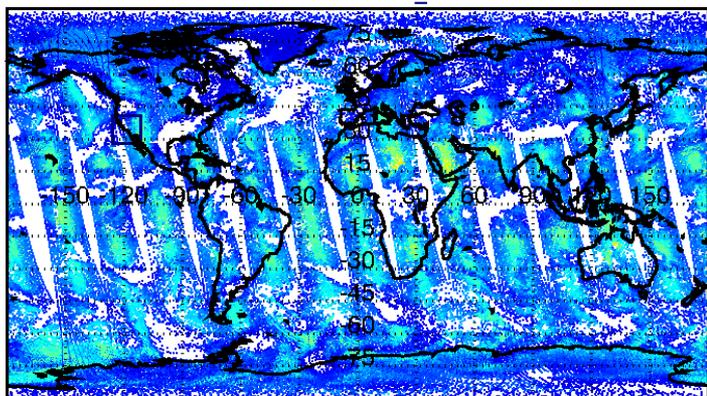
after



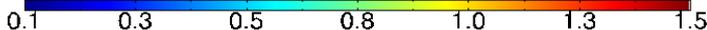
DOFs increase after the re-selection of channels

Averaging Kernels and DOFs – CO₂

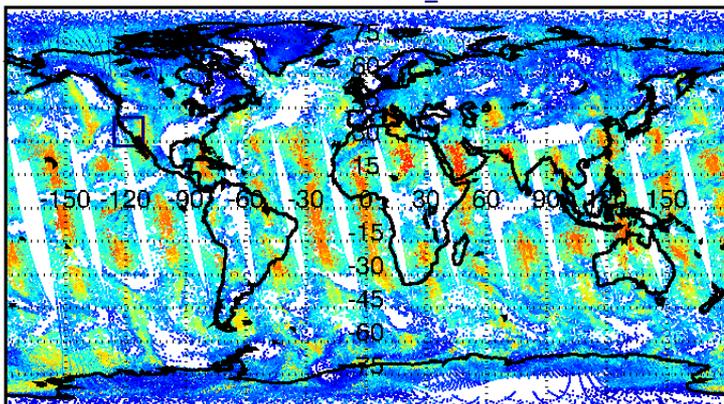
DOF 20151024_co2



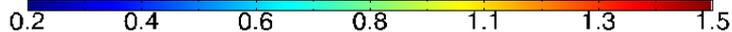
DOF



DOF 20151024_co2

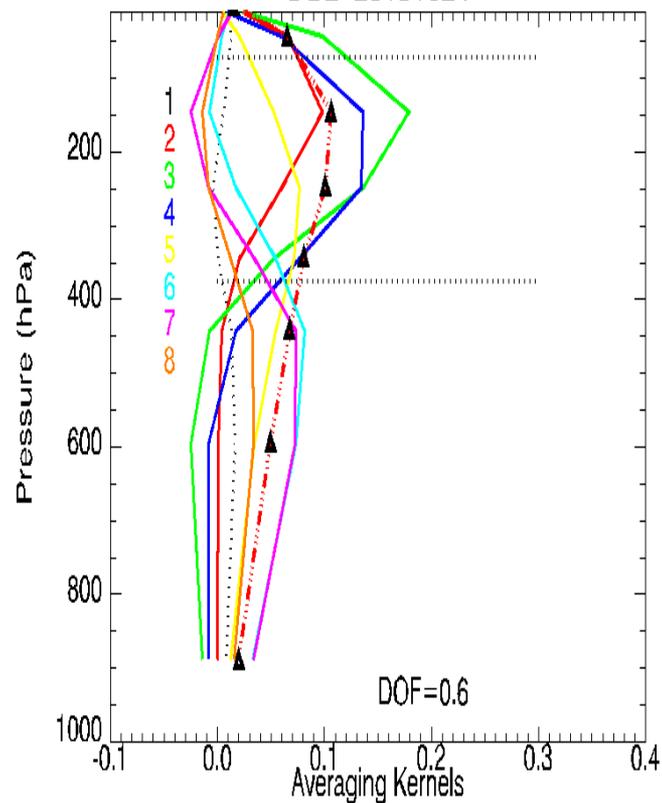


DOF



More works need to be done for CO₂

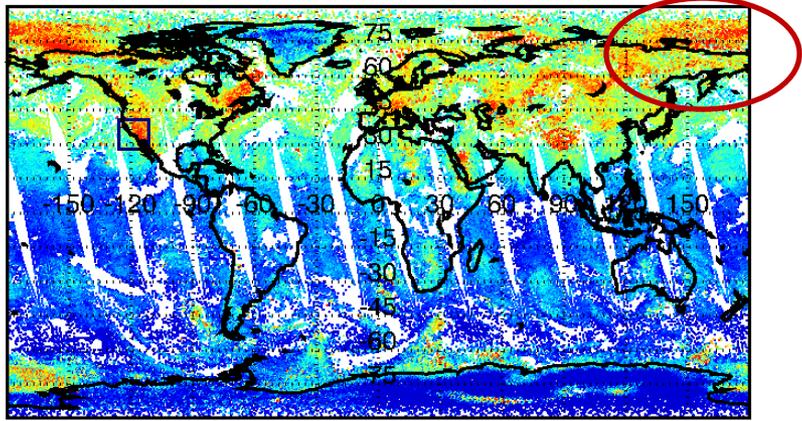
CO2 20151024



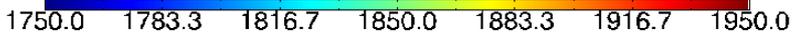
Changes of CH₄ Distribution after the re-selection of channels and update of QC (+10 ppb)

current

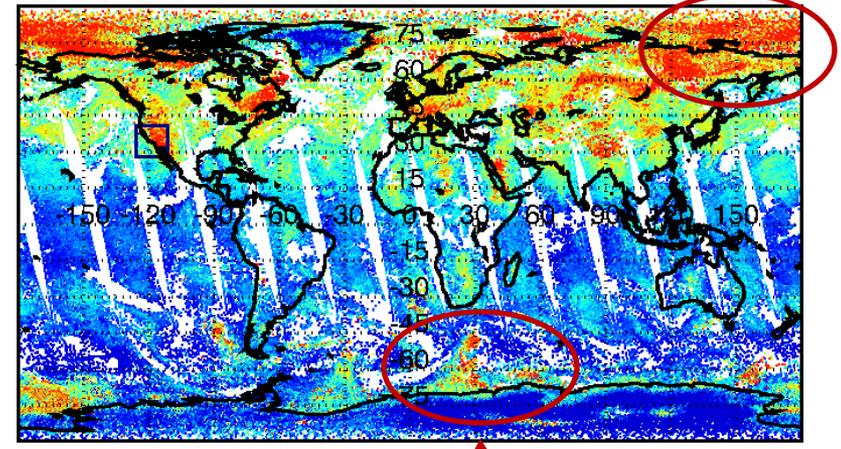
CH4 515.720 20151023



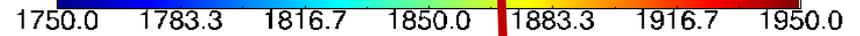
ppb



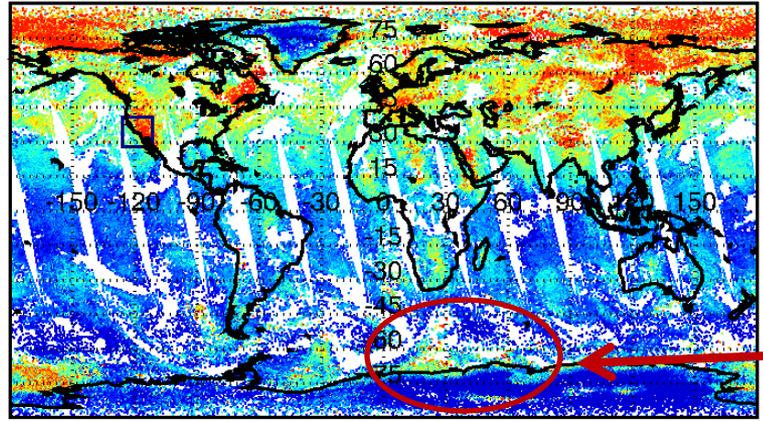
CH4 515.720 20151023



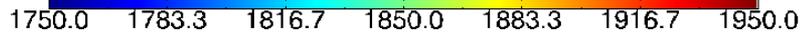
ppb



CH4 515.720 20151023



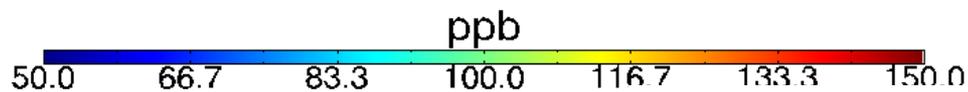
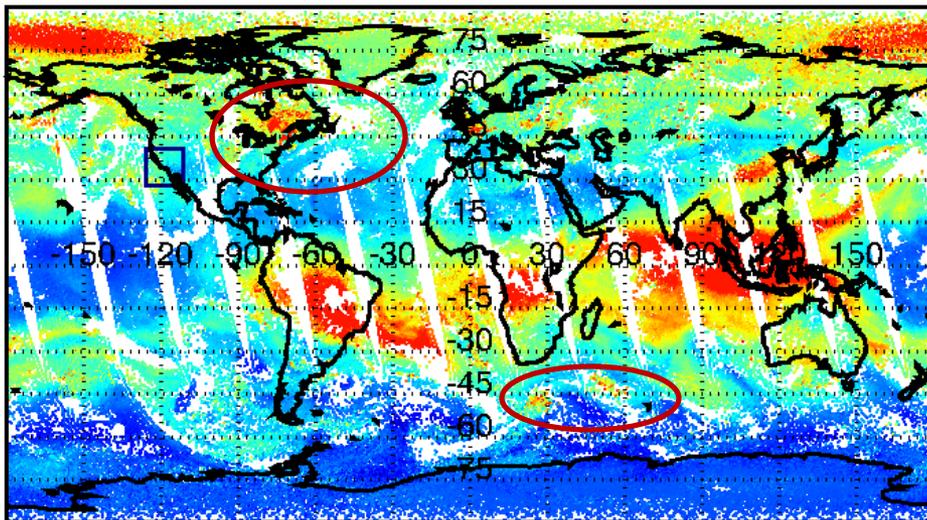
ppb



after the re-selection of channels

New QC

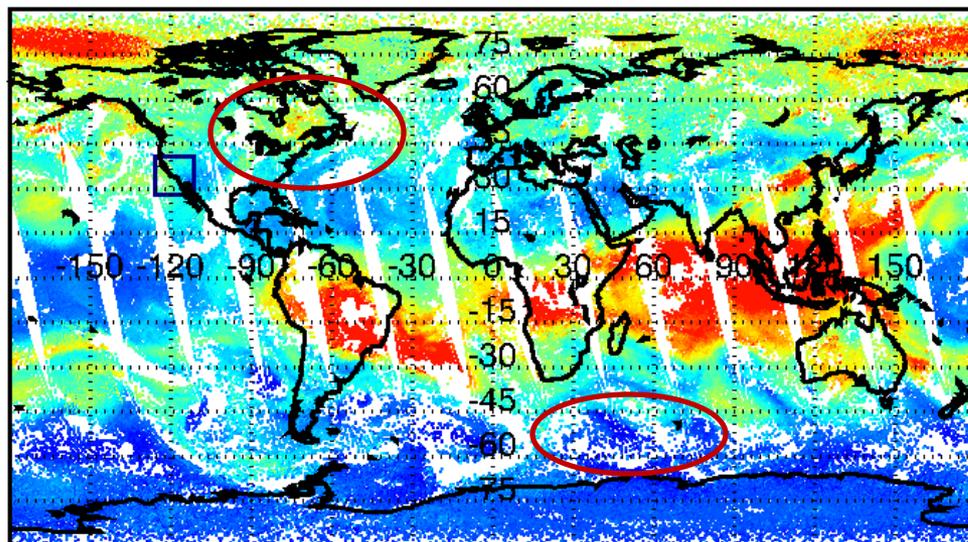
CO 515.720 20151023



**Change of CO distribution
after re-selection of
channels and update of QC**

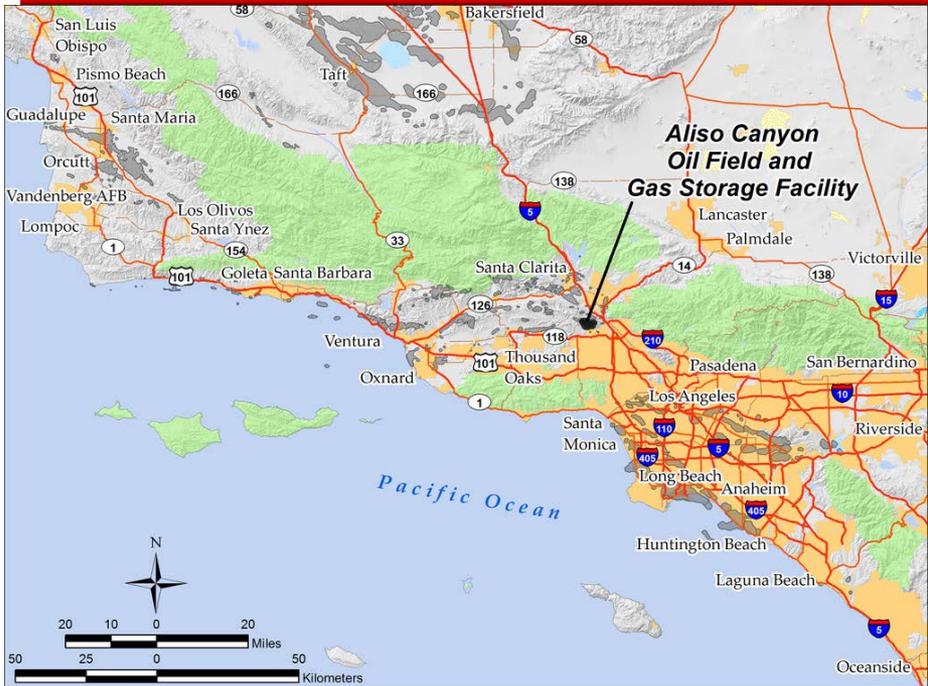
CO 515.720 20151023

After



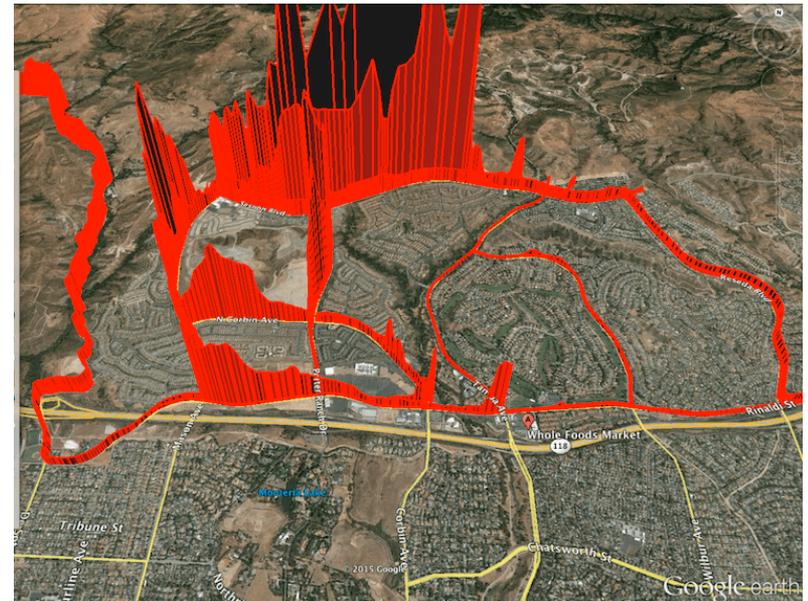


Aliso Canyon Gas Leakage (10/23/2015- 2/18/2016)



CH₄ increase from ground measurement

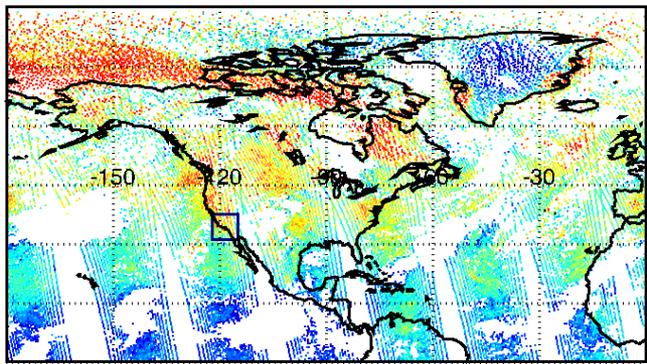
- Historically largest gas leakage -- a good case to test if NUCAPS can capture this leakage;
- CrIS retrievals for two days before the leakage (10/23/2015) and 1 week after have been made in this analysis;





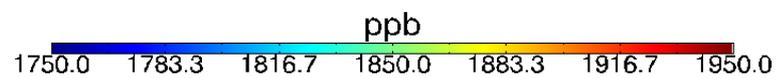
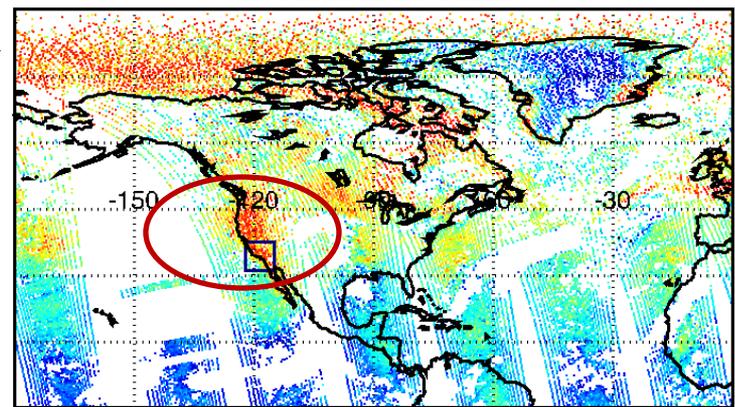
CH₄ from Ascending Node – enhanced CH₄ started in Oct.22,2015

CH4 515.720 20151021

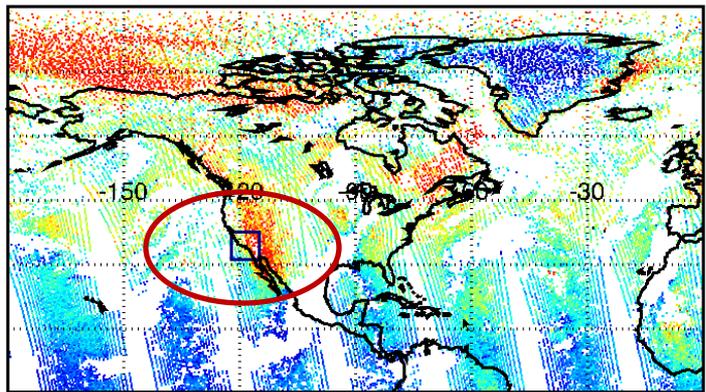


Unknown sources

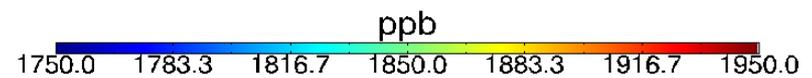
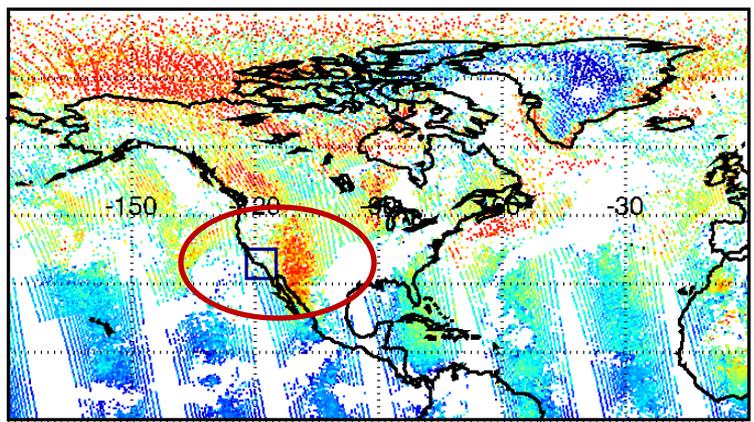
CH4 515.720 20151022



CH4 515.720 20151023



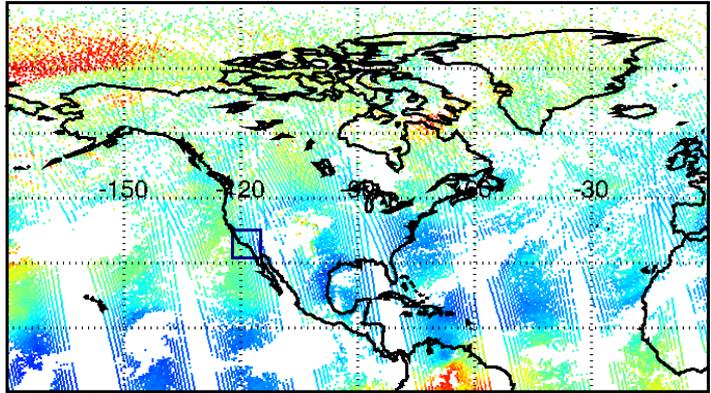
CH4 515.720 20151024





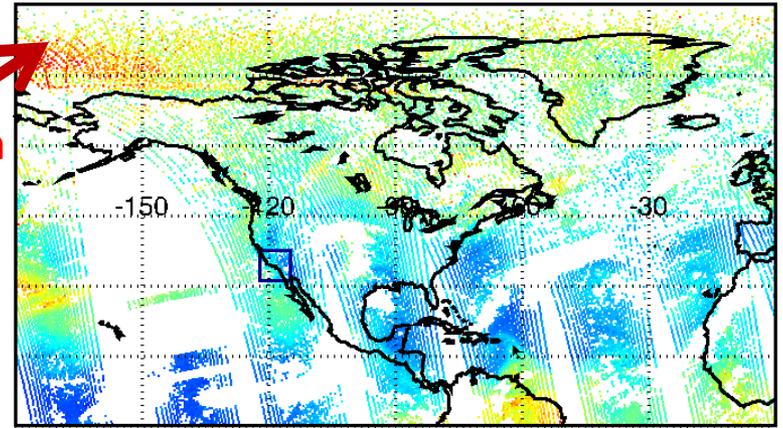
CO from Ascending Node – similar transport of CO, but sources are unknown

CO 515.720 20151021

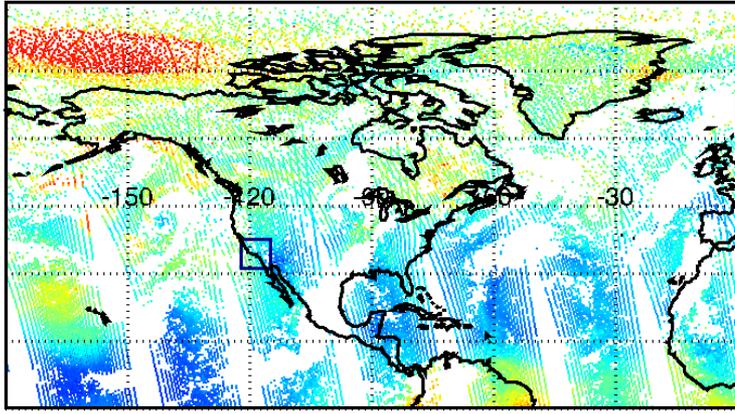


CO 515.720 20151022

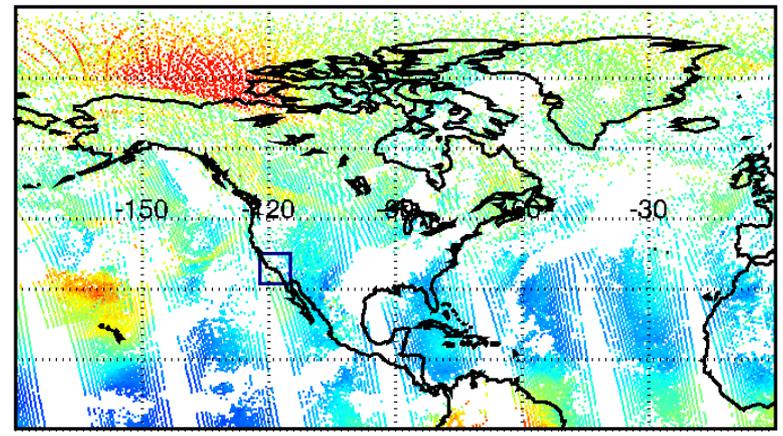
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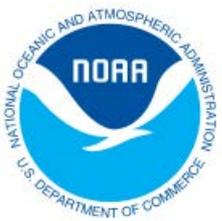


CO 515.720 20151023



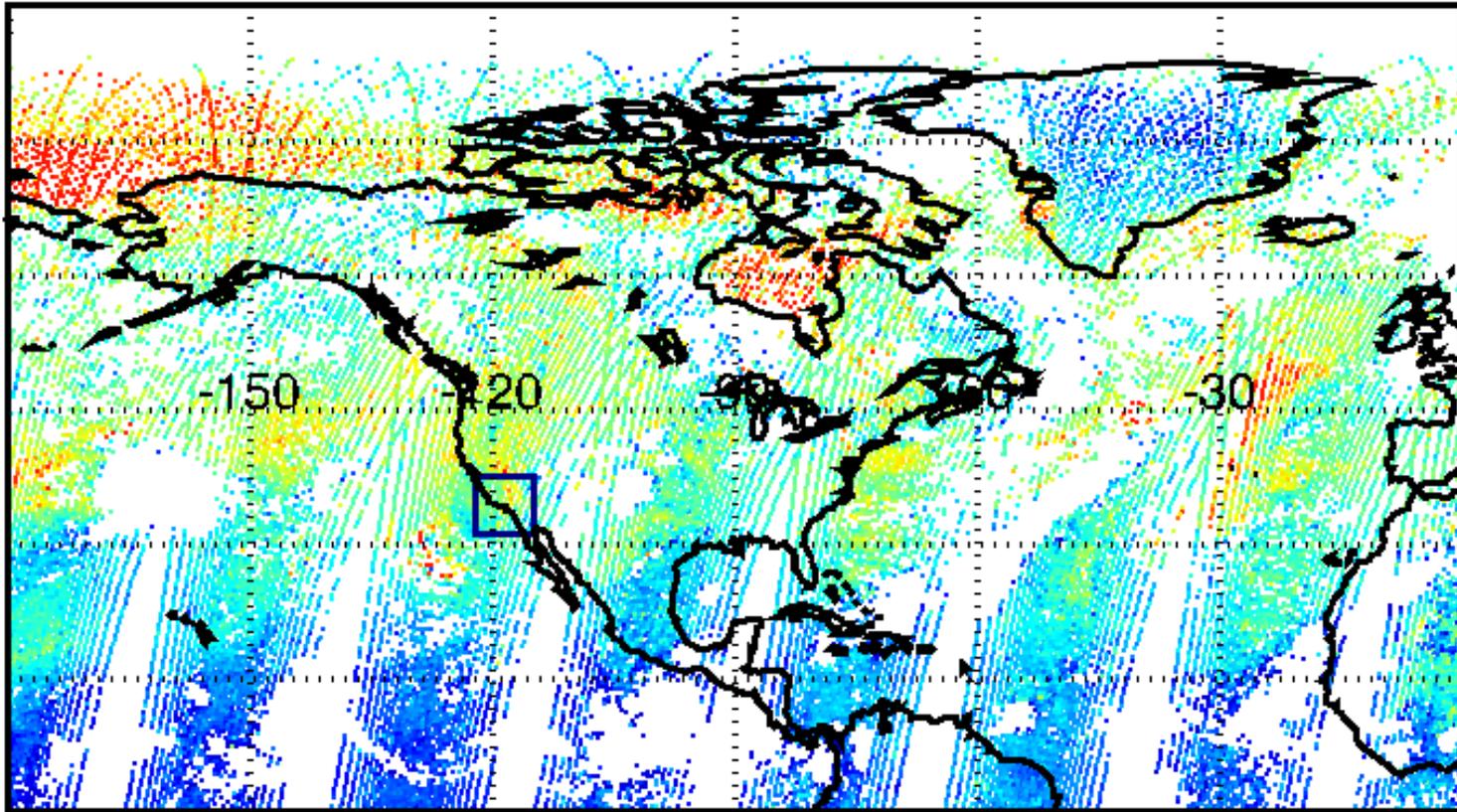
CO 515.720 20151024



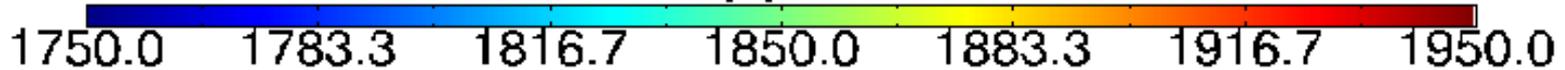


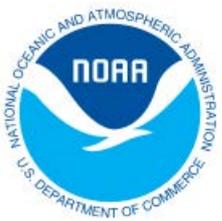
CH₄ from 10/21 – 10/29/2015

CH4 515.720 20151021



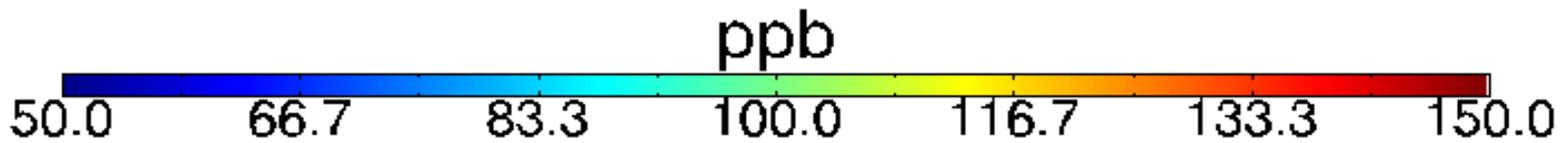
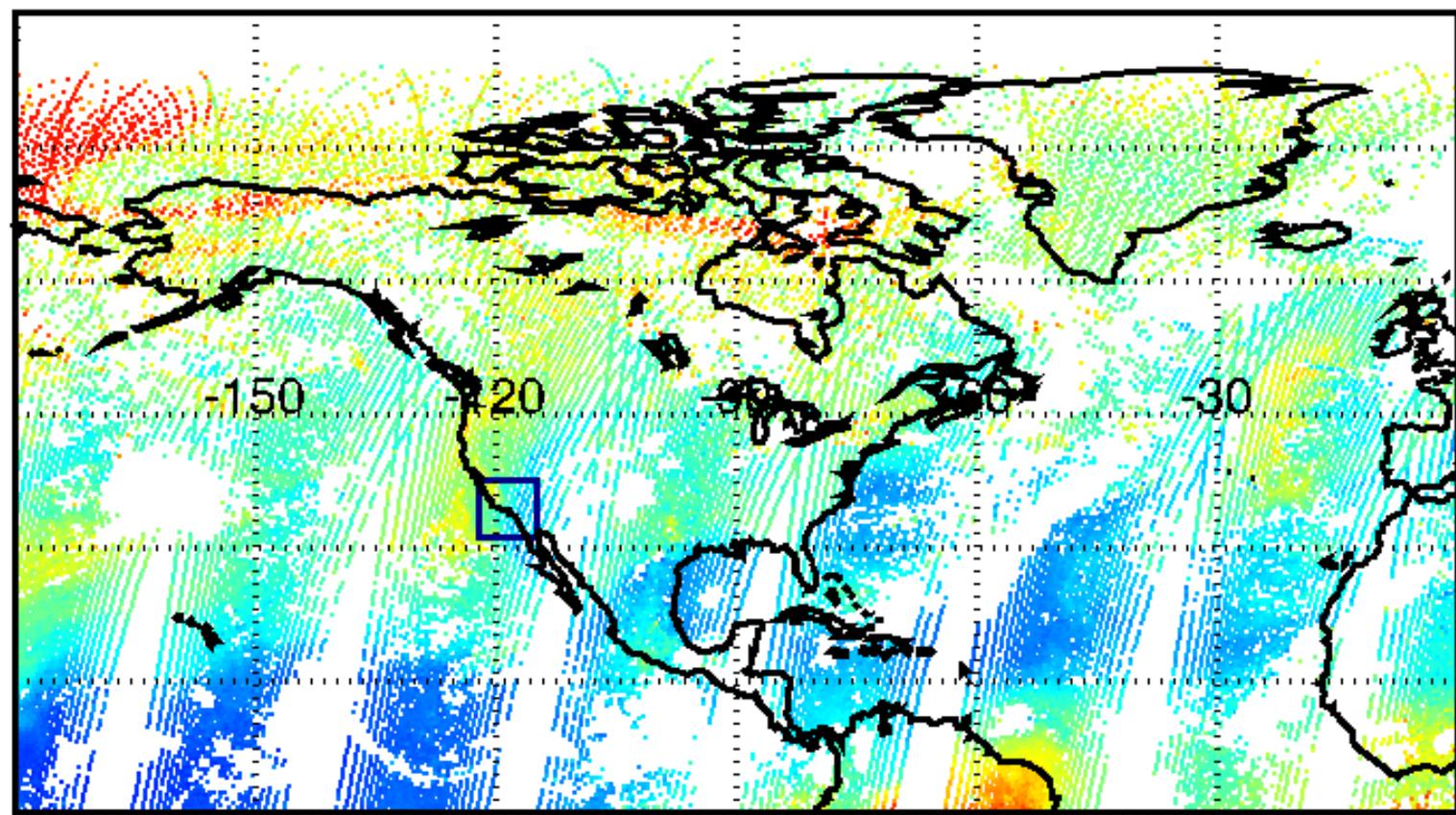
ppb





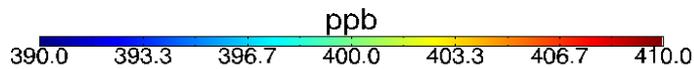
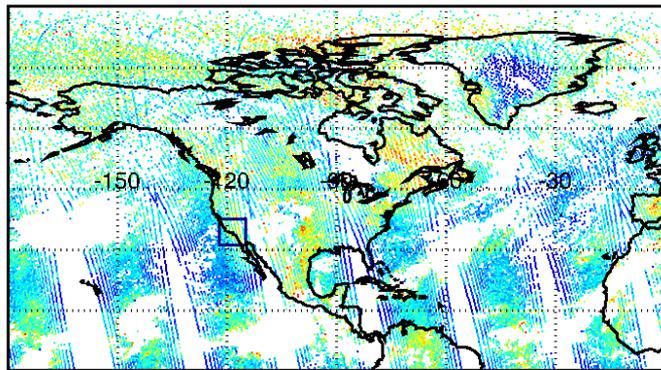
CO from 10/21 – 10/29/2015

CO 515.720 20151021

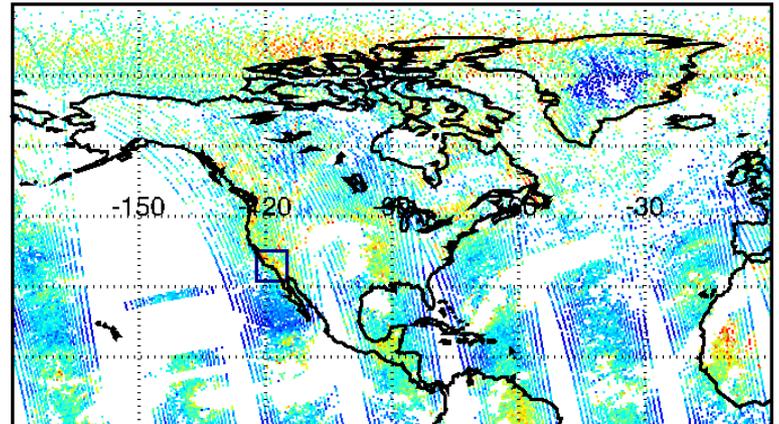


CO₂ from Ascending Node

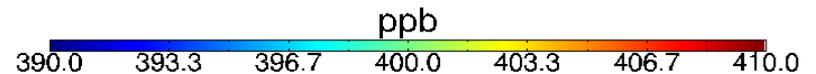
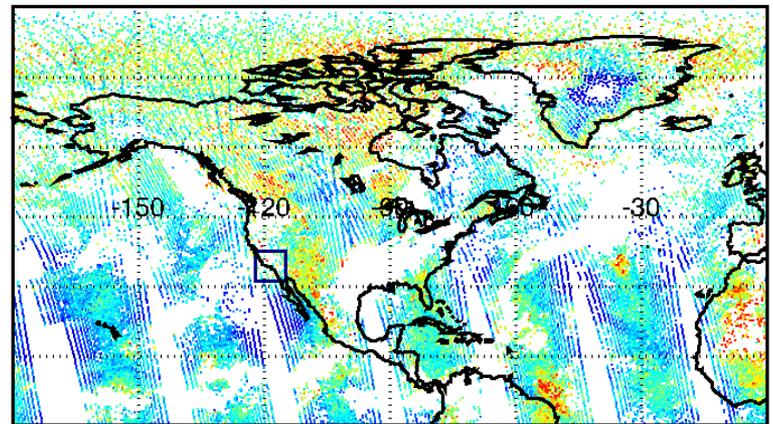
CO2 20151021

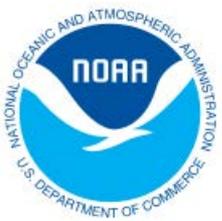


CO2 20151022



CO2 20151024





Summary and Future Works

1. CrIS full spectrum data can be used to retrieve trace gases with similar DOFs as AIRS and IASI, with its major sensitivity in the *mid-upper troposphere*; however, to combine these three sensors to make a consistent product from 2002 to beyond need more works (*larger disparity existed in the Arctic between AIRS and IASI retrievals*);
2. It is promising to use CrIS full Spectrum data to detect the leakage of CH₄ during the historically largest Gas leakage from **Aliso Canyon Oil Field and Gas Storage Facility in 2015**. **However**, more checks to other possible uncertainties need to be done (cloud-clearing, transport);
3. Preliminary improvements in channels selection and QC have been made, which show positive impacts to the retrieval products;
4. Validation is a key step but hampered due to lack of the measurements of trace gases profiles. Improvement to QC will be one focus of future works.

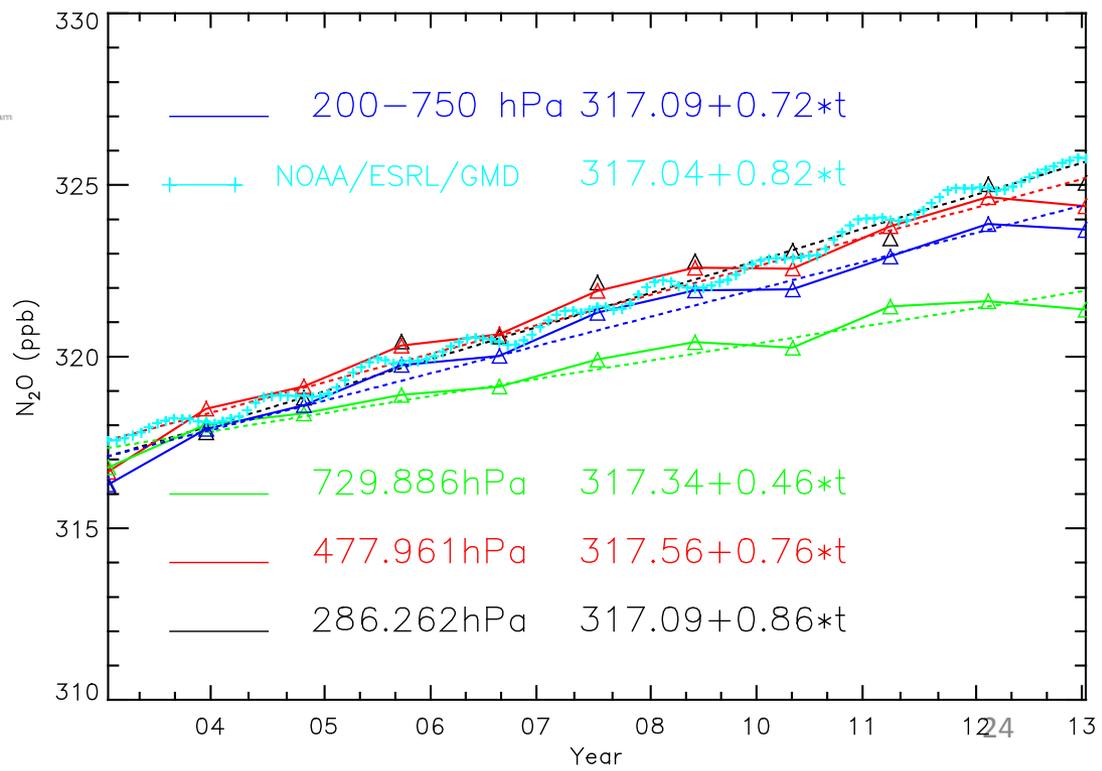
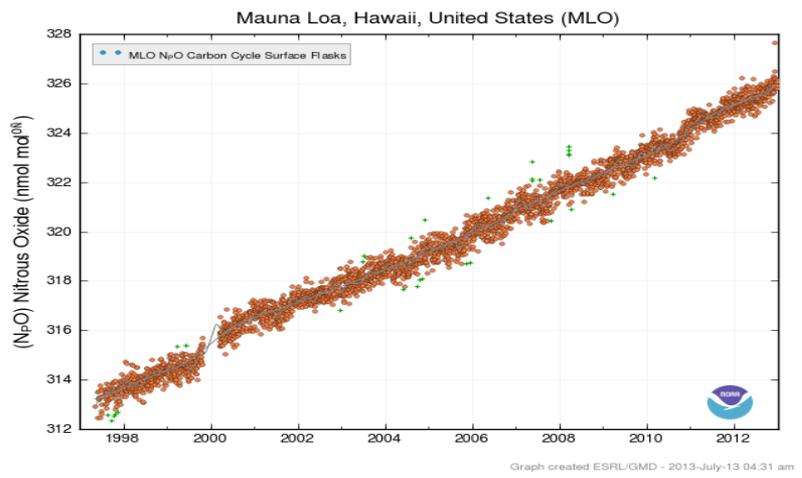


Questions/Suggestions





3. Monitoring of N₂O trend using AIRS



Xiong, X. et al., 2014, Retrieval of Nitrous Oxide from Atmospheric Infrared Sounder: Characterization and Validation, JGR-atmosphere, 119, doi:10.1002/2013JD021406.

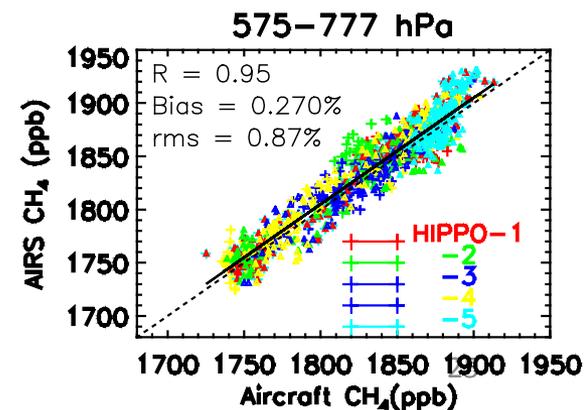
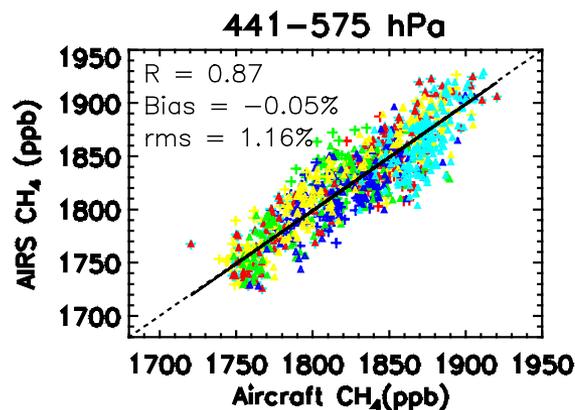
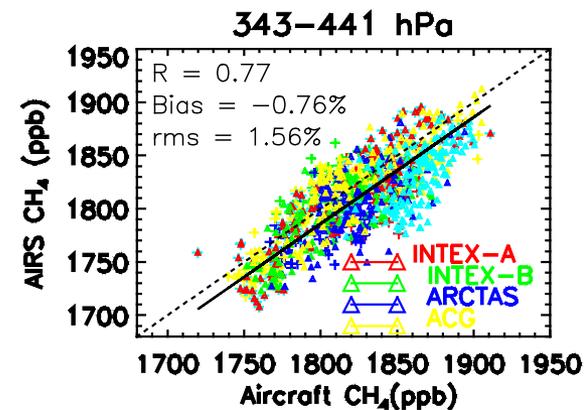
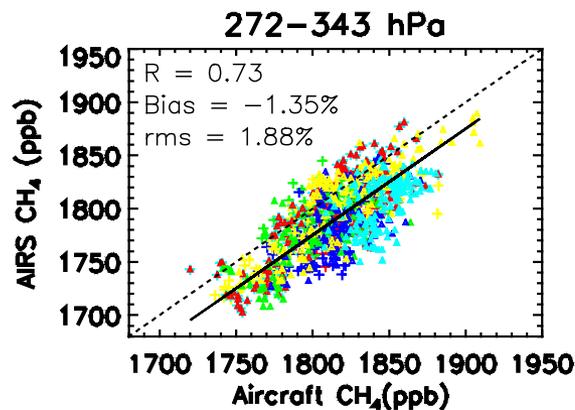
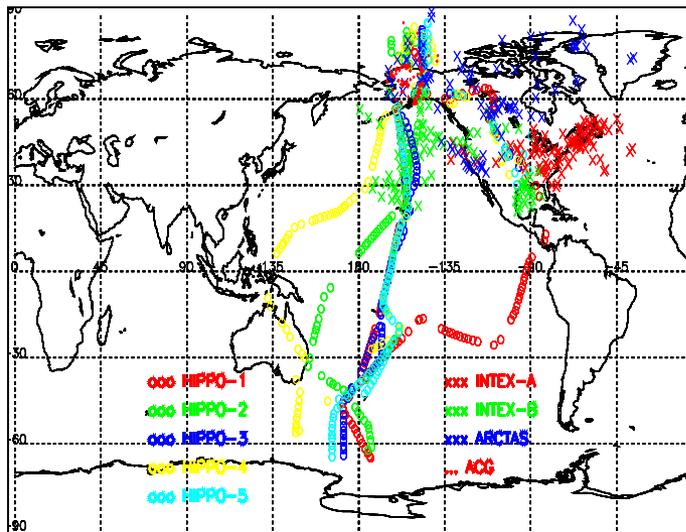


Validation: one Key step to evaluate the trace gases products



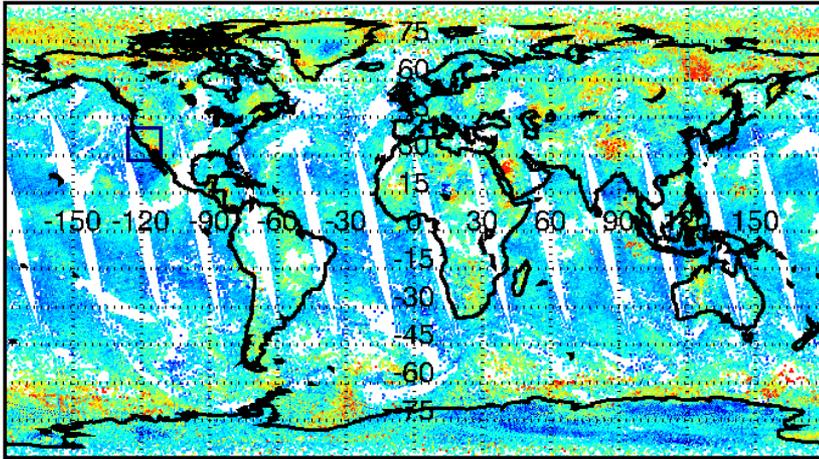
AIRS-V6 CH₄

Locations of Validation Profiles

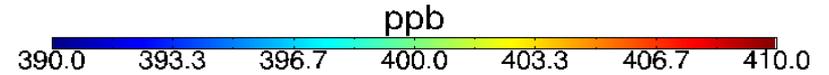
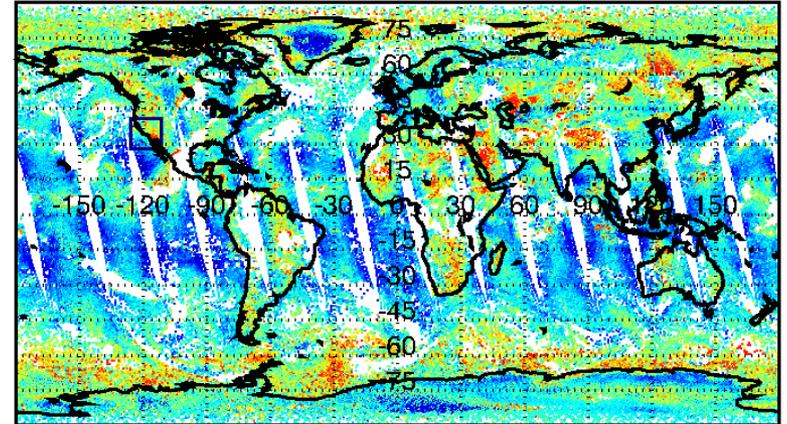


Change of CO₂

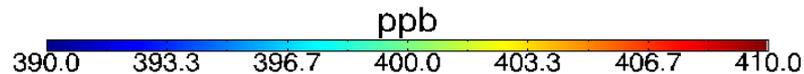
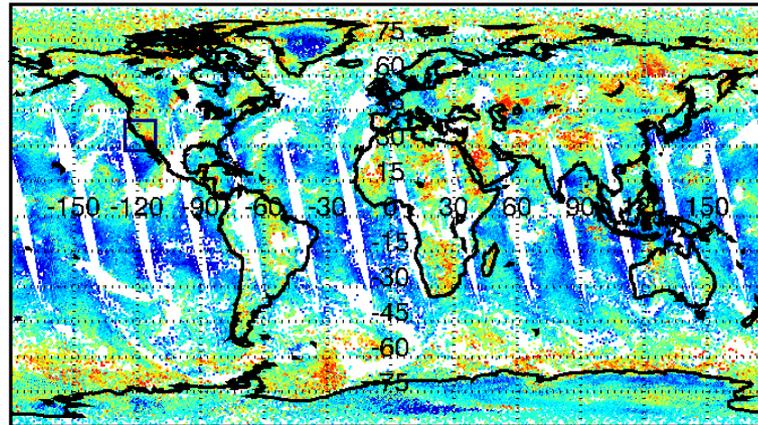
CO2 20151023



CO2 20151023



CO2 20151023

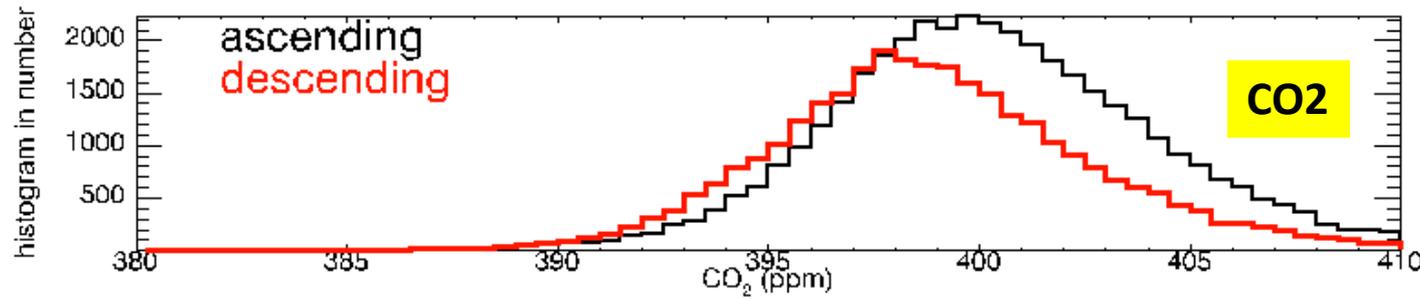
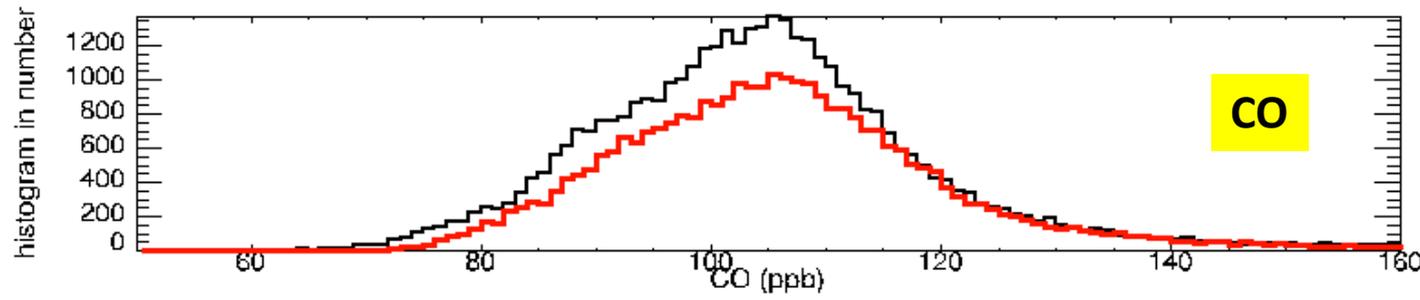
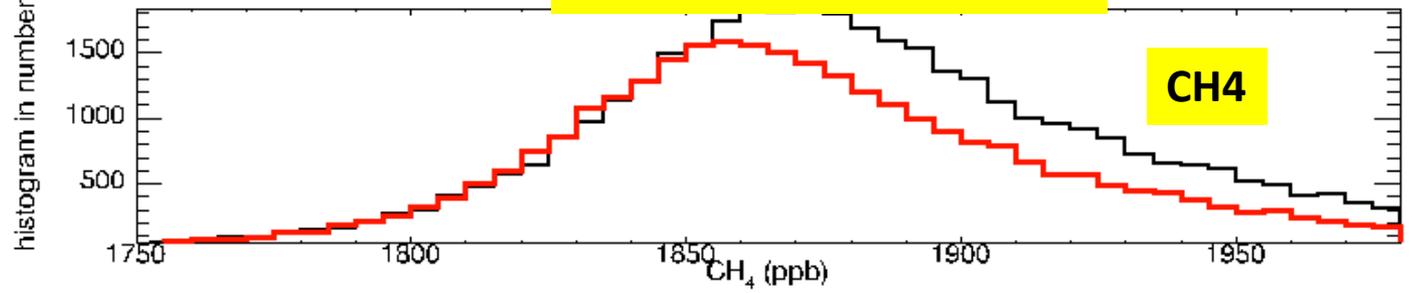


More works need to be done for CO₂



Day-night Difference

20151024, Latitude > 30 °



Daytime CH4 and CO2 are larger than night time, but not CO



The NOAA Operational High-Resolution CrIS Channel Selection: Impacts On NUCAPS Trace Gas Retrievals

Jonathan W. Smith¹

Antonia Gambacorta¹, Chris Barnett¹, Nadia Smith¹,
Brad Pierce², Walter Wolf², Mitch Goldberg³

Thursday, August 11, 2016

¹ Science and Technology Corporation

² NOAA/NESDIS STAR

³ NOAA JPSS Program

Introduction

- **The Cross-Track Infrared Sounder (CrIS)** is a Fourier spectrometer covering the longwave (655-1095 cm⁻¹, “LW”), midwave (1210-1750 cm⁻¹, “MW”), and shortwave (2155-2550 cm⁻¹, “SW”) infrared spectral regions.
- **NUCAPS Phase I, II and III operations:**
 - Maximum geometrical path difference $L = 0.8$ cm (LW), 0.4 cm (MW) and 0.2 cm (SW)
 - Nyquist spectral sampling ($1/2L$): 0.625 cm⁻¹, 1.25 cm⁻¹ and 2.5 cm⁻¹
 - Total number of channels: 1305
- **NUCAPS Phase IV operations:**
 - Maximum geometrical path difference $L = 0.8$ cm in all three bands
 - Nyquist spectral sampling ($1/2L$): 0.625 cm⁻¹ in all three bands
 - Total number of channels: 2211 + 12 guard channels
- **Motivation for a channel selection:**
 - Assimilation of full radiance spectra is not computationally efficient for near real time data processing.
 - A channel selection is required to expedite both data assimilation and retrieval processes.
 - Attention must be paid to minimizing the loss of information content such that the final retrieval quality is not deteriorated.



Channel Selection Methods: Two Schools of Thought



Jacobians or Physical method

- physically-based methodology
 - channels are selected upon their spectral properties
 - each atmospheric species, we perform a spectral sensitivity analysis and retain the spectrally purest channels.
- Other than spectral purity, priority is given to:
 - vertical sensitivity properties,
 - instrumental noise
 - RTA errors.
- Jacobian method is suited for sequential steps retrieval methodologies
- works for simultaneous optimal estimation retrieval techniques.

Rodgers method

- follows a statistical iterative approach
 - channels are incrementally added after being tested against an increase in degree of freedom.
- This methodology is suited for simultaneous optimal estimation retrieval techniques.

Both methods:

- a constant channel selection is normally used
- derived as an average from multiple optimal selections computed over different geophysical regimes (polar, mid latitudes, tropical, land, ocean, desert).

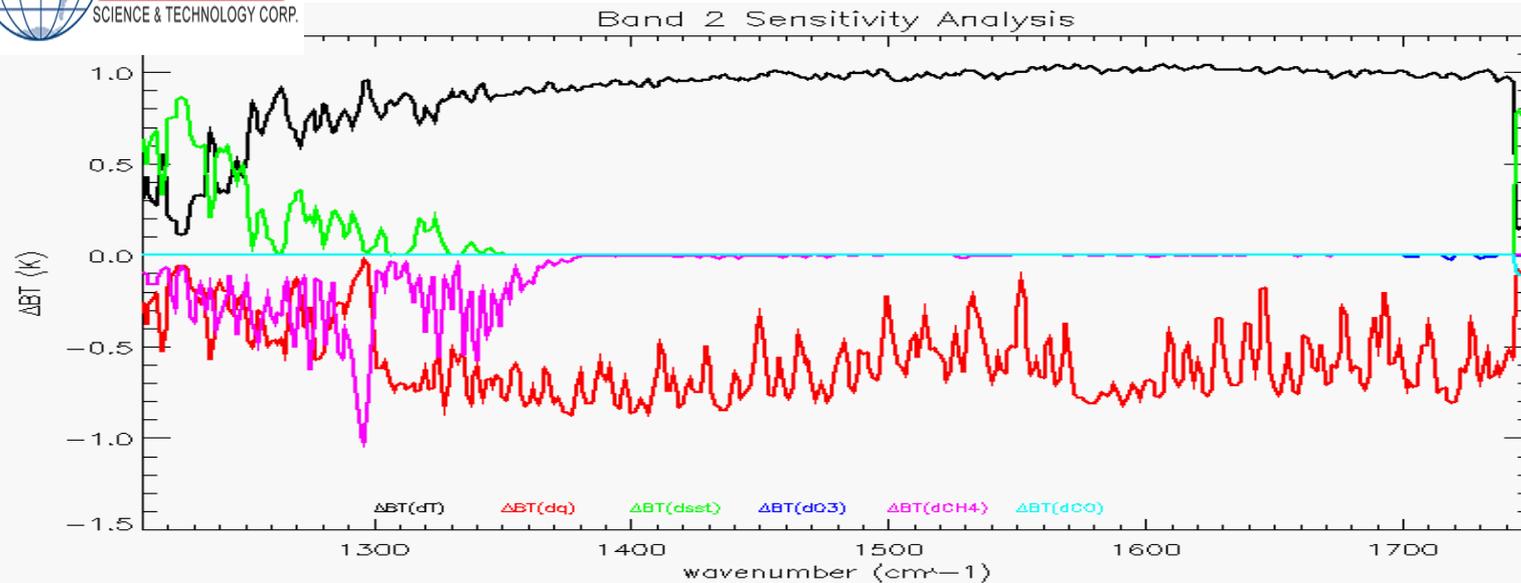
Why do we use the Jacobians method?

- NUCAPS required all sky operational products:
 - Cloud cleared radiances
 - Cloud top pressure and fraction
 - Surface temperature
 - Vertical temperature
 - Water vapor
 - Trace gases: O_3 , CH_4 , CO , CO_2 , SO_2 , N_2O , HNO_3
 - Future candidates:
 - NH_3 (Ammonia), HCO_2H (Formic Acid), CH_3COONO_2 (“PAN”)
- Most channels are largely contaminated by clouds, temperature and water vapor signals.
- A “**trace gas**” is a gas which makes up less than 1% of the volume of the Earth’s atmosphere.
- Trace gas radiative signals are in the range of the instrument noise.
- *Answer: Spectral purity combined with a sequential retrieval approach is essential for the retrieval of the full list of NUCAPS products, particularly for trace gases, under all sky conditions.*
- In depth description available in:

A.Gambacorta and C.Barnet, Methodology and information content of the NOAA NESDIS operational channel selection for the Cross-Track Infrared Sounder (CrIS), IEEE Transaction on geoscience and remote sensing.

Vol. 51, No. 6, 2013. DOI: 10.1109/TGRS.2012.2220369

Spectral Purity Analysis (band 2)



SST	1K
T	1K
H2O	10%
O3	10%
CH4	2%
CO	1%

Brightness temperature difference (ΔBT) terms represent the sensitivity of each channel to a given perturbation species and are indicative of the degree of “spectral purity” of each channel.

- Perturb these gases (left column) by that amount or percentage (right column), you obtain a perturbation (ΔBT) in brightness temperature (figure above).
- The magnitude of ΔBT describes how sensitive a channel is to the perturbed species.
- You select those channels that tend to be sensitive to only your species of interest with minimum interference from the other species.
- You still account for the residual interference as an error term in the retrieval measurement error covariance.

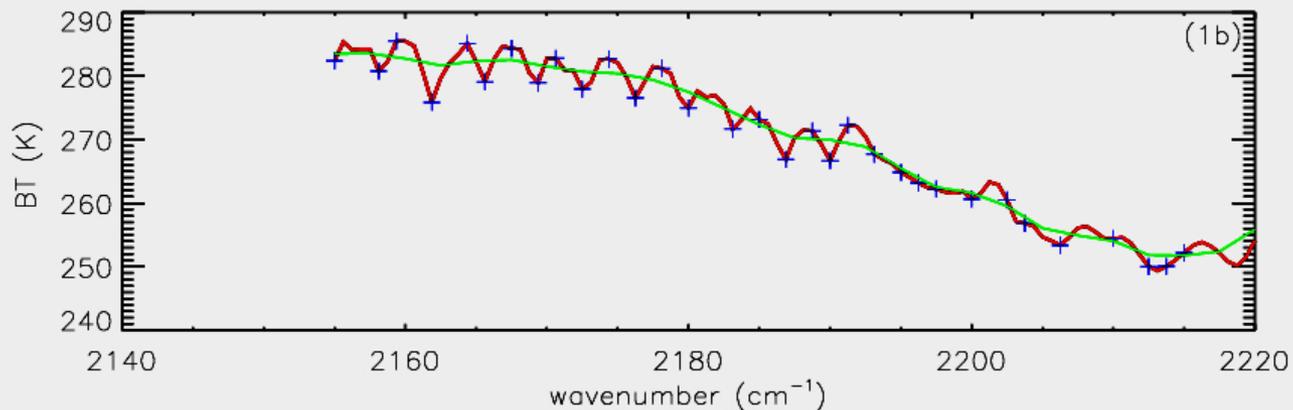
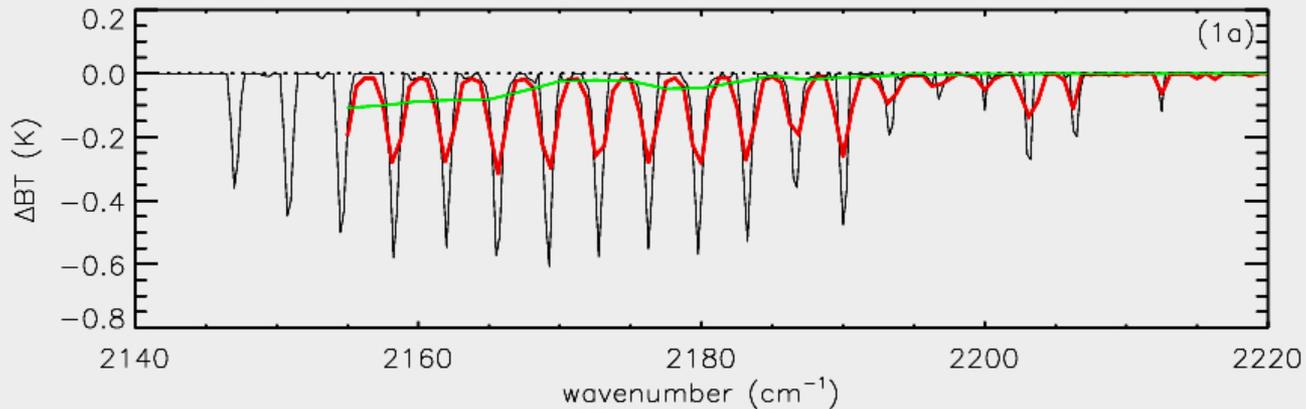


CO Channel Selection

A test case study from the 1 May
2016 (Ft. McMurray, Alberta Fire
Case)

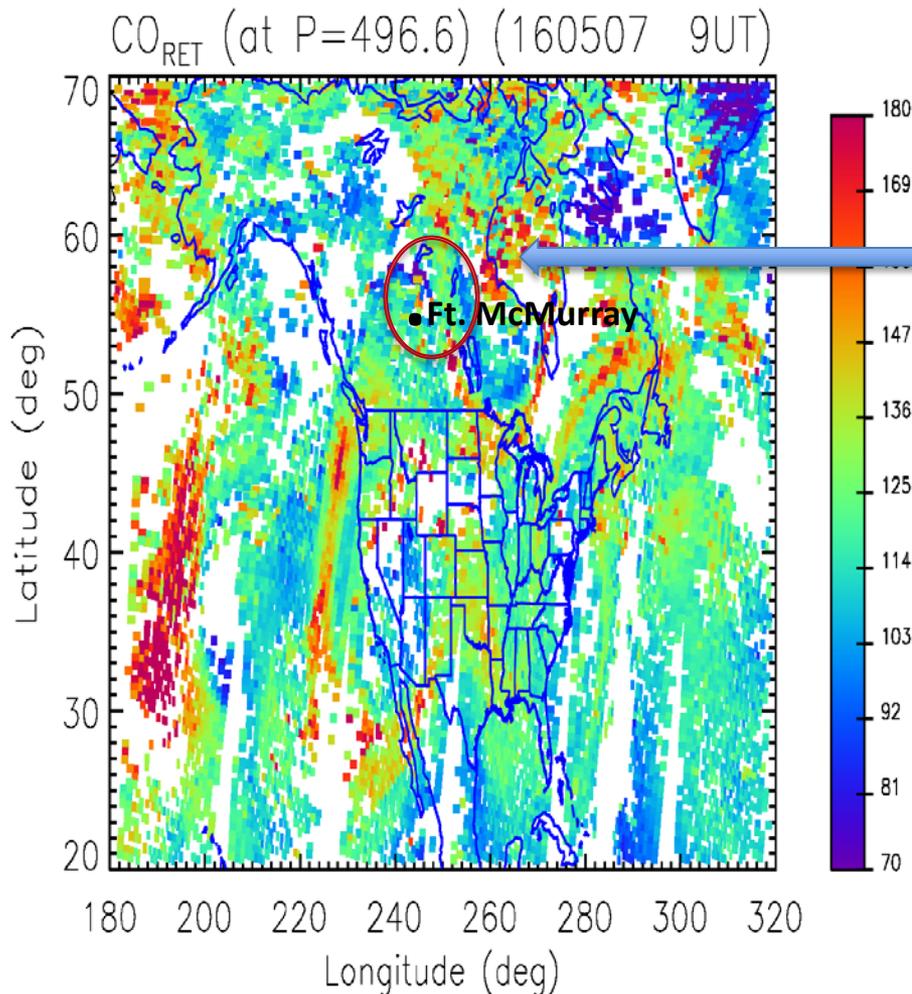
Sensitivity Analysis to 1% CO perturbation

2.5cm⁻¹ 0.625 cm⁻¹ 0.25cm⁻¹



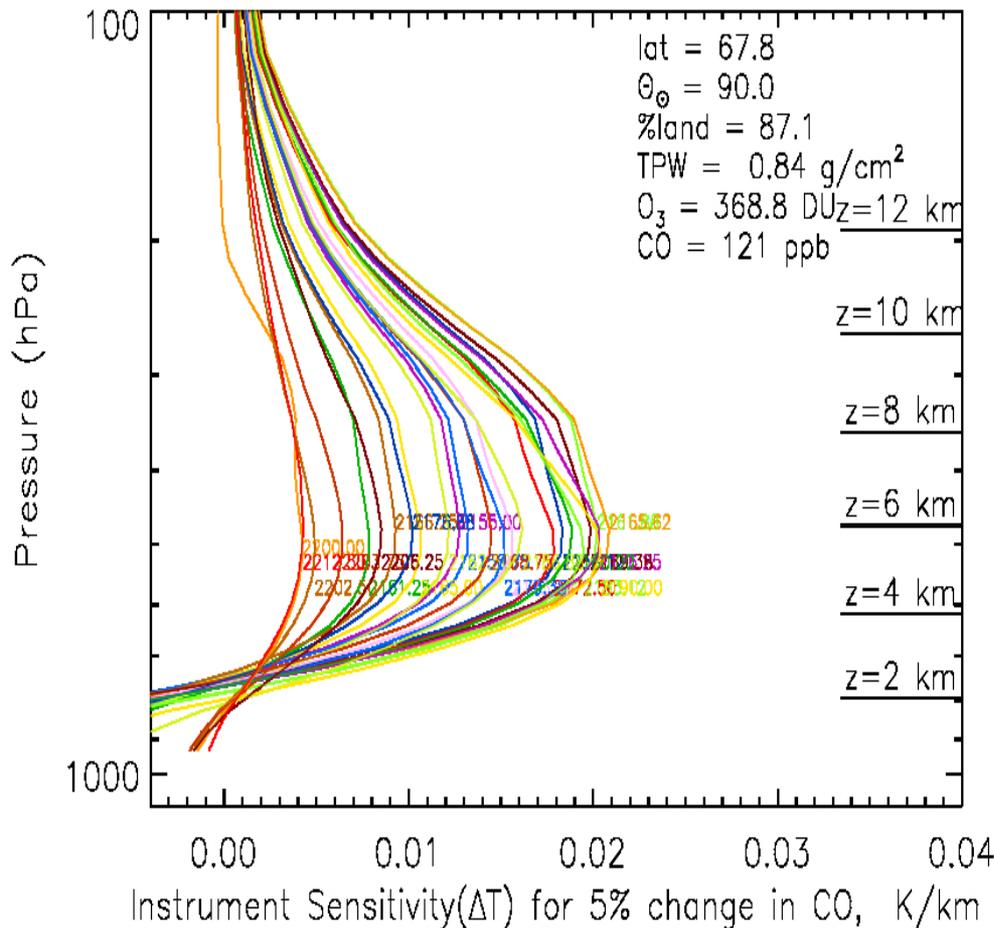
- Why you are showing the CO case?
 - Only when switched to high spectral resolution, CrIS spectrum (red curve, bottom part) shows the distinctive signature of CO absorption (red and black curve, top figure).
 - Blue cross symbols: CO high resolution channel selection.

Fire Case Study



- 7 May 2016 NUCAPS retrieval over North America
- Highlighting the Ft. McMurray, Alberta Fire
- Pressure level: 496.62 hPa
- 120+ ppbv over fire

CO channel selection for Ft. McMurray, Alberta fire case



- The selection was made on multiple geophysical regimes (polar, mid-latitude, tropics, and fire) to
 - ensure global applicability.
 - examine polluted vs relatively clear regimes.
- We are testing CO selection over focus areas to ensure global optimality and to serve users needs



NUCAPS High Res Trace Gas Product Evaluation



- Initiative is based on 2 recently funded JPSS proposals.
 1. Greg Frost: “Understanding emissions and tropospheric chemistry using NUCAPS and VIIRS”
 2. Brad Pierce: “High Resolution Trajectory-Based Smoke Forecasts using VIIRS Aerosol Optical Depth and NUCAPS Carbon Monoxide Retrievals “
- Models are used to interpolate the sparse aircraft observations to the satellite temporal, spatial, and vertical sampling characteristics for detailed validation
- NUCAPS (and AOD f/ VIIRS) will be used within IDEA (Infusing Satellite Data into Envir. AQ Applications)

<http://www.star.nesdis.noaa.gov/smcd/spb/aq/>



Future Work:

Maintenance and Optimization

- *We will re optimize and deliver the channel selection once the new version of the RTA is delivered*
- Expected improvements
 - NON LTE and water vapor regions
- Continue to run NUCAPS various global cases
- Channel selection for IASI
- Continue to ensure that users obtain the best products



Acknowledgements



Walter Wolf

Larabee Strow

Tom King

Lihang Zhou



Lessons from the Field: Tailoring NUCAPS trace gas products to user needs

Nadia Smith

In collaboration with:

Chris Barnet, Antonia Gambacorta (STC)
Greg Frost, Stuart McKeen (NOAA/ESRL/CSD)
Brad Pierce (NOAA/NESDIS/STAR)
Van Dang, Brian Kahn (NASA/JPL),
Colby Francoeur, Jonathan Smith (STC), etc.

STAR JPSS 2016 Annual Science Team Meeting 8–12 August, NCWCP, College Park, MD

Doing Science within an Operational Framework

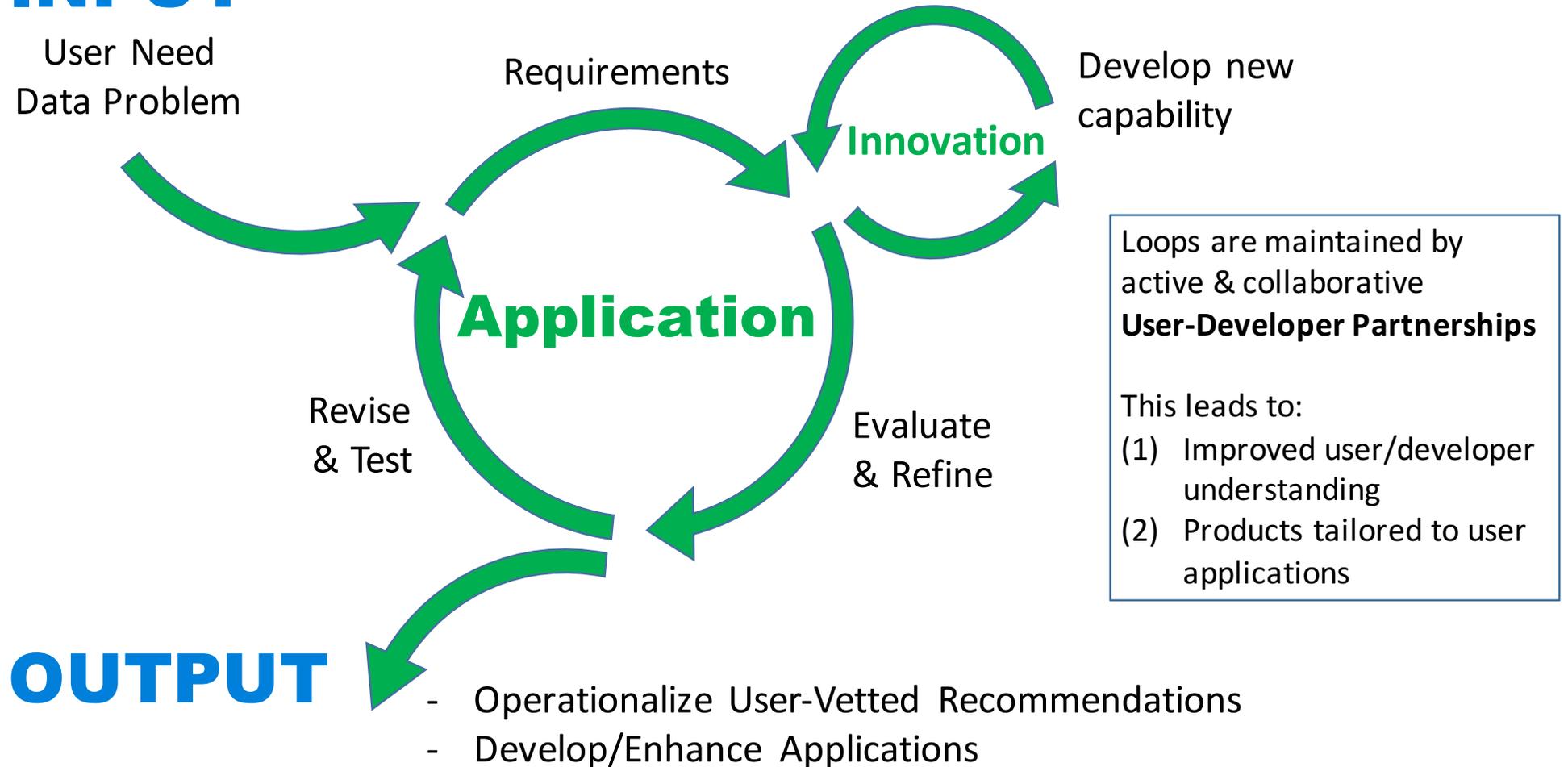
- Who cares about this problem?
- Can we find a **robust, stable** scientifically credible solution?
- Is the solution **operationally viable**, i.e. cost effective?

Sounding Initiative: A User-Oriented Approach to Development

See NOAA Test Bed Concept in Ralph et al. 2013 BAMS

INPUT

User Need
Data Problem



Loops are maintained by active & collaborative **User-Developer Partnerships**

This leads to:

- (1) Improved user/developer understanding
- (2) Products tailored to user applications

NOAA PGRR Sounding Initiative: NUCAPS CO and CH4

INPUT

Need for Averaging Kernels (AK)
and Quality Control (QC)

What are the fundamental, physical limits?

What are things we can change & tailor?

Application

Generate
experimental
products

Try, Test, Evaluate
Revise, Refine

STC NUCAPS Team in
collaboration with:

NESDIS/STAR
NOAA/ESRL/CSD
CIRES + CIMSS

Working with multiple users
in multiple applications to
ensure that everyone
benefits

OUTPUT

Present NOAA/STAR with fully vetted recommendations and solutions

Operationalize AK product and QC changes

Auxiliary Data Distribution – Averaging Kernels

Our primary partners in this initiative:

Brad Pierce (PGRR PI): High resolution trajectory-based smoke forecasts

Greg Frost (PGRR PI): Understanding emissions and tropospheric chemistry using NUCAPS and VIIRS

- At present, the NUCAPS trace gas user community is largely made up of scientists, not forecasters or air quality monitoring agencies yet
- Users have need for Auxiliary products that are not available in Operational CLASS product to cast light on the quality of products and aid in evaluation/characterization – Specifically the Averaging Kernels (AK) and Degrees of Freedom (DOF), both metrics of uncertainty and information content
- We developed the capability to distribute AK and DOF to users in netCDF files.

NUCAPS stores all the building blocks with which to calculate AK and DOF in binary files (that are currently discarded for operational products, but available when run off-line)

For each granule of measurement and a target parameter (e.g., CO, CH₄), we generate a netCDF file that contains all the relevant retrieval and auxiliary information that enables users to do meaningful characterization.

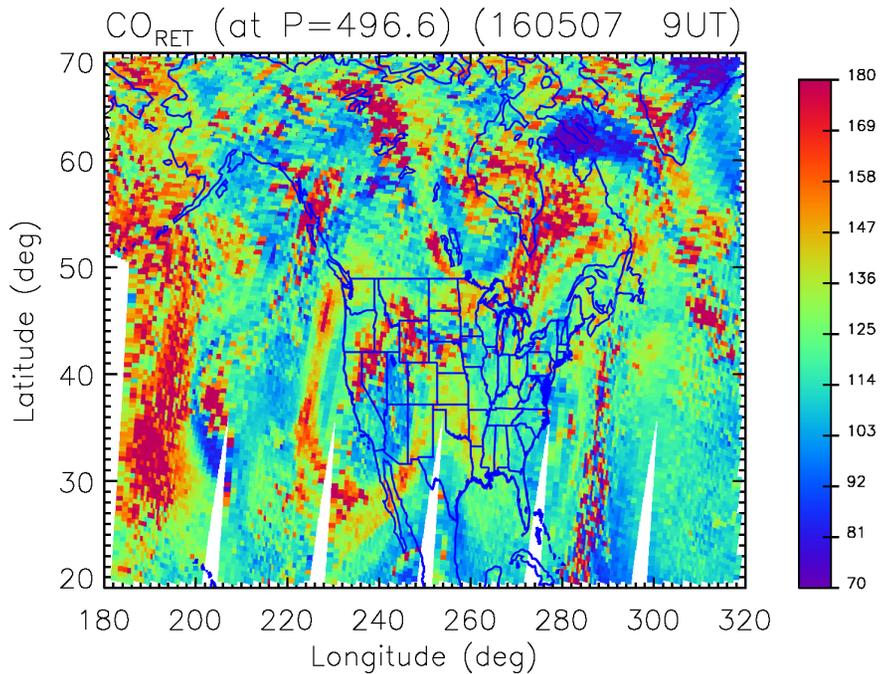
Each netCDF files is ~2.5MB in size

These netCDF files are [experimental products](#) and available only upon user request.

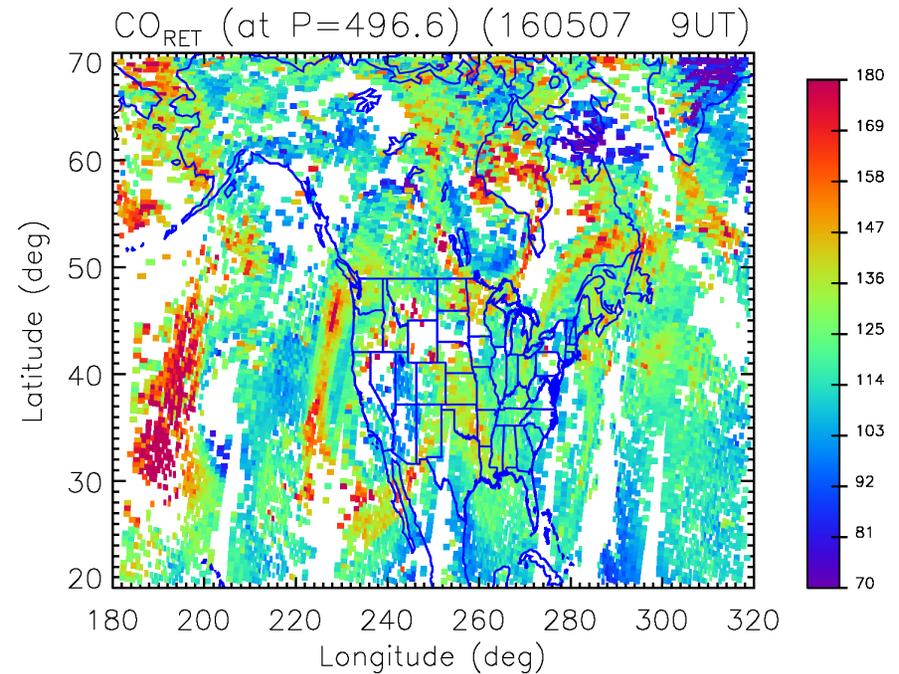
We will evaluate product value, fine tune its design and eventually make recommendations for operationalization

Quality Control – A necessary step in using Satellite Data

NUCAPS CO without QC



NUCAPS CO with QC

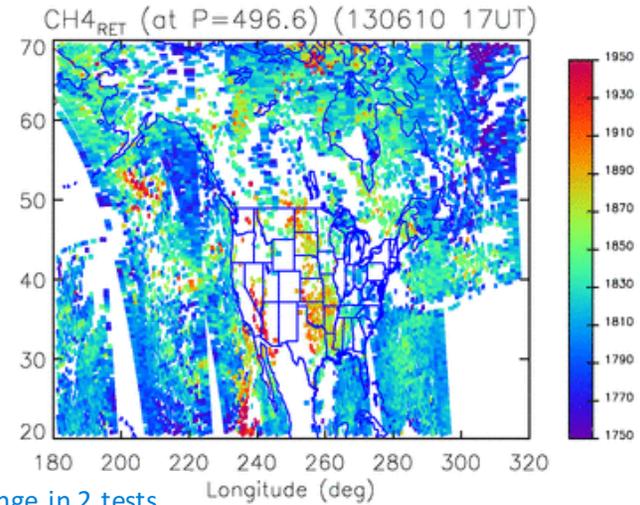
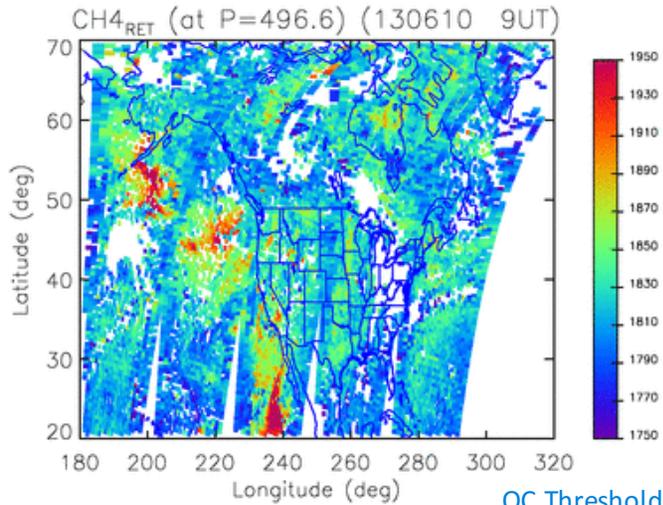


NUCAPS QC indicates quality of T/q from IR and MW retrieval steps
Designed to meet system requirements for global retrieval statistics; 1K T and 10% q

Can we adjust NUCAPS QC and improve Retrieval Yield?

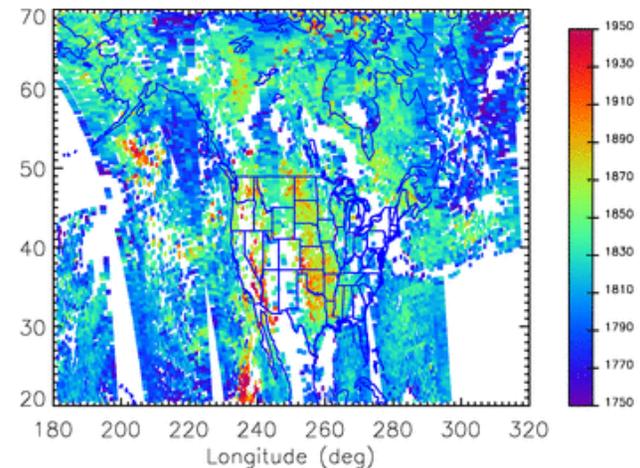
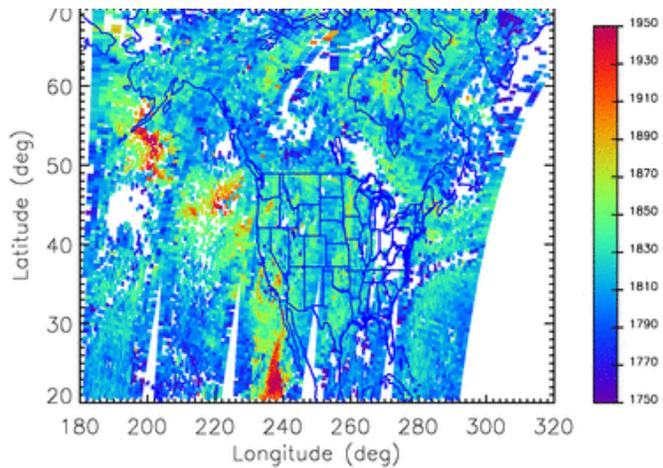
Night Time
AM orbit
(~01h30)

NUCAPS has
17 QC tests
throughout
retrieval
process



Day Time
PM orbit
(~13h30)

~4% increase in
retrieval yield



~12% increase
in retrieval yield

Can we tailor QC to specific parameters? – CO

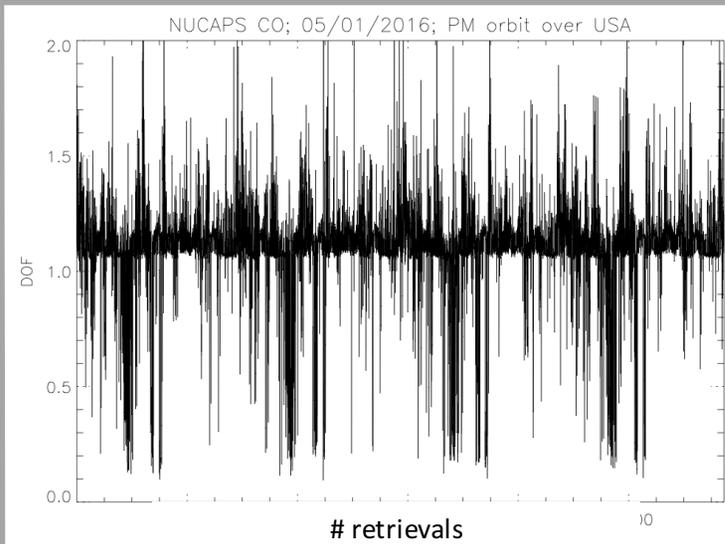
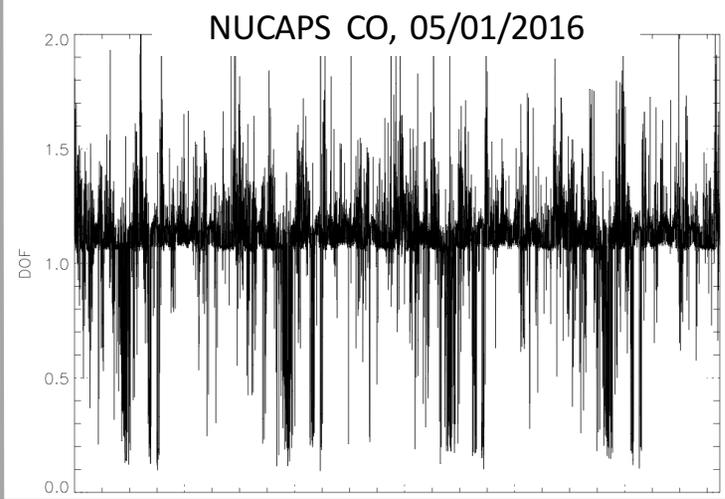
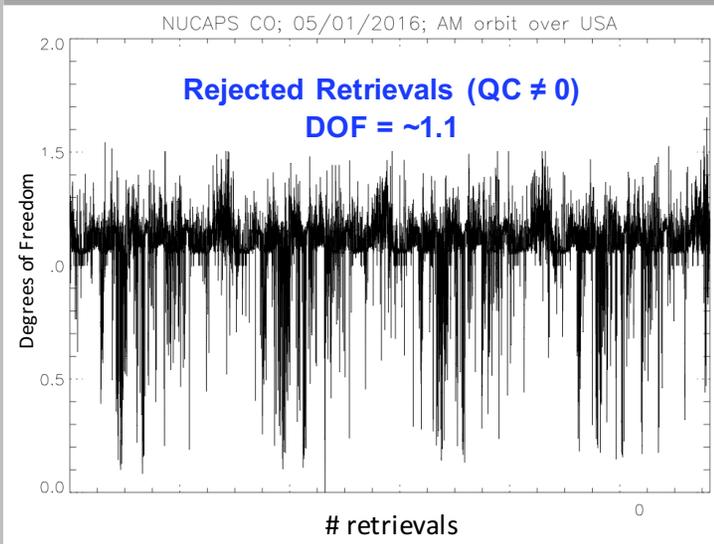
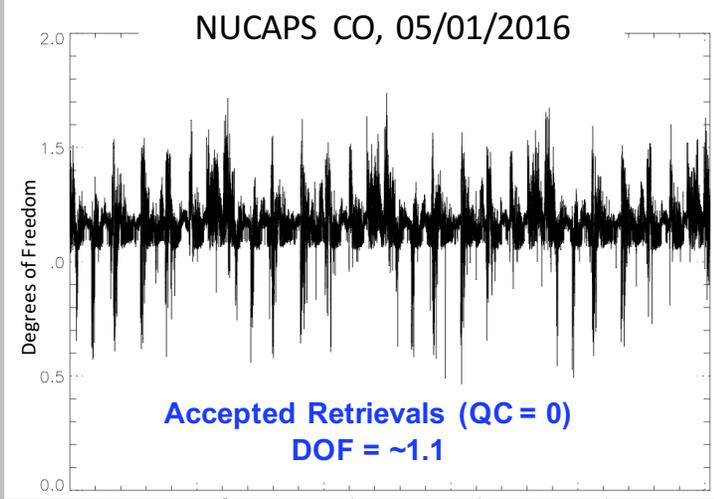
Night Time
AM orbit
(~01h30)

Night time DOF for accepted cases has less variation

There is a clear difference between night time DOF for accepted vs rejected cases

QC should typically filter out those retrievals with low DOF (or quality) and retain those with high DOF

The larger the DOF, the more information is available in the radiances



Day Time
PM orbit
(~13h30)

Degrees of Freedom (DOF) as indicator of information content

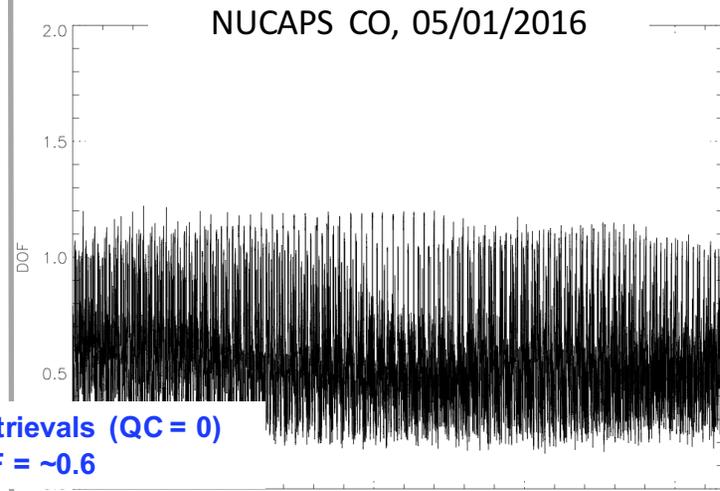
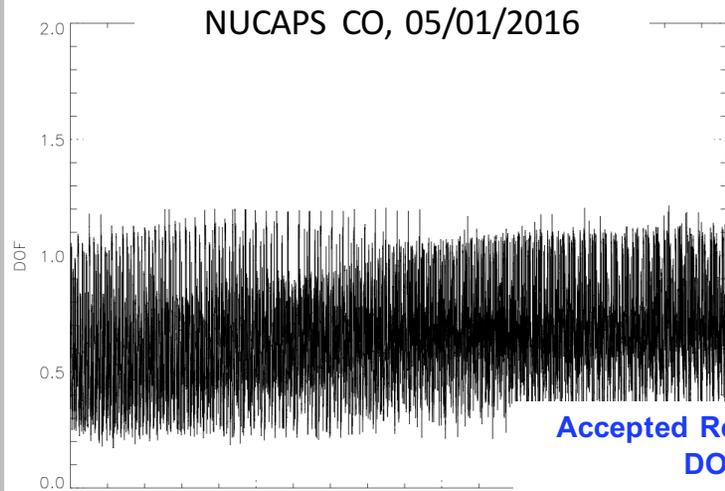
Mean DOF = 1.2
No matter what the time of day or QC

Daytime DOF has the same variation and systematic pattern irrespective of QC

There are many CO retrievals with DOF > 1 in rejected cases (and vice versa) suggesting opportunity to develop CO-tailored QC. The quality of NUCAPS CO appears to be largely independent of T/q QC

Can we tailor QC to specific parameters? – CH4

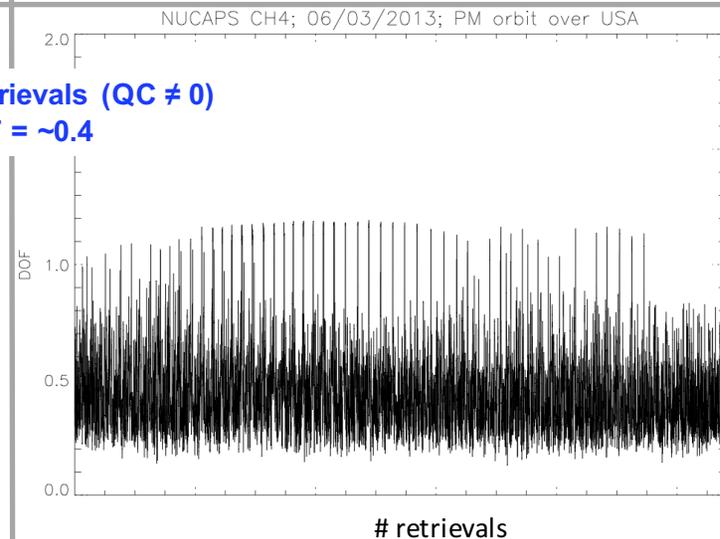
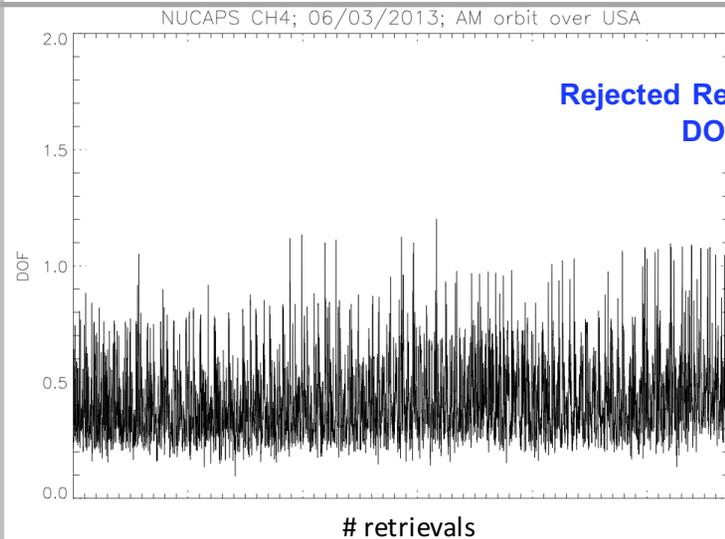
Night Time
AM orbit
(~01h30)



Day Time
PM orbit
(~13h30)

Accepted retrievals have higher DOF than rejected cases for both day and night time suggesting a stronger dependence of CH4 on T/q QC

DOF for rejected cases has less variation and the average is lower than the DOF for accepted cases suggesting that current QC successfully filters out the low quality CH4 retrievals



Accepted retrievals have high DOF variability suggesting a strong dependence on prevailing atm conditions

There are some CO retrievals with DOF > 0.5 in rejected cases suggesting opportunity to tailor QC for CH4

NOAA PGRR Initiative: NUCAPS CO and CH4

INPUT

Need for data at multiple scales

Application

Data at range of space-time scales to model dynamic processes

Innovation

Develop objective methods for non-uniform data

OUTPUT

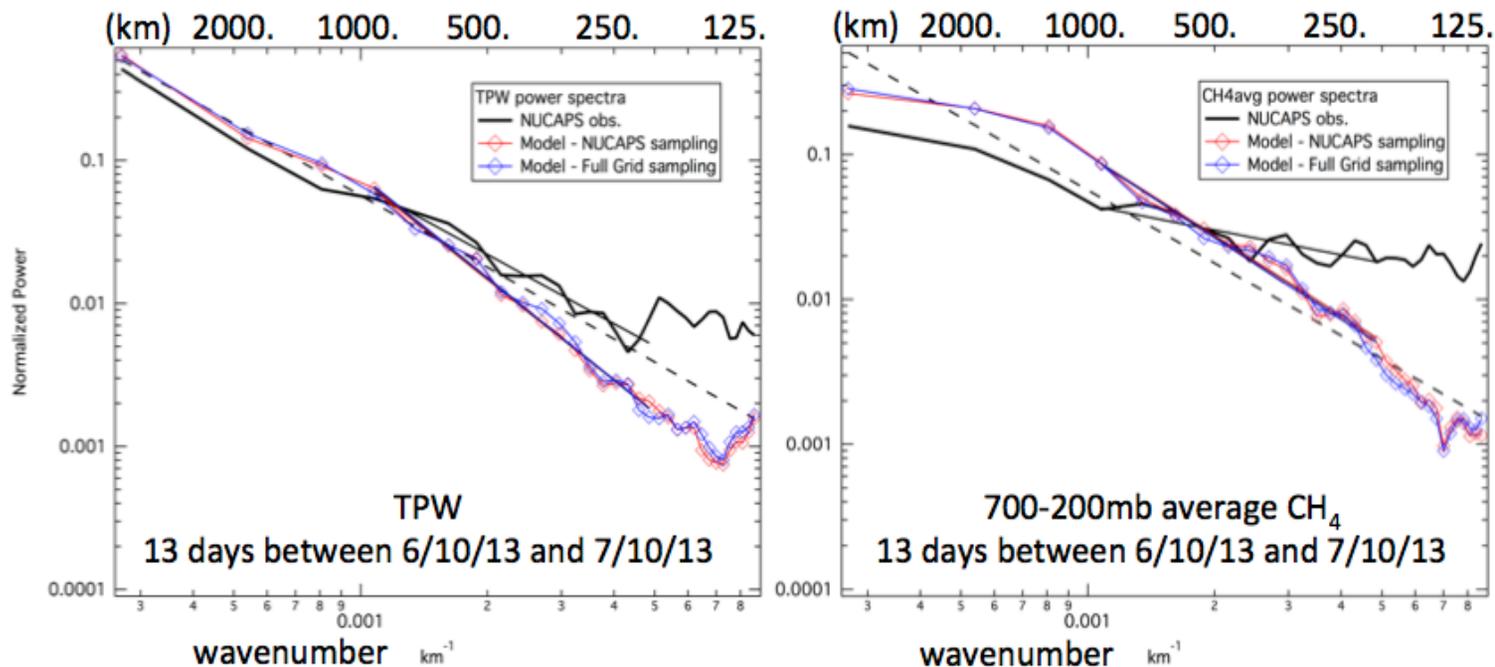
- Empowered Users/Developers
- Adoption of new methods
- Improved Trace Gas Climatologies, etc

STC NUCAPS Team in collaboration with:

NOAA/ESRL/CSD
CIRES
NASA/JPL, etc.

Characterizing Atmospheric Chemistry

The objective is to understand how NUCAPS trace gases scale with respect to TPW in order to constrain the modeling of emission, chemistry and transport.



Average **normalized power spectra** for TPW (left) and 700-200 mb average CH₄ (right) for the NUCAPS data and the WRF-Chem model output. Dashed line is the $-5/3$ power law, and length scale is shown on the top axis. Thin lines are regression fits between 200 and 1000 km length scales.

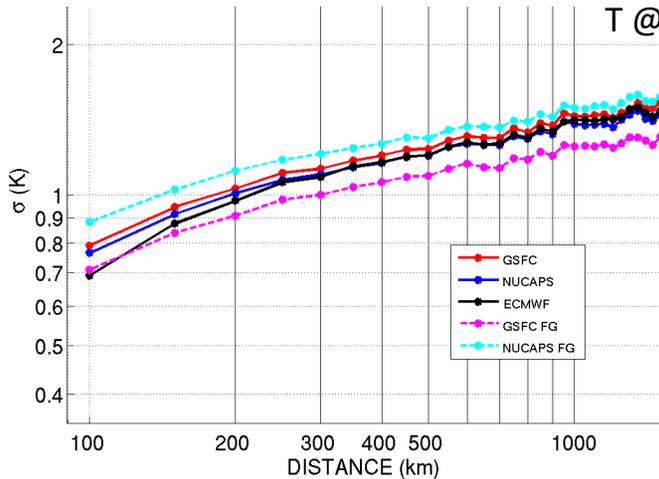
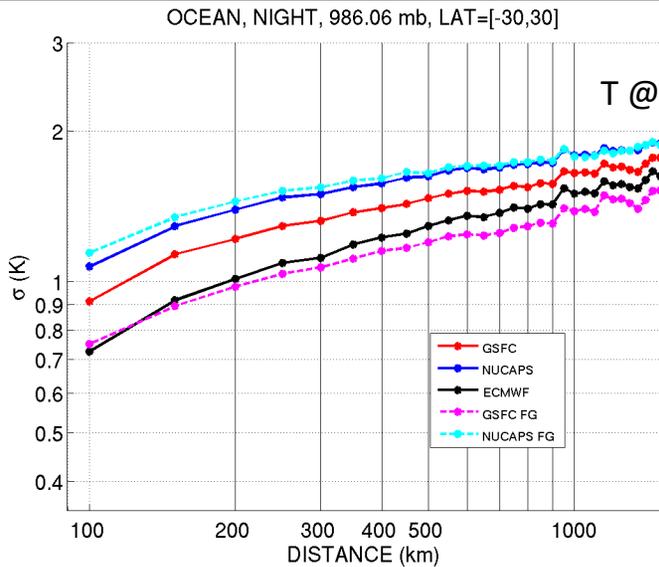
Figures by Stuart McKeen

Spatial Variability in Satellite Data

Night Time
AM orbit
(~01h30)

Standard deviation of
NUCAPS T at different
spatial scales

“Variance scaling”
methods allow the
characterization of
nonlinear
atmospheric
processes and cross-
scale energy transfer.



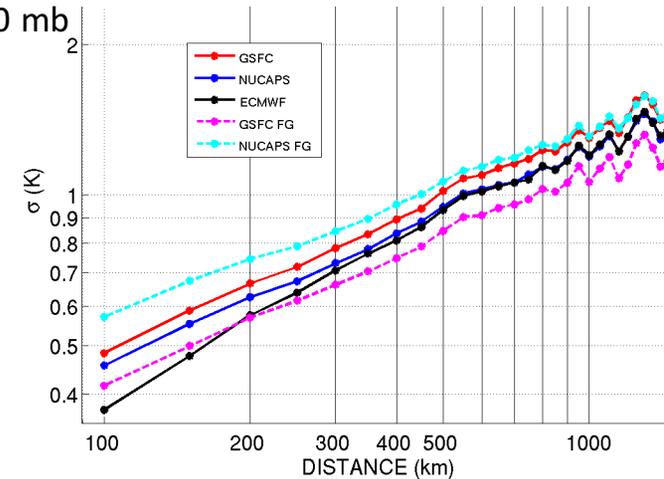
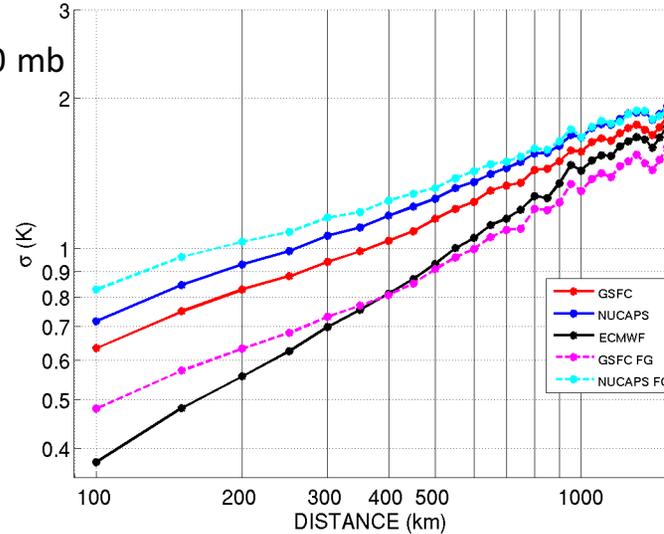
OCEAN, DAY, 986.06 mb, LAT=[-30,30]

Day Time
PM orbit
(~13h30)

Satellite data have
sampling challenges
different to any
other data source.

We need to find
methods that
aggregate spatially
non-uniform data in
objective manner
and do not introduce
systematic effects in
end result.

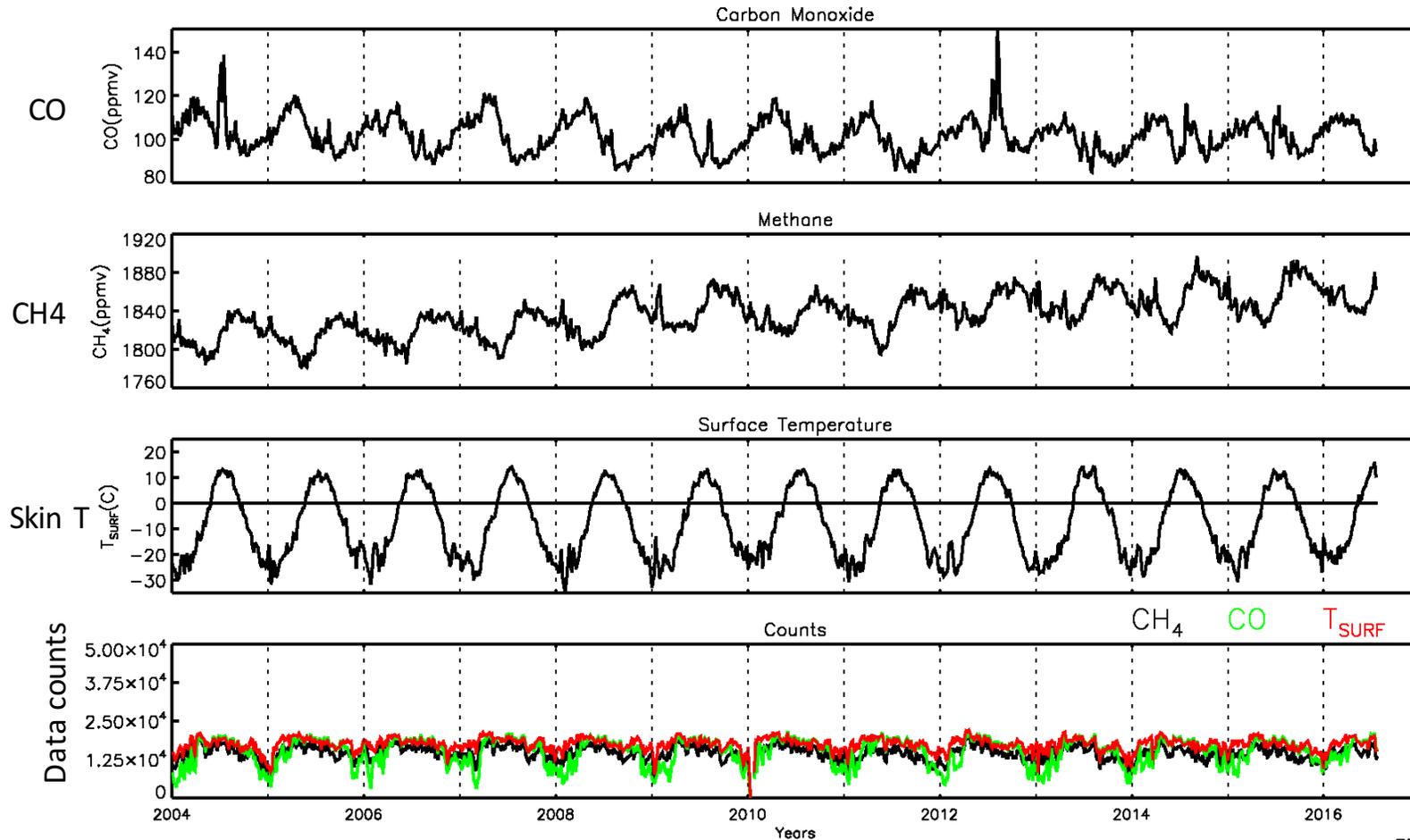
Collaboration with
Stuart McKeen
(ESRL, CIRES)
Brian Kahn and Van
Dang (NASA/JPL)



Figures by Van Dang
NASA/JPL

Temporal Variability in Satellite Data

12 years of AIRS retrievals Alaska (60–70N, 165–90W), 5 day average



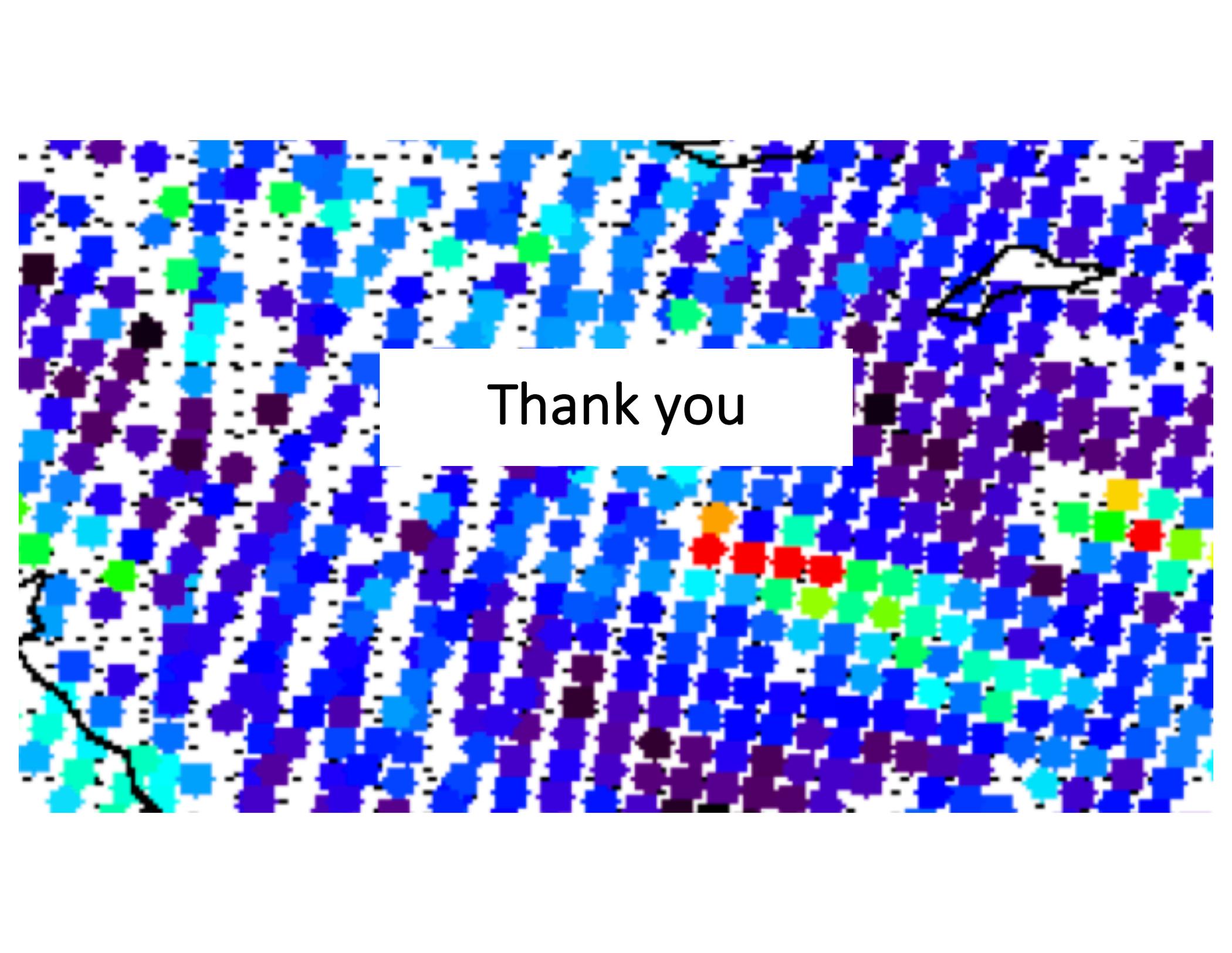
Experiments in temporal averaging.

Aqua and SNPP have repeat cycles of 16 days. How does the long term temporal pattern change when we average different sets of days together?

Figure by Colby Francoeur, STC

Lessons Learned

- The NOAA Sounding Initiative allows Users and Developers to collaborate and more effectively work towards solutions – we are all learning in the process
- There is a user need to not only improve the retrieval quality, but also the data product design, i.e., to tailor the type of information made available in the data product files
- Given that QC removes data, we need to understand how the systematic patterns in data sampling affect analyses and propagate into applications, especially those that are concerned with dynamic, complex processes
- Our efforts will lead to products tailored to user needs AND applications tailored to satellite data

The background is a dense, pixelated pattern of various colors including shades of blue, purple, green, cyan, and red, set against a white background. The colors are scattered in a somewhat random but textured manner. A white rectangular box is centered horizontally and vertically, containing the text "Thank you".

Thank you

Evaluation of NUCAPS CO Retrieval and High Resolution Smoke Trajectory Forecasting

Brad Pierce (NOAA/NESDIS/STAR)

Collaborators:

Nadia Smith, Antonia Gambacorta and
Chris Barnet (STC)

Jim Davies and Kathy Strabala (CIMSS)

Greg Frost and John Holloway
(NOAA/ESRL)

Shobha Kondragunta (NESDIS/STAR)

Fort McMurray wildfire Case study

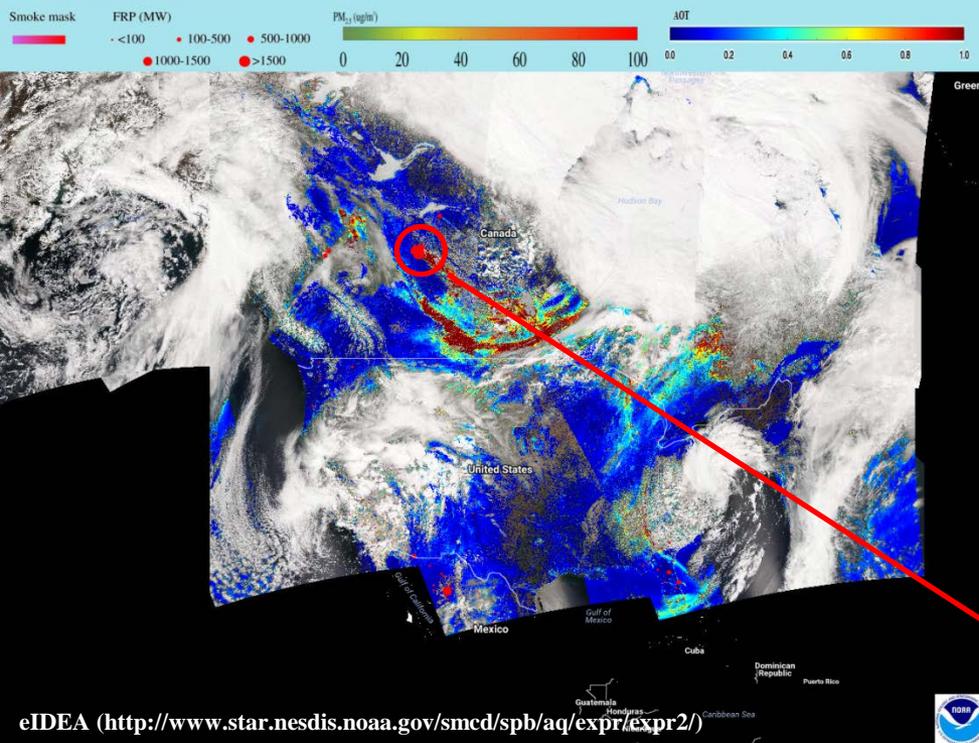
(May 1, 2016) – 9:57 p.m., Mayor Blake has declared a State of Local Emergency in Fort McMurray localized to Gregoire.

(May 4, 2016) –Mandatory evacuation of Anzac, Gregoire Lake Estates and Fort McMurray First Nation.

(May 16, 2016) The evacuation zone has increased north of the city of Fort McMurray.

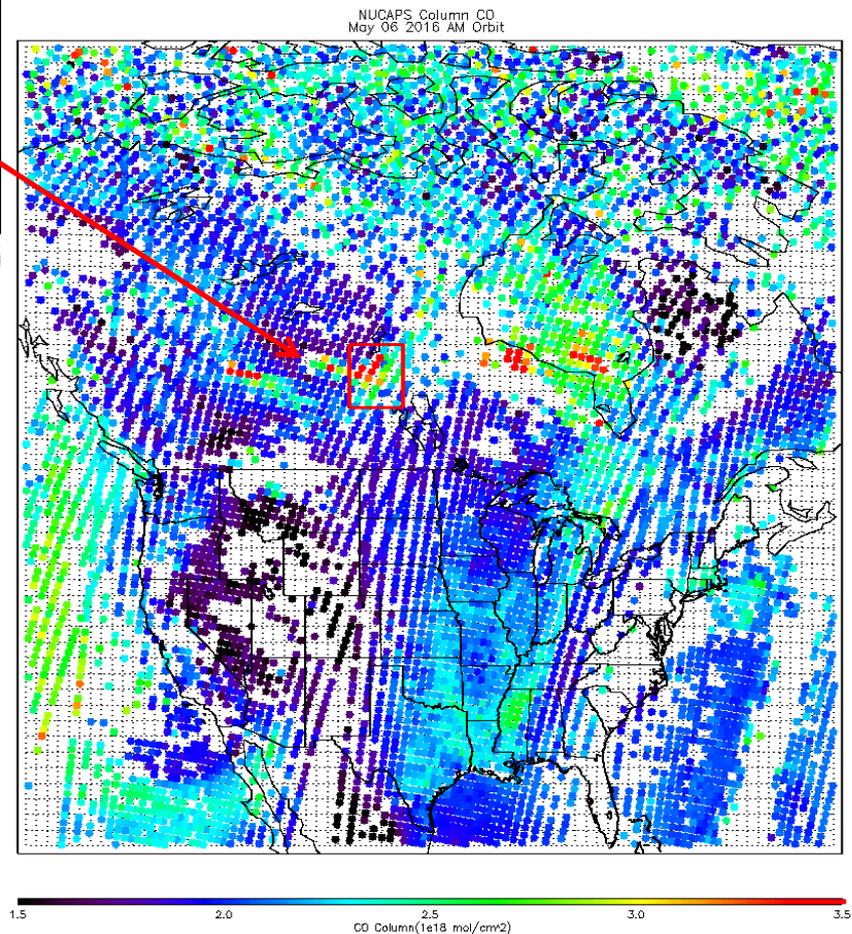
(May 18, 2016) A voluntary, phased re-entry for the safe return of Fort McMurray residents will begin June 1 if future wildfire conditions do not delay restoration efforts.



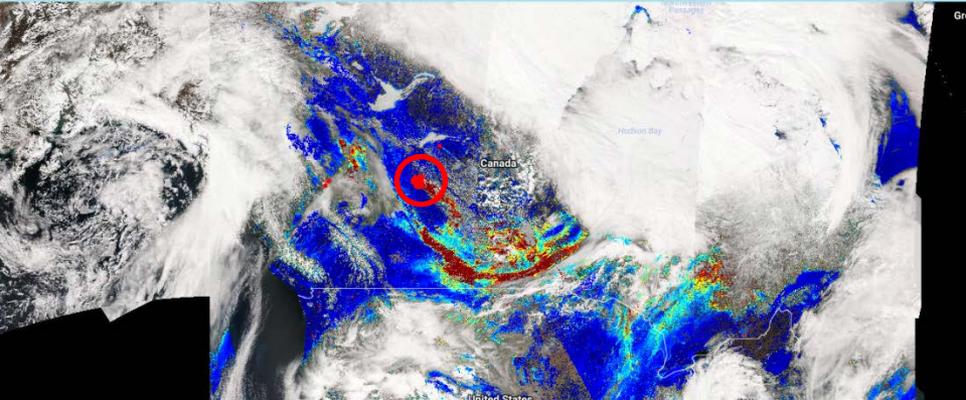
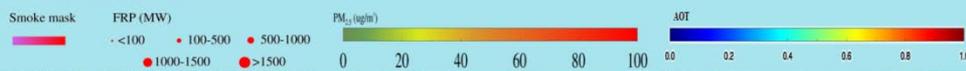


CSPP NUCAPS trace gas EDR

- ☐ Include averaging kernel, apriori, interpolation and inverse matrices for applying to model (or insitu) profiles for data assimilation (or validation) activities.

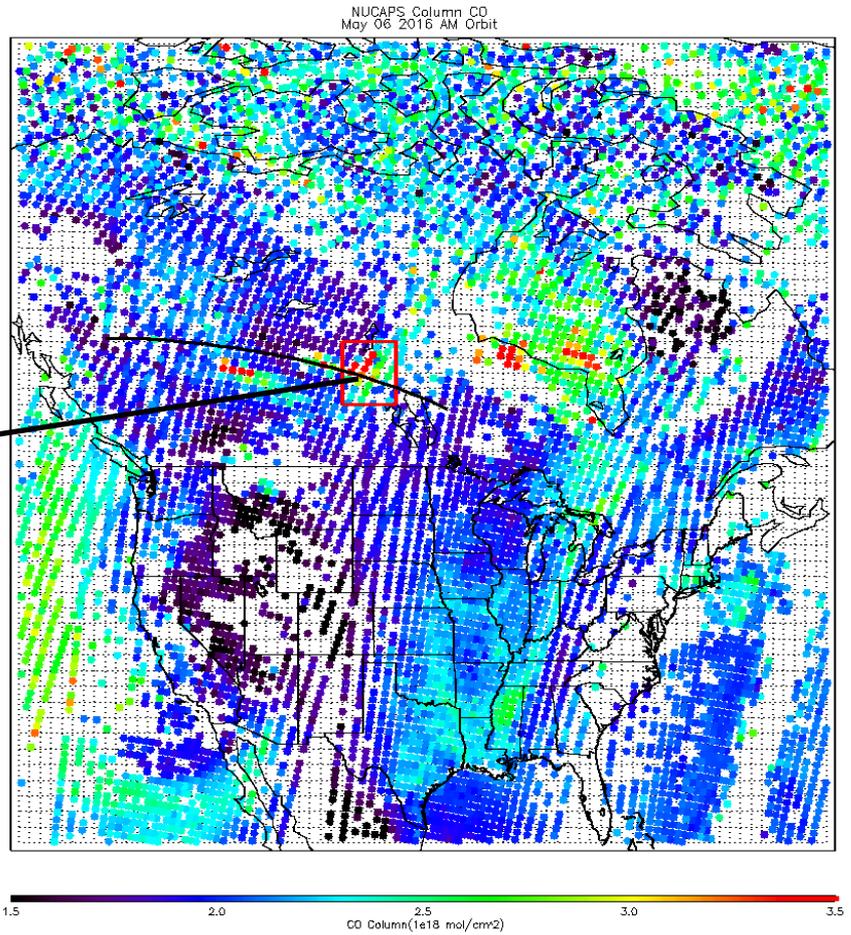
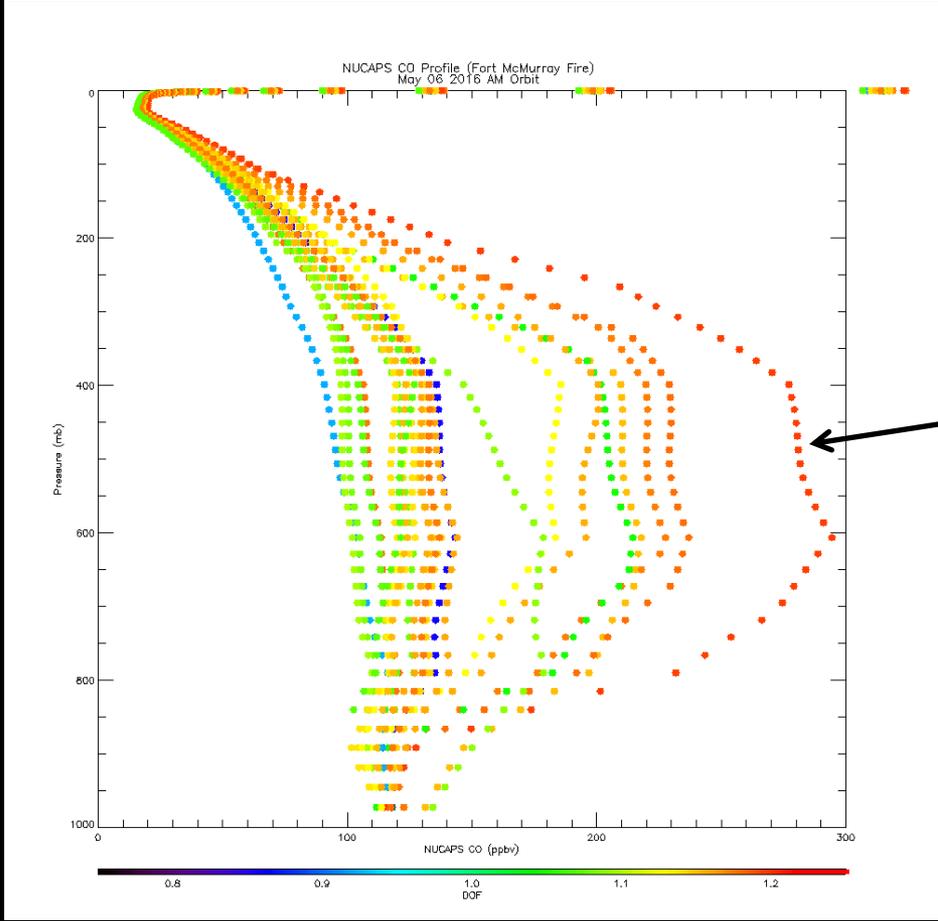


- ☐ Files also include surface parameters, degrees of freedom, and combined microwave and infrared quality flags.
- ☐ Will be used within CSPP for IDEA-I NUCAPS smoke forecasts and also in collaboration with colleagues at NOAA/ESRL for NUCAPS CH₄ and CO retrieval validation activities.



CSPP NUCAPS trace gas EDR

- ☐ Include averaging kernel, apriori, interpolation and inverse matrixes for applying to model (or insitu) profiles for data assimilation (or validation) activities.



Satellite Retrievals

Global Assimilation

Regional Prediction

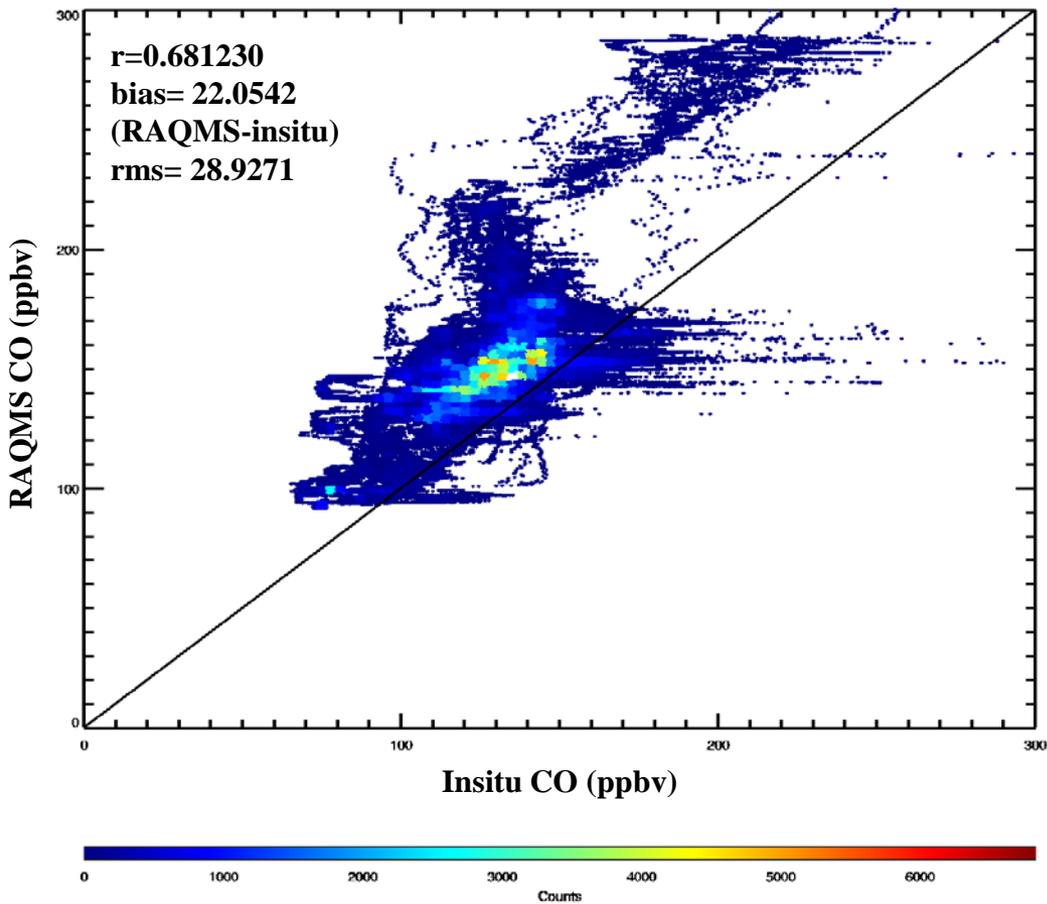
Validation

RAQMS

Realtime Air Quality Modeling System

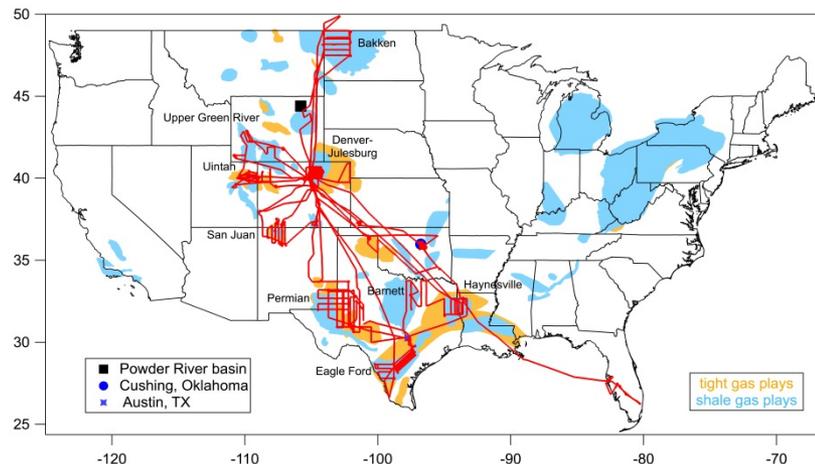
Evaluate RAQMS vs insitu CO during NOAA/ESRL SONGNEX 2015 for indirect NUCAPS CO validation

RAQMS vs Insitu SONGNEX 2015 (March 19-April 27, 2015)

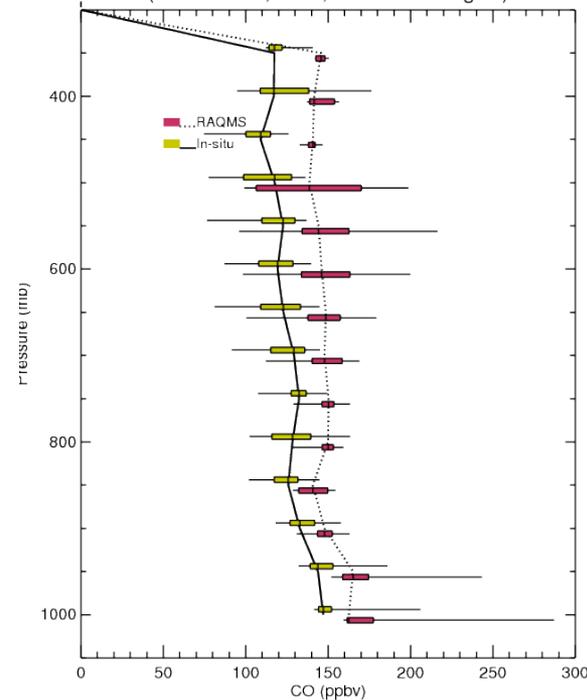


SONGNEX 2015

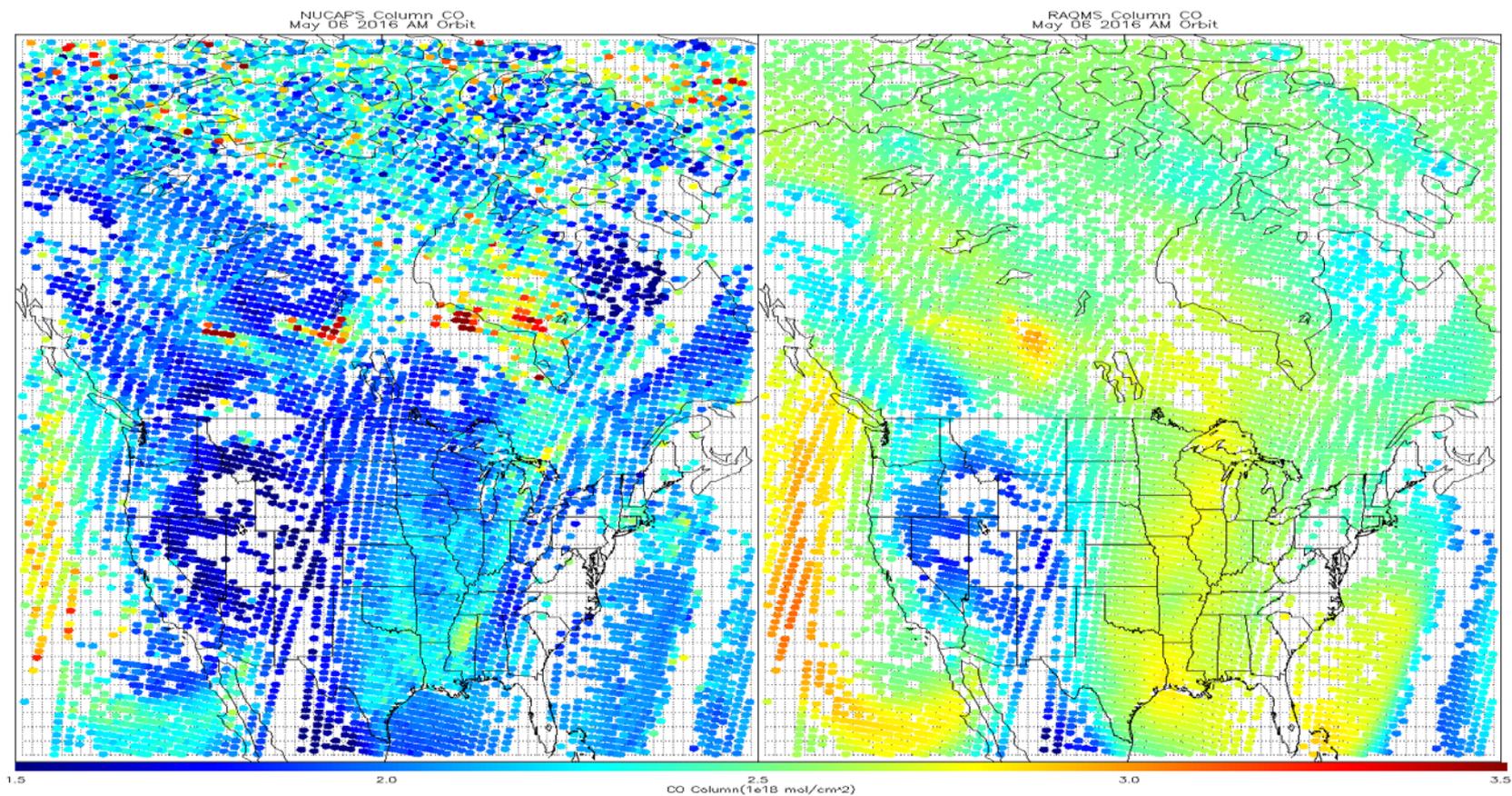
Shale Oil and Natural Gas Nexus



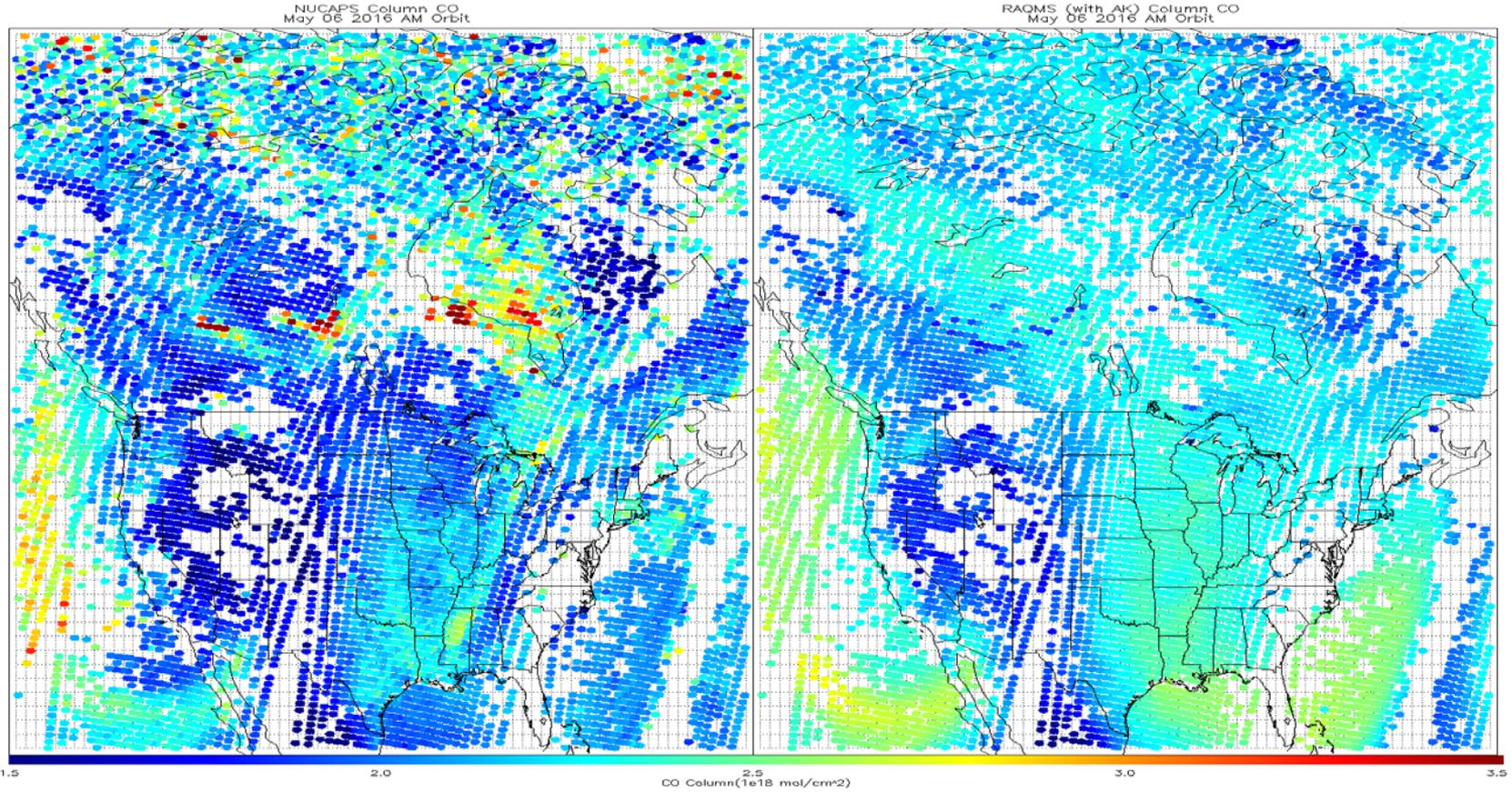
RAQMS/NOAA P3 Insitu CO (Holloway)
(03/19-04/27, 2015, SONGNEX Flights)



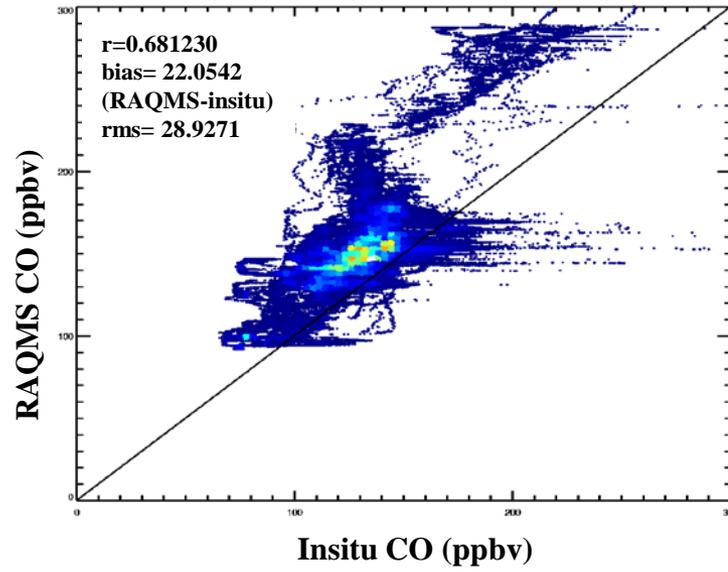
NUCAPS verses RAQMS Column CO May 06, 2016 AM Orbit



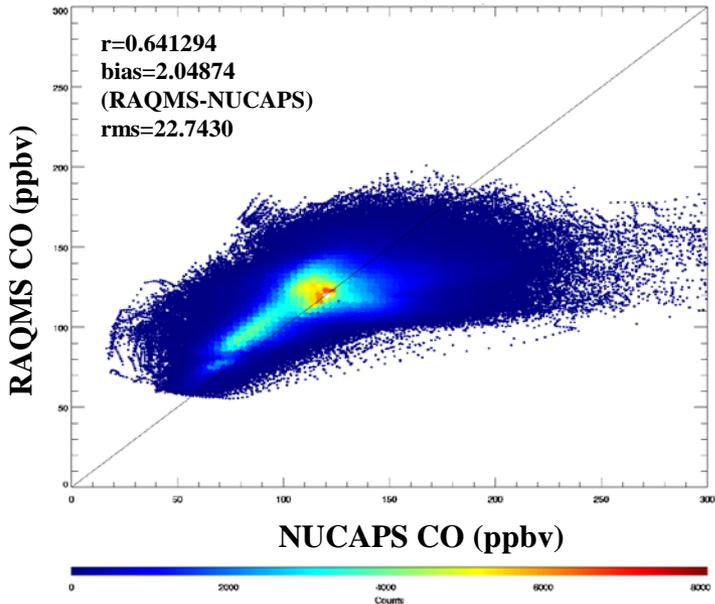
NUCAPS verses RAQMS (AK) Column CO May 06, 2016 AM Orbit



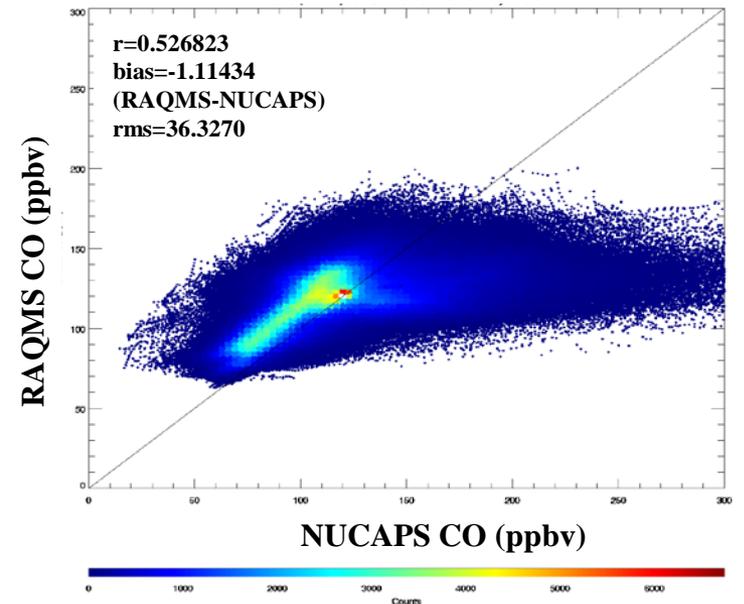
**RAQMS vs Insitu SONGNEX 2015
(March 19-April 27, 2015)**



**RAQMS vs NUCAPS AM Orbit
(May 1-16, 2016)**



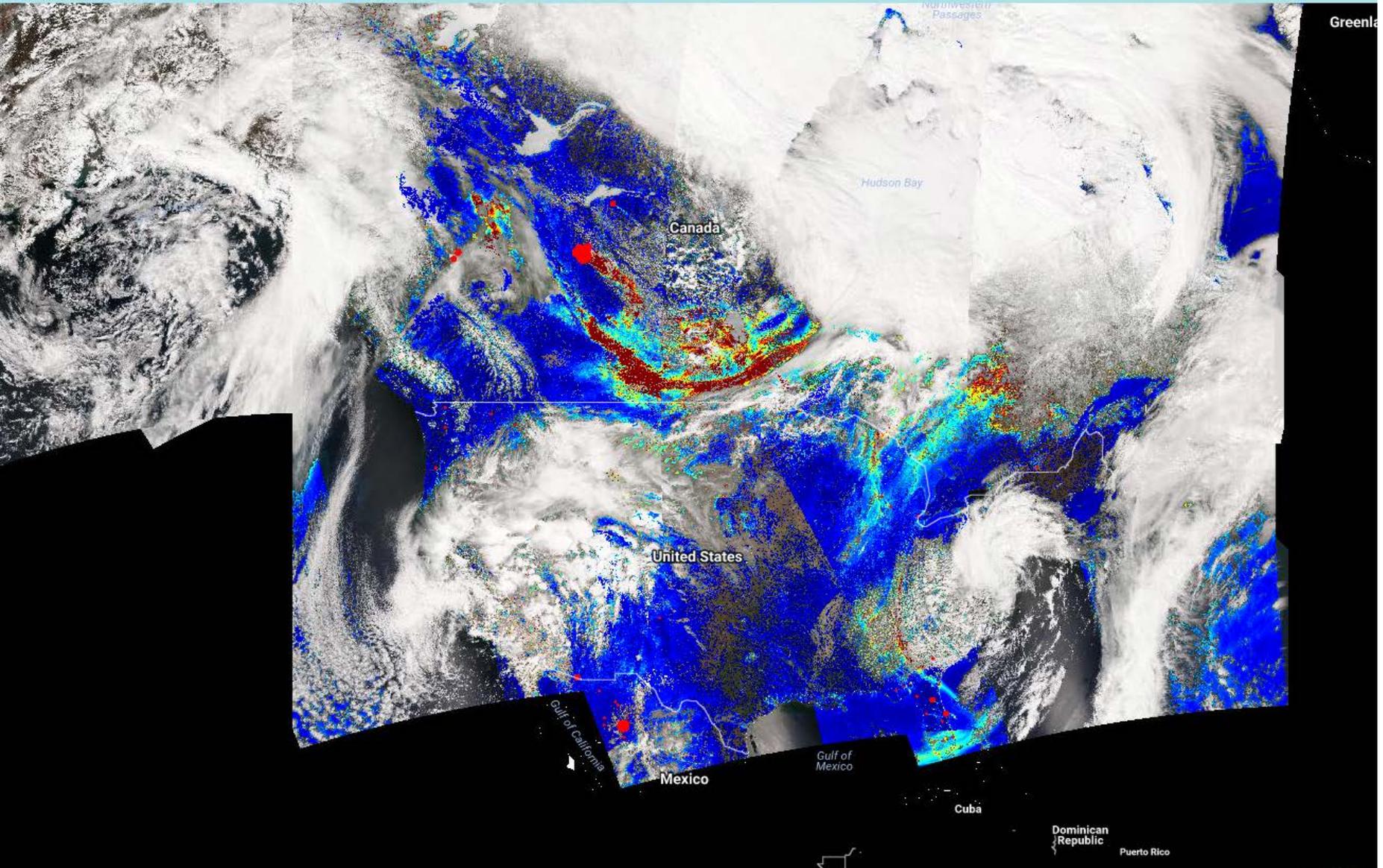
**RAQMS vs NUCAPS PM Orbit
(May 1-16, 2016)**



High Resolution Trajectory-Based Smoke Forecasts

- **Goal:** Provide low latency, web-based, high resolution forecasts of smoke dispersion for use by NWS Incident Meteorologists (IMET) to support on-site decision support services for fire incident management teams.
 - Project utilizes VIIRS AOD and NUCAPS CO retrievals to initialize trajectory-based, high spatial resolution smoke dispersion forecasts.
 - Project is an extension of Infusion of satellite Data into Environmental Applications-International (IDEA-I) trajectory based aerosol forecast capabilities and will be tested and released within CSPP prior to transition to Operations at NESDIS.

May 06, 2016

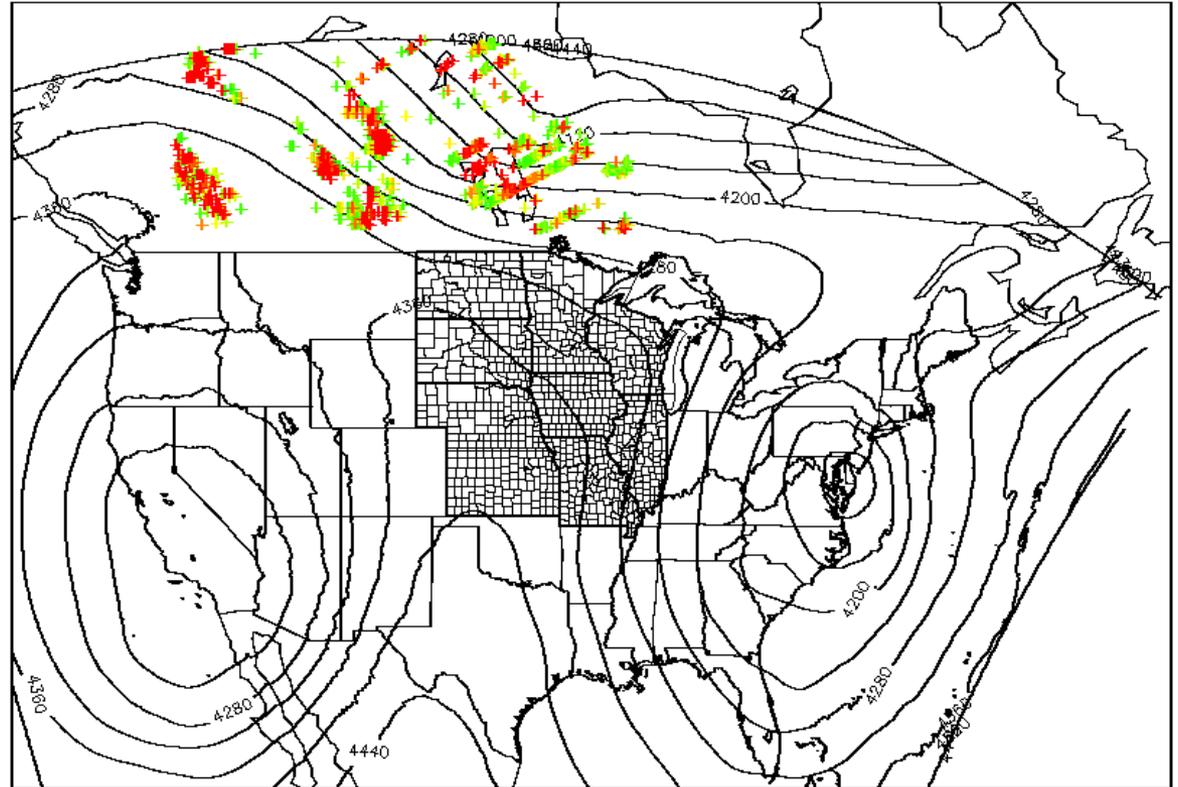


IDEA-I High resolution (NAM 4km) trajectory forecast

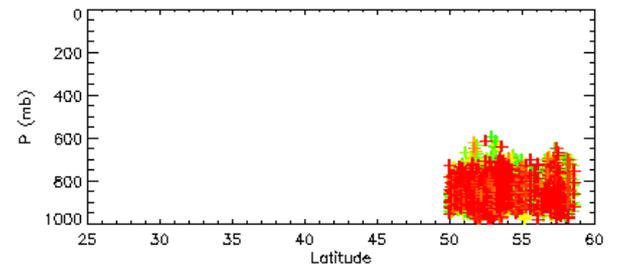
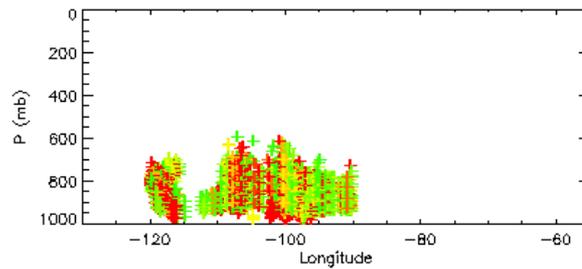
Fort McMurray Wildfire

May 06, 2016

2016050617 High Resolution VIIRS AOD Trajectories
NAM 600mb Heights Contoured



+



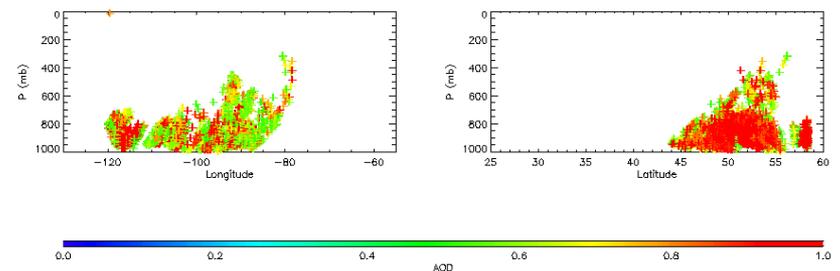
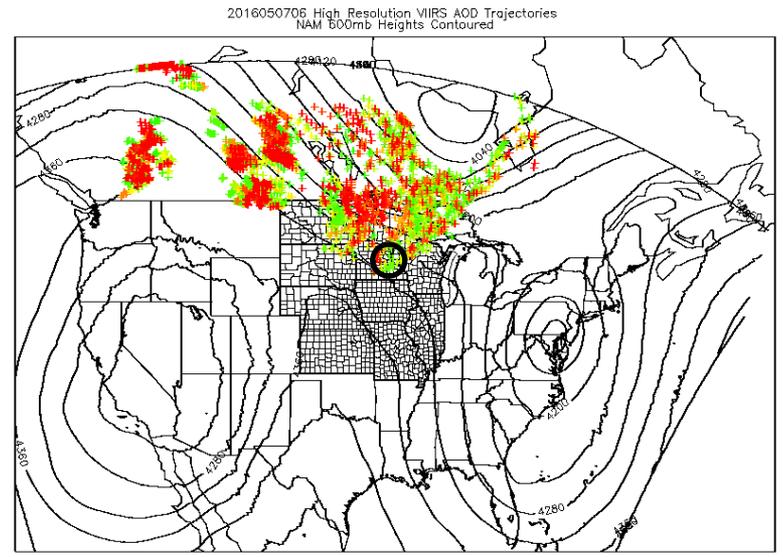
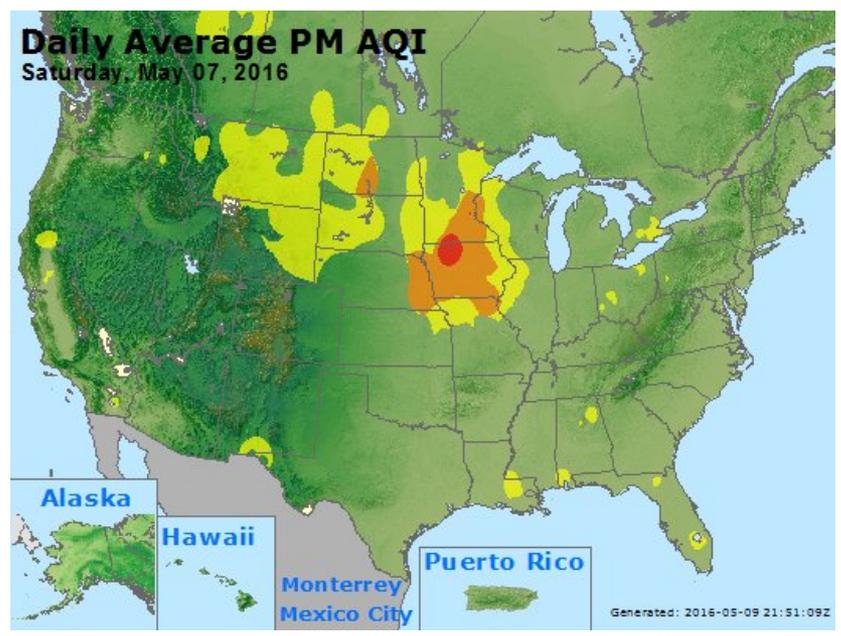
- IDEA-I high resolution trajectories initialized at each 6km VIIRS pixel (only AOD>0.5 initialized)
- Upper panel shows NAM 600mb heights
- Lower panels show longitude and latitude cross sections
- IDEA-I high resolution trajectory forecast colored by initial AOD

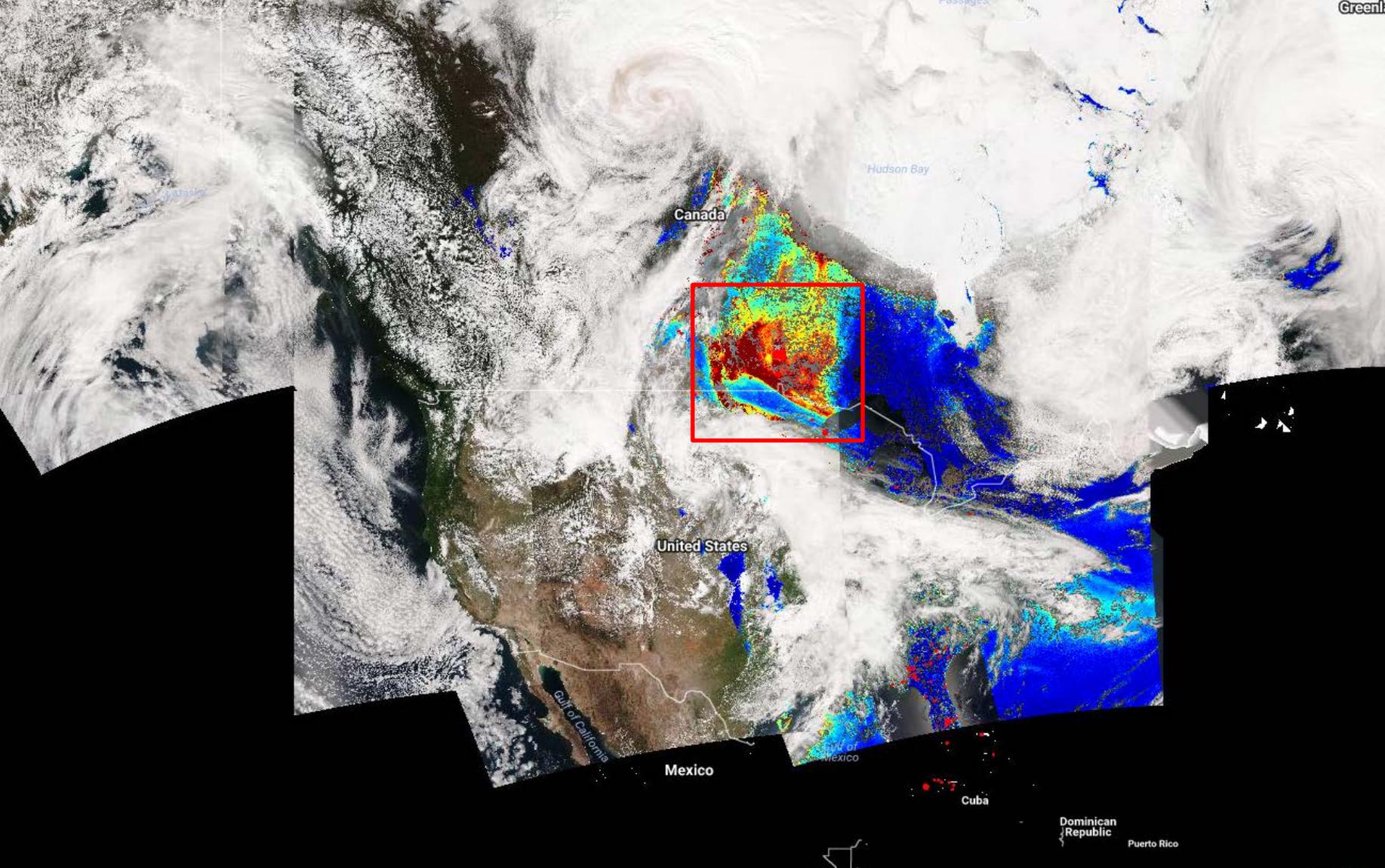
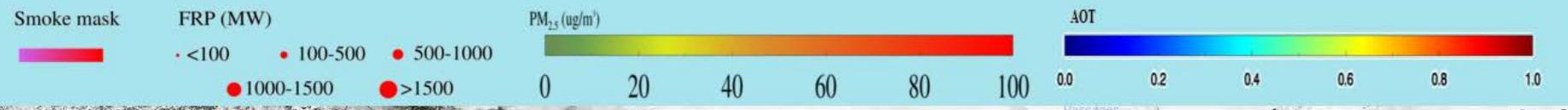
From Andy Edman/NWS

**SPECIAL WEATHER STATEMENT
NATIONAL WEATHER SERVICE TWIN CITIES/CHANHASSEN MN
127 AM CDT SAT MAY 7 2016**

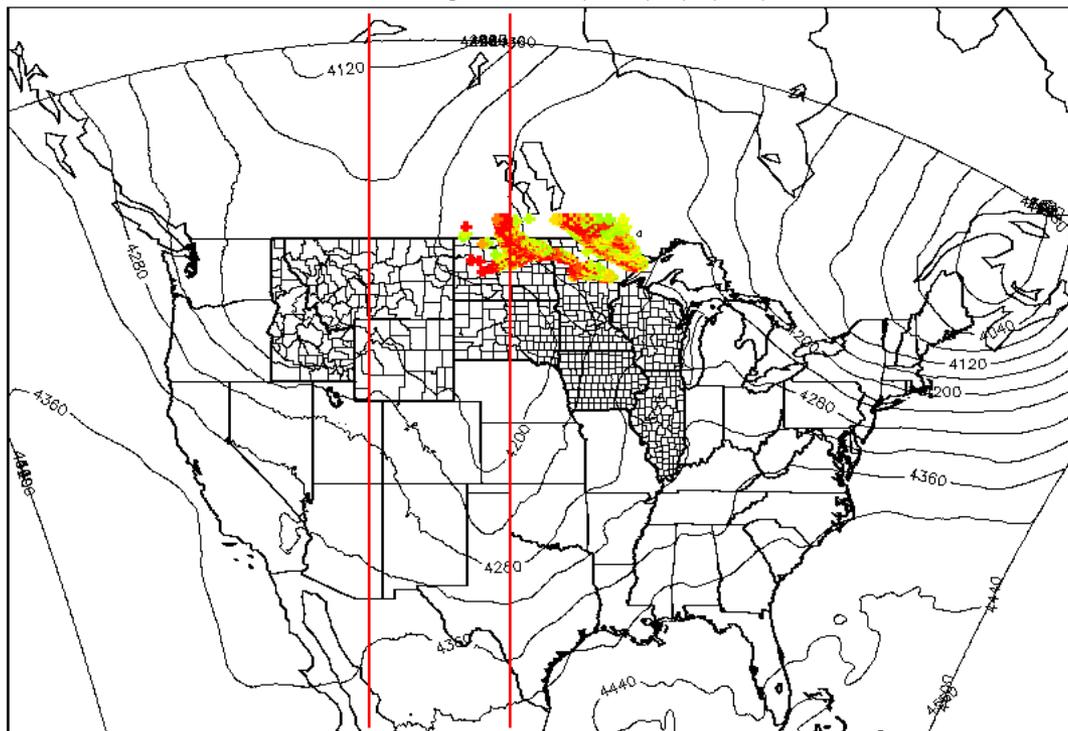
...SMOKY CONDITIONS TO PERSIST THROUGH THE OVERNIGHT HOURS...

WIDESPREAD SMOKE FROM BOTH THE LARGE CANADIAN WILDFIRES AND A SMALLER WILDFIRE NEAR LAKE HATTIE IN HUBBARD COUNTY MINNESOTA HAS BLOWN INTO CENTRAL MINNESOTA...PARTICULARLY WITHIN AND NEAR THE TWIN CITIES METROPOLITAN AREA...DUE TO STRONG WINDS FROM THE NORTHWEST. VISIBILITIES HAVE BEEN REDUCED TO BETWEEN 1 AND 3 MILES...AND AIR QUALITY HAS BEEN SIGNIFICANTLY IMPACTED.

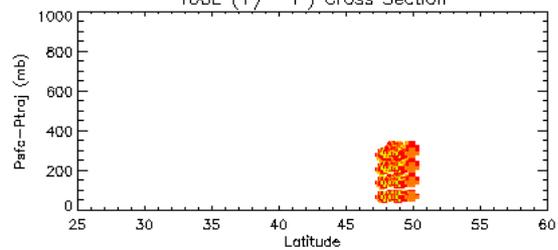




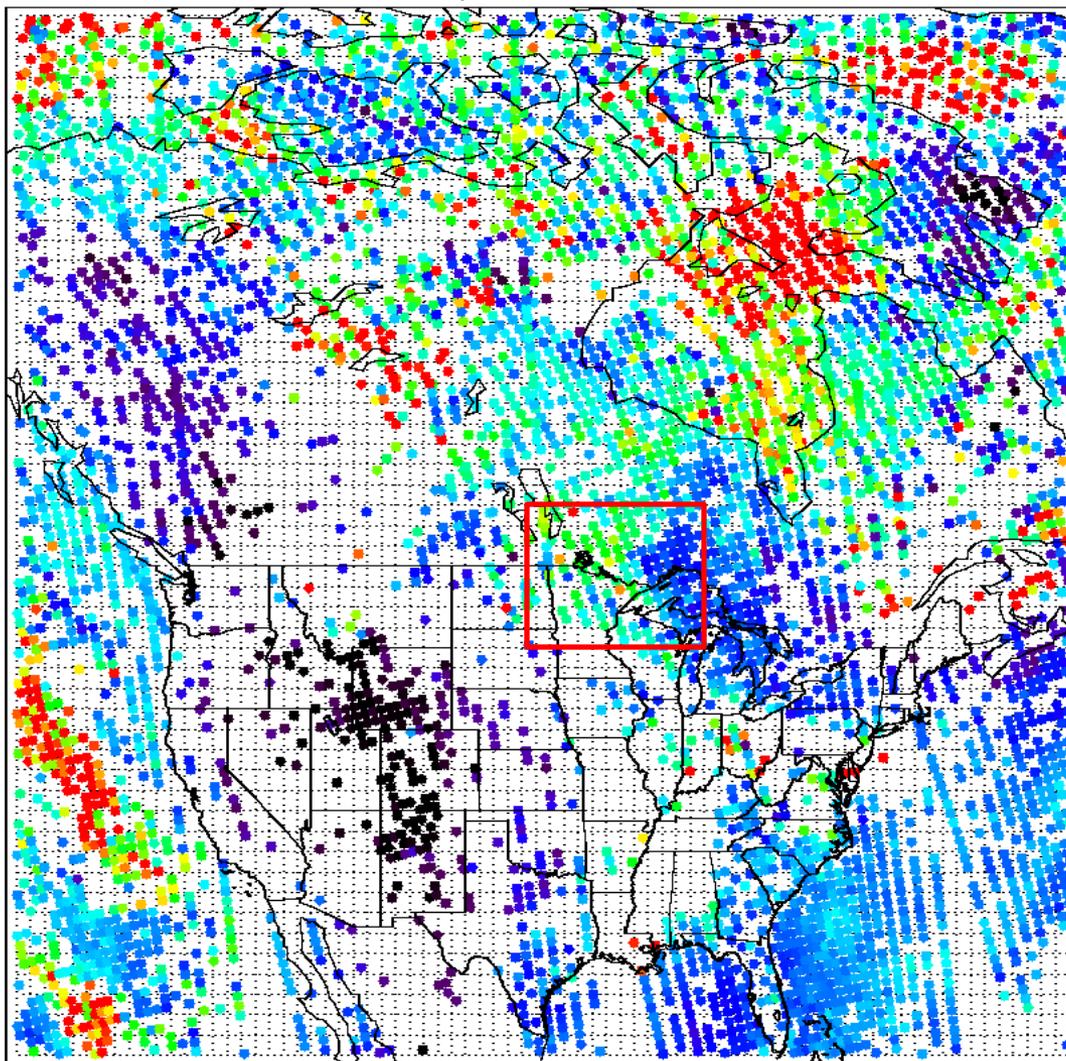
2016050919 High Resolution VIIRS AOD Trajectories
NAM 600mb Heights Contoured/PCP (mm/hr) Purple



100E (+/- 1°) Cross Section

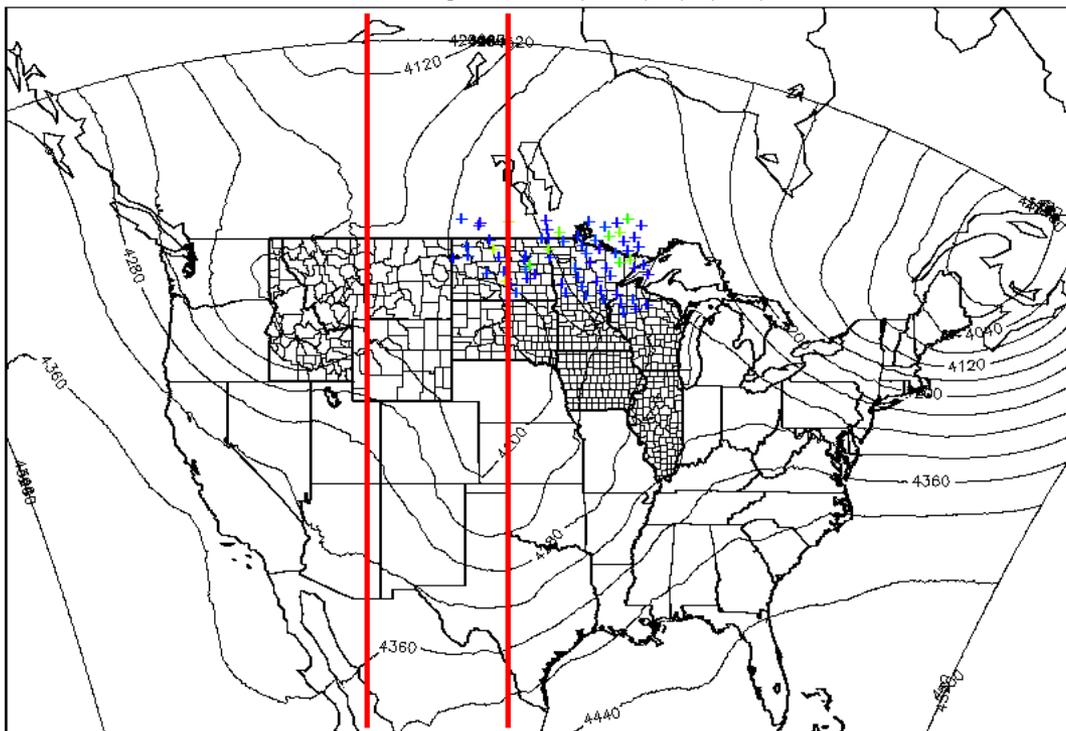


NUCAPS Column CO
May 09 2016 PM Orbit

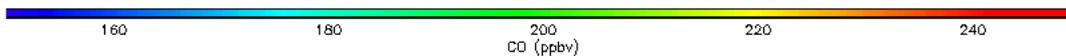
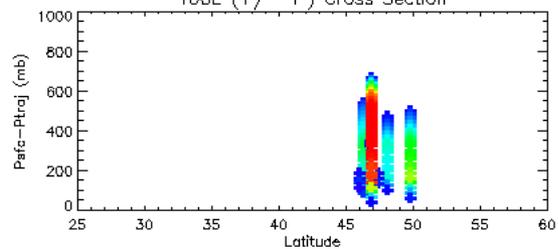


1.5 2.0 2.5 3.0 3.5
CO Column(1e18 mol/cm²)

2016050918 High Resolution NUCAPS_CO Trajectories
NAM 600mb Heights Contoured/PCP (mm/hr) Purple



100E (+/- 1°) Cross Section



VIIRS True Color Image May 9, 2016 20:15 UTC

Smoke from Fort McMurray fire imbedded with low pressure system over northern Canada

Questions?



NOAA/NASA

(From NOAA Environmental Visualization Laboratory)



Understanding Emissions and Tropospheric Chemistry using NUCAPS and VIIRS

A JPSS Proving Ground/Risk Reduction Project

NOAA OAR ESRL: *G. Frost, S. McKeen, S.-W. Kim, R. Ahmadov, M. Trainer, Y. Cui, W. Angevine, T. Ryerson, J. Roberts, C. Warneke, C. Granier, K. Rosenlof, J. Brioude*

STC: *C. Barnett, N. Smith, A. Gambacorta*

NOAA NESDIS STAR: *R. B. Pierce*

NOAA NESDIS NCEI: *C. Elvidge*

Project Overview

Goal: Use aircraft data and atmospheric models to characterize NUCAPS CH₄ and CO retrievals

Objectives:

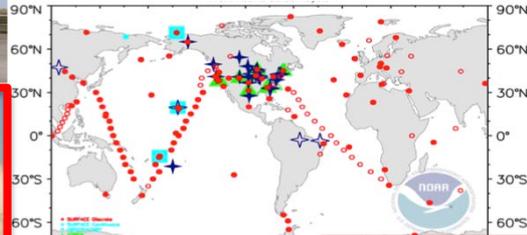
- Validate atmospheric chemical-transport models with aircraft observations
- Simulate spatial and temporal variability of CH₄ and CO
- Evaluate NUCAPS CH₄ and CO retrievals with validated model
- Assess ability of JPSS datasets to constrain modeled CH₄ and CO

End Users: Researchers and forecasters at NOAA and elsewhere

Close collaboration of NOAA ESRL team with [STC NUCAPS retrieval team](#) and [NESDIS STAR analysis team](#) is **absolutely critical** to this project's success and **adds value to PGRR investment**

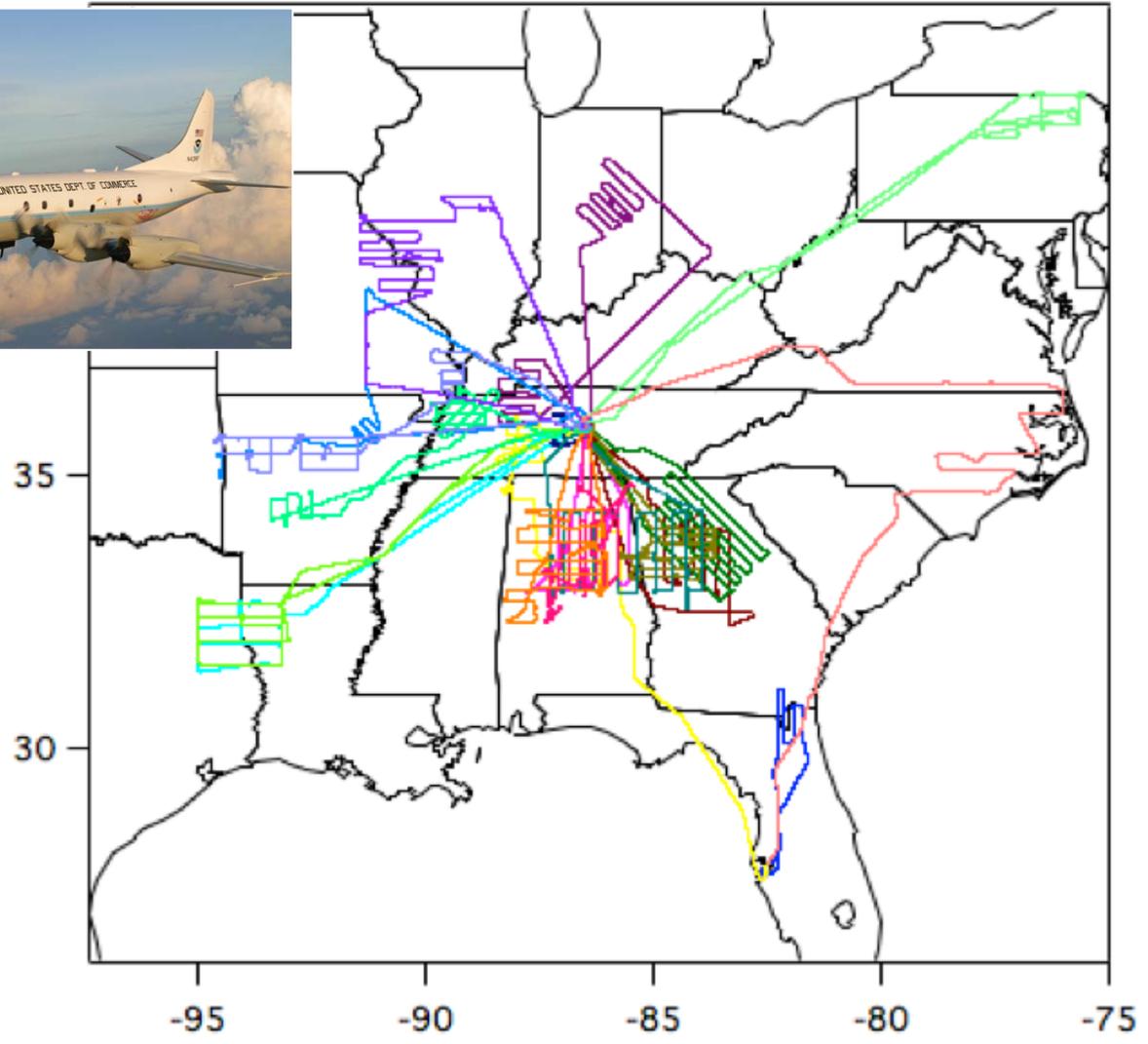
ESRL Research Assets

ESRL employs unique combination of observational platforms, analysis approaches, and human expertise



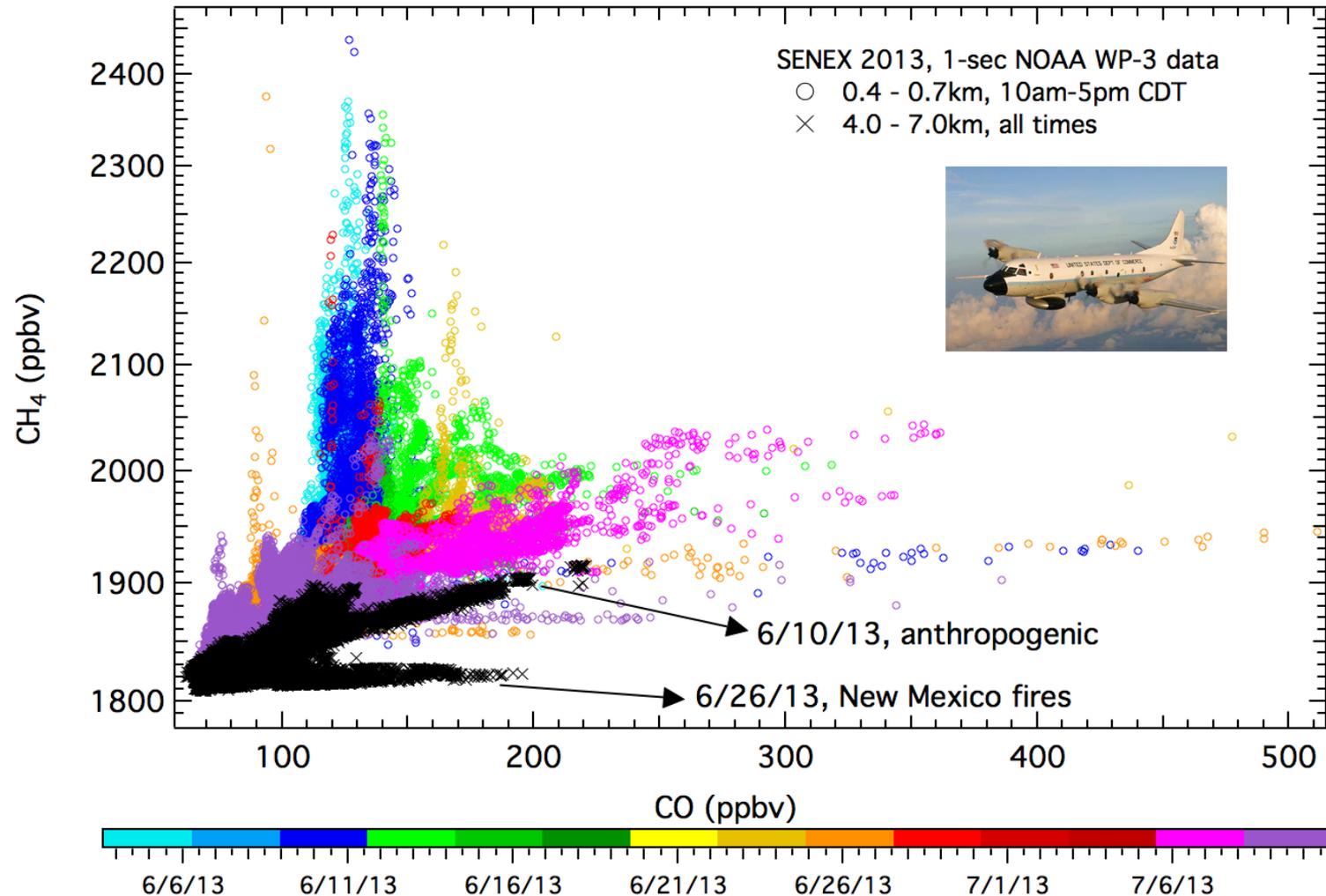


SENEX 2013 NOAA WP-3 Flights

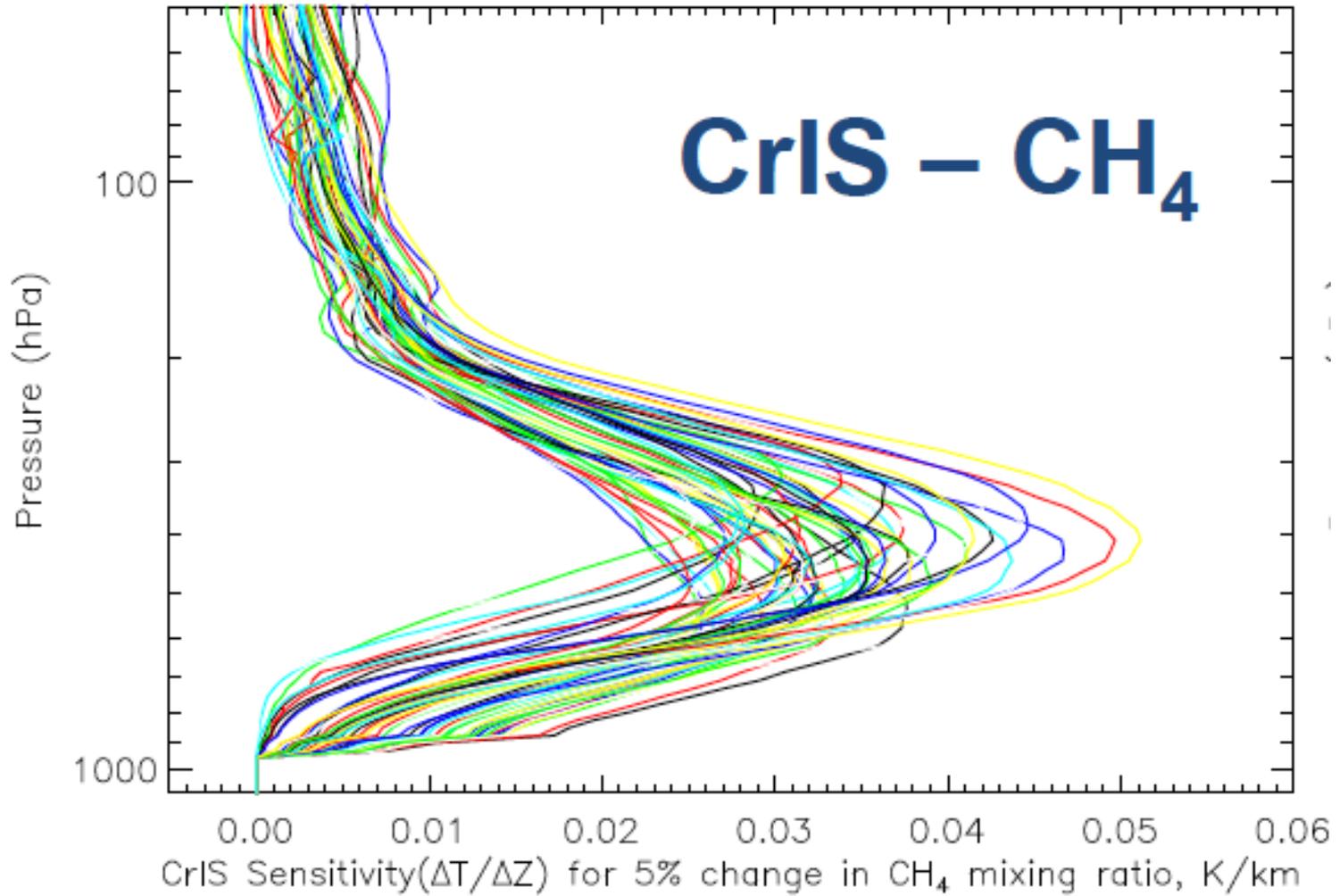


<http://www.esrl.noaa.gov/csd/projects/senex/>

Detecting Source Signatures with Aircraft Data



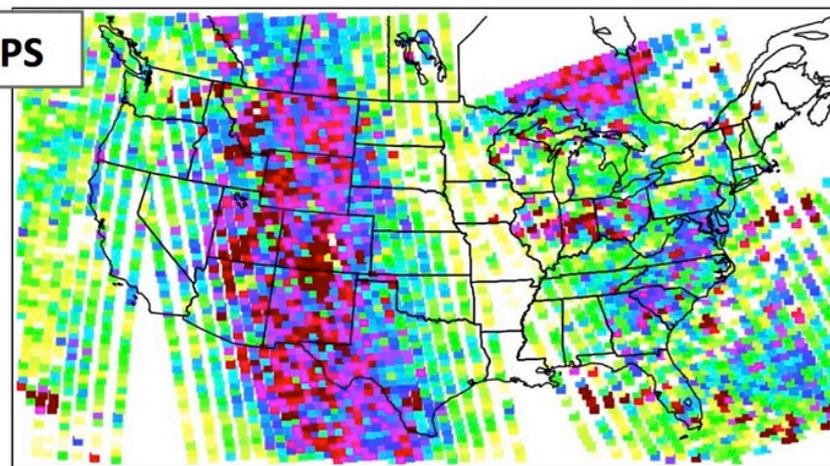
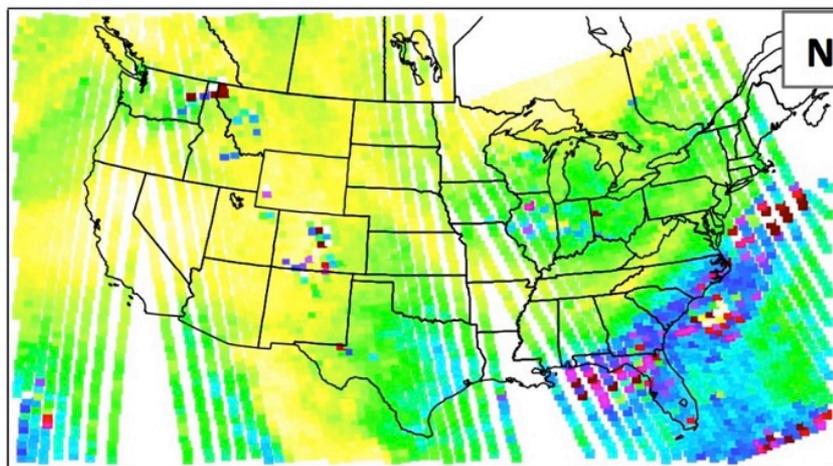
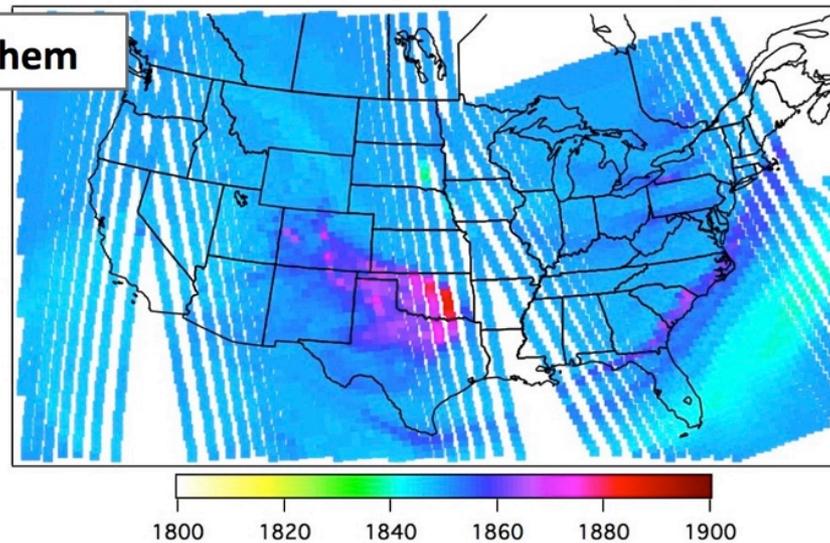
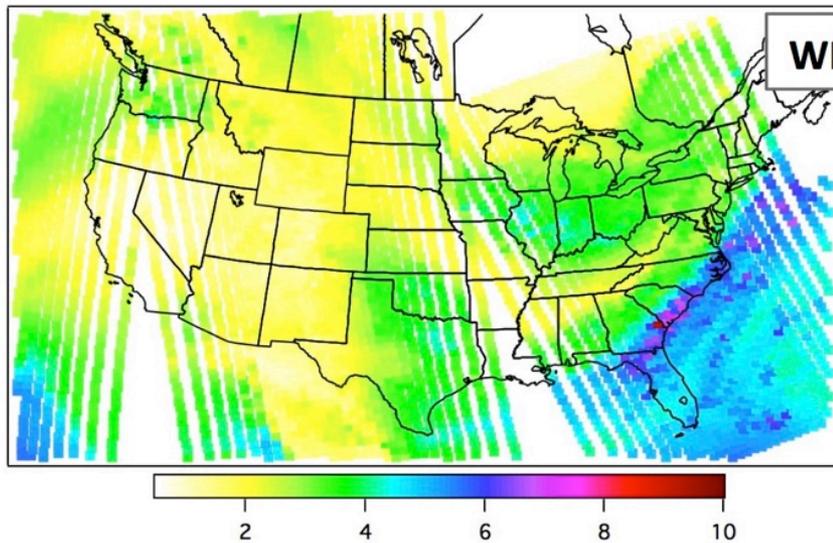
CrIS CH₄ Vertical Sensitivity



NUCAPS vs. WRF-Chem Model Comparison

6/29/13, 16:38-21:46 UTC, Total Precipitable Water (cm)

6/29/13, 16:38-21:46 UTC, mid-trop. CH₄ (ppbv)

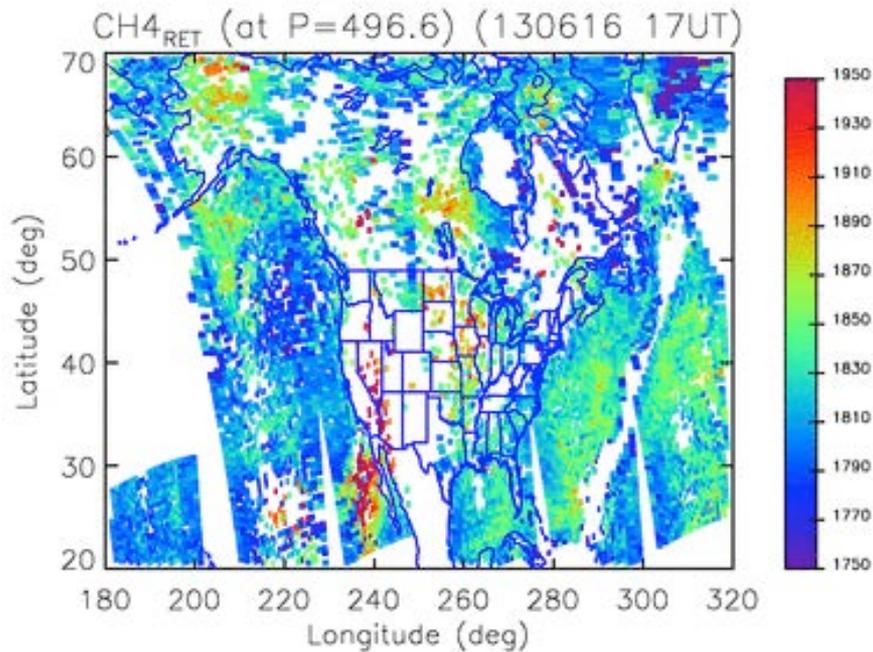


NUCAPS CH₄ Science Retrievals: Initial Data Processing Issues

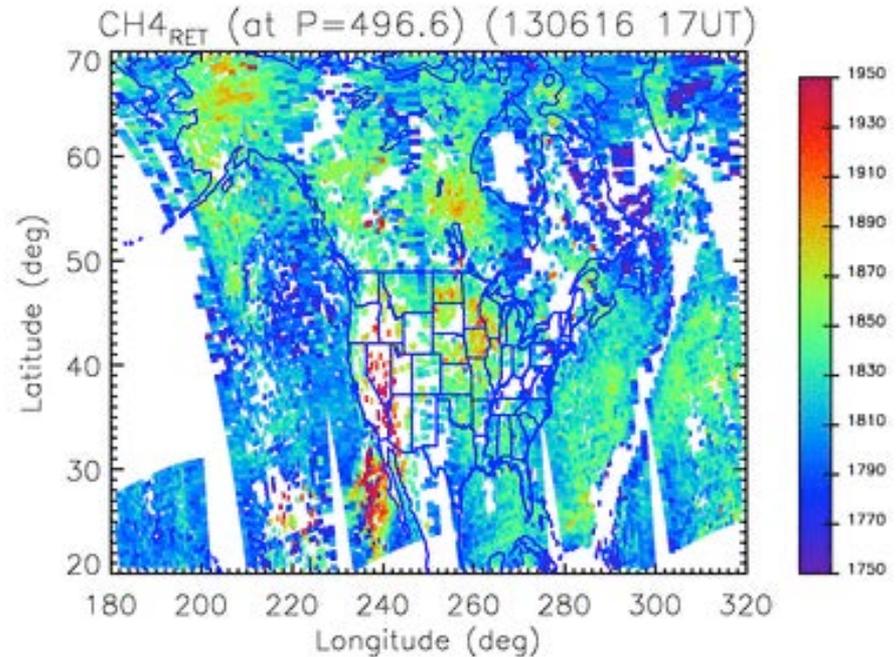
- Many granules not processed due to failures in pre-processor code, possibly from too stringent ATMS QC threshold
- “Acceptable” QC (QC = 0): Daytime data rejection >> nighttime over land, likely from too stringent CrIS QC threshold
- Very noisy CH₄ signal. Noise filter or averaging may be needed.
- CrIS averaging kernels not initially available

Improved NUCAPS Science Code Quality Control Thresholds

Before QC Changes

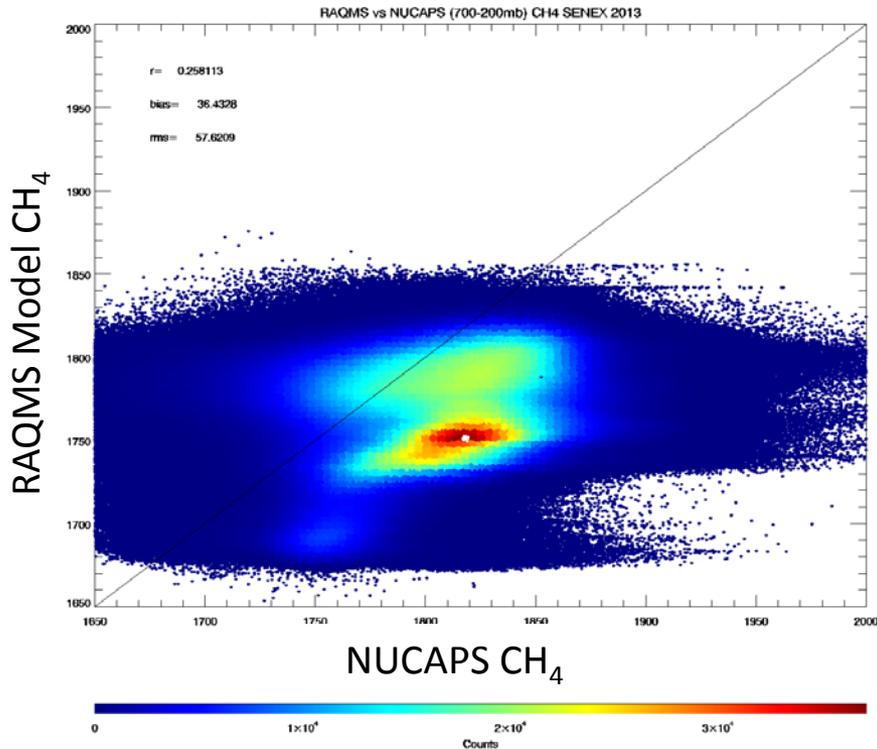


After QC Changes

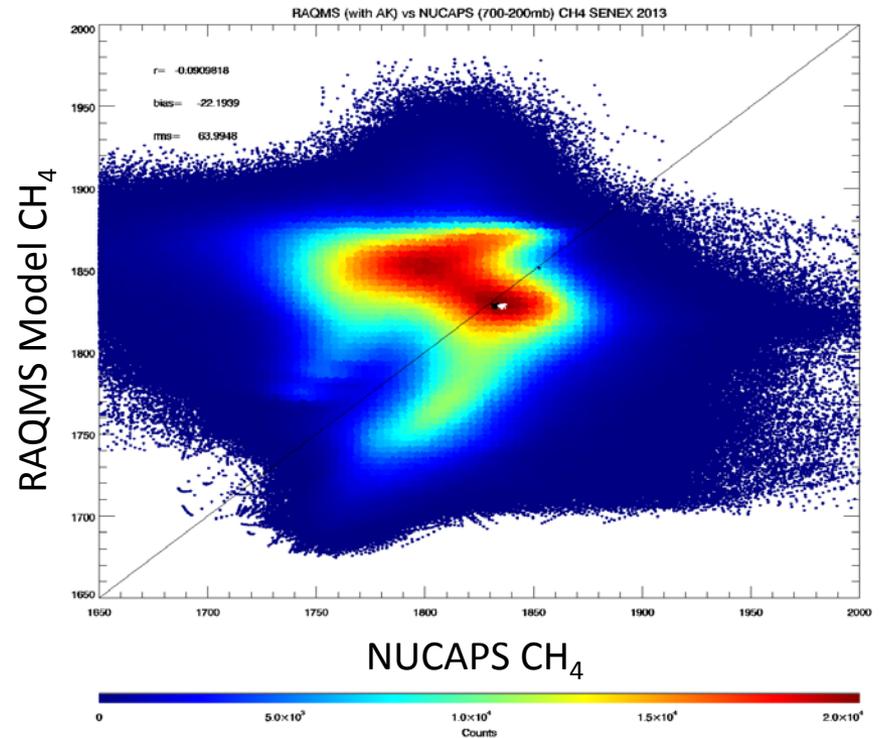


CrIS Averaging Kernels Now Available in Science Code Output

Model without AKs



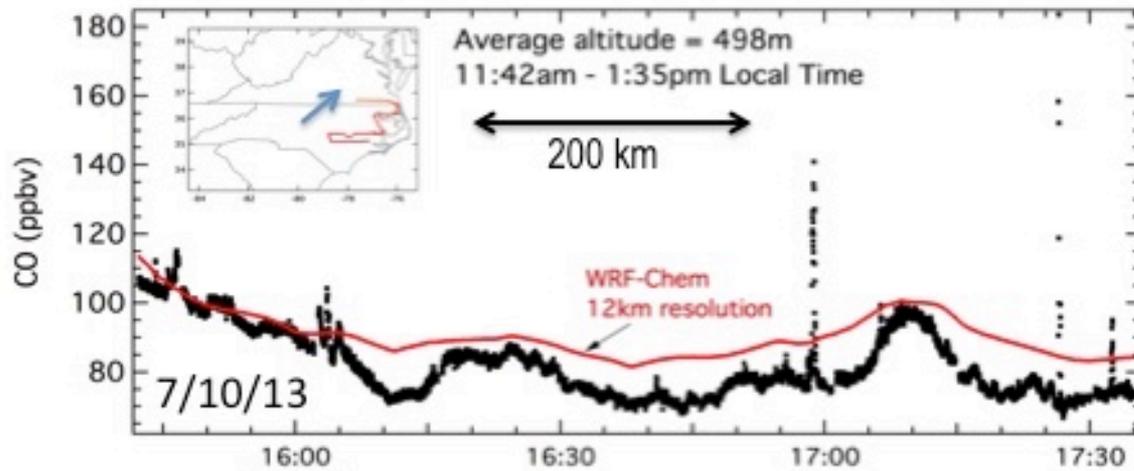
Model with AKs



Analyzing Scale Dependence of Variance

Compare SENEX-2013 aircraft and WRF-Chem model CO

Time Series



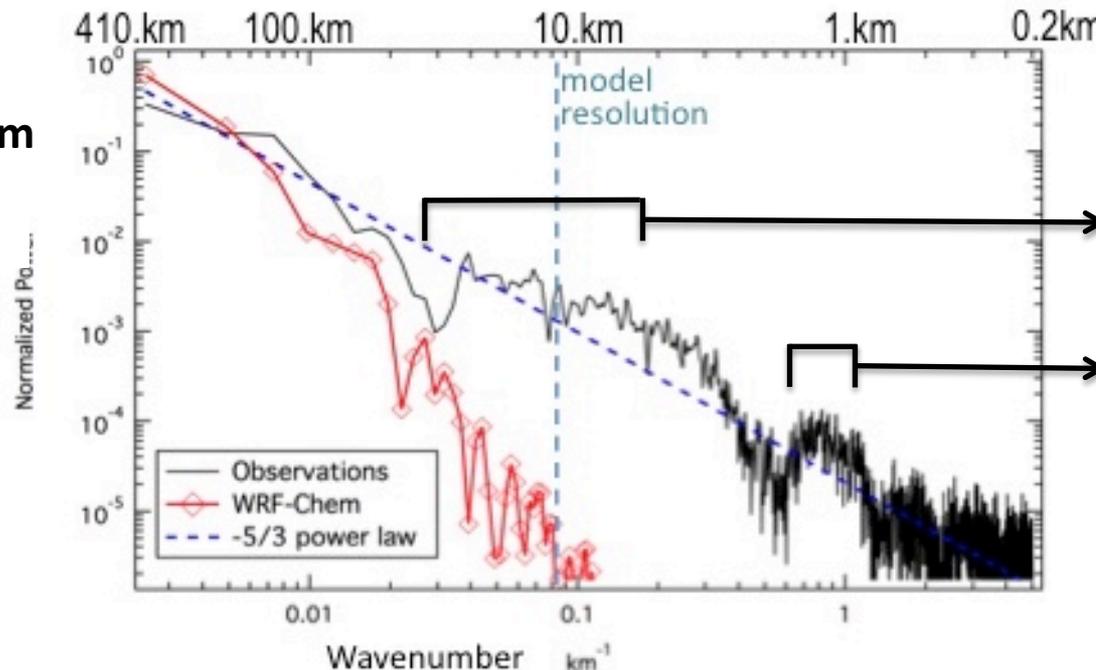
Urban Plumes:

15:50 Raleigh/Durham
16:20 Greenville
17:10 Fayetteville

Burning Plumes:

Throughout transect

Fourier Transform Power Spectra



Length Scale

5-30 km scale:

combustion source areas
(cities and towns)

1-2km scale:

Agricultural burn plumes

Power Spectra of CO depends on both emissions and transport

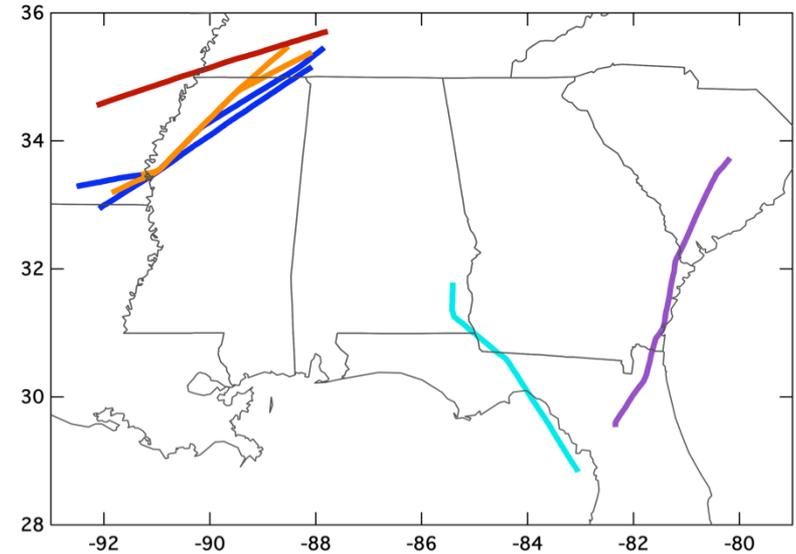
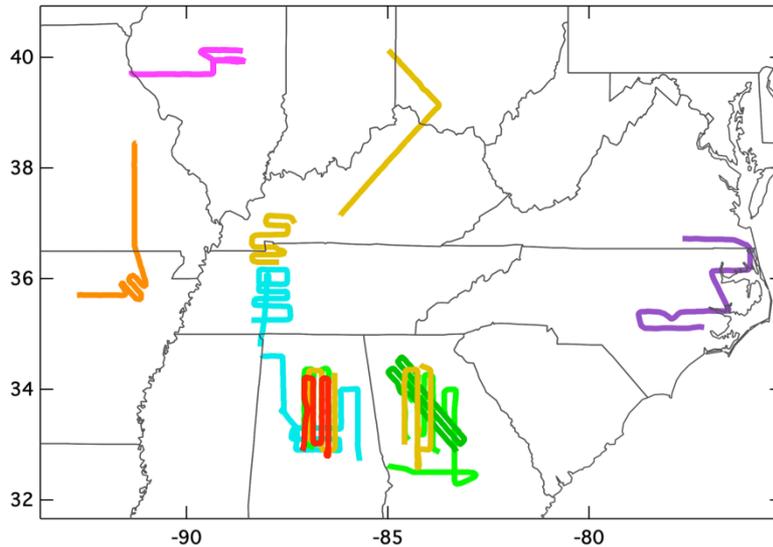
Model spectra somewhat similar to observations for length scales $> 4\Delta x$

Comparing Average Power Spectra: Aircraft and Model

SENEX 2013 flights within the boundary layer and at high altitude (~500mb)

14 Daytime PBL transects (300-700 m AGL)

7 Hi Altitude transects (480-530 mb)



14 transects, 10:00am-6:00pm EDT,
with $N > 4096$ for 1-Hz data

21.6 Hours of flight time

7 transects, day and night,
with $N > 2048$ for 1-Hz data

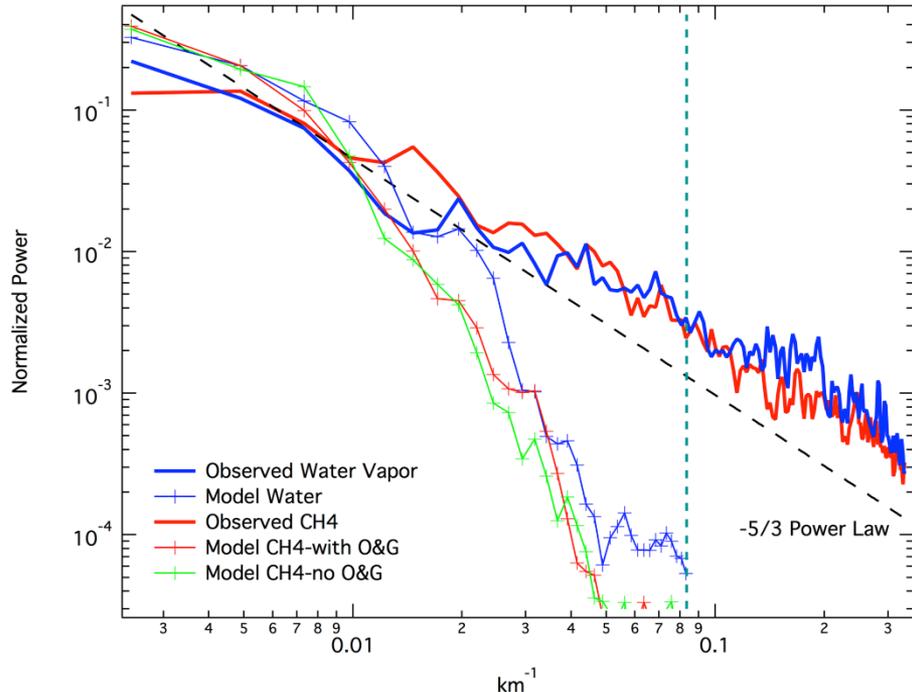
5.4 Hours of flight time

Comparing Average Power Spectra: Aircraft and Model

CH₄ and H₂O mixing ratios within the boundary layer and at high altitude (~500mb)

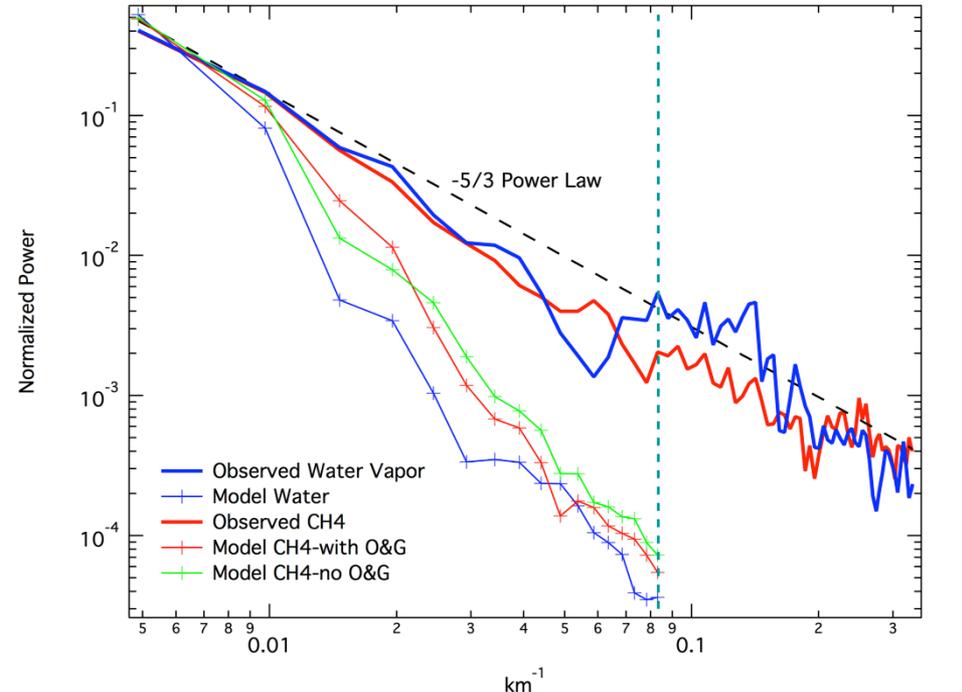
14 Daytime PBL transects (300-700 m AGL)

410.km 100.km 33.km 10.km 3.3km



7 Hi Altitude transects (480-530 mb)

200.km 100.km 33.km 10.km 3.3km



Power spectra for CH₄ and H₂O show similar slopes and tendencies.

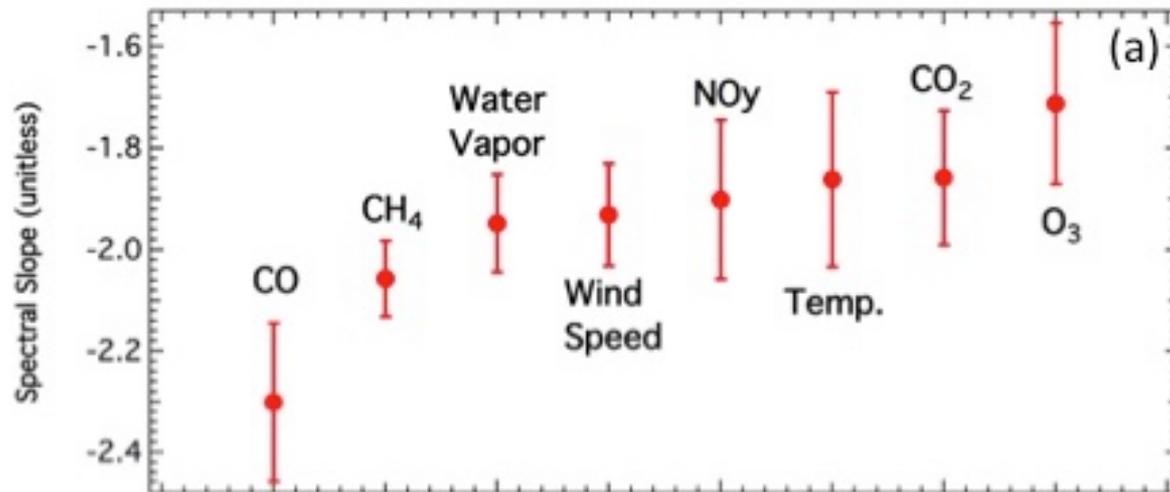
At high altitude the slope is about -5/3 for longer (>50 km) length scales.

Model H₂O vapor captures variability for length scales > 3ΔX in the PBL, > 7ΔX at 500mb.

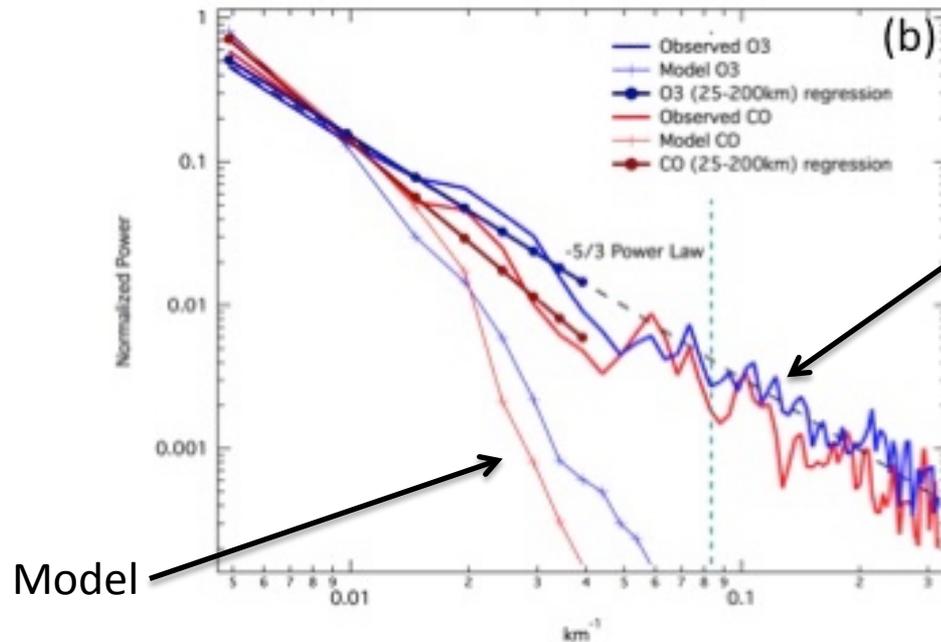
Adding/Removing model Oil/Gas emissions impacts CH₄ power spectra for both the PBL and high altitude transects.

Comparing Average Power Spectra: Aircraft and Model

Data at high altitude (~500mb)



Aircraft power spectral slopes

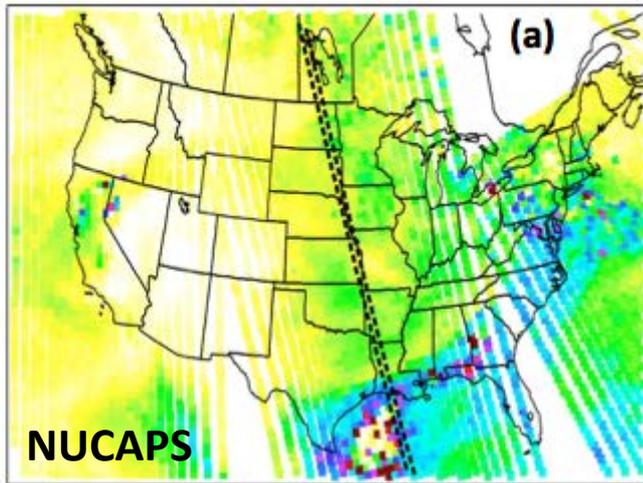


Aircraft

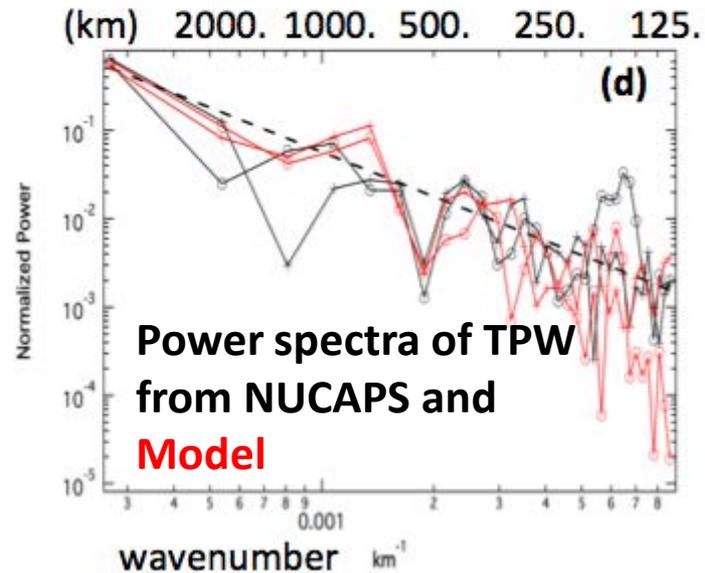
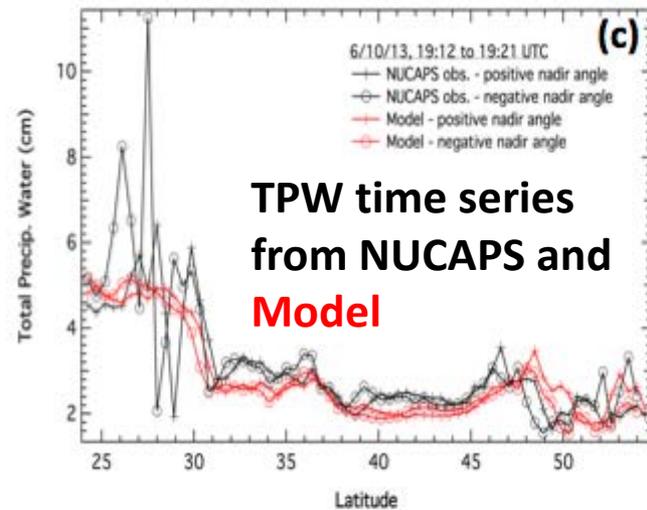
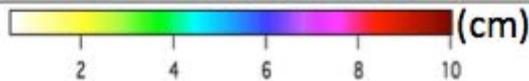
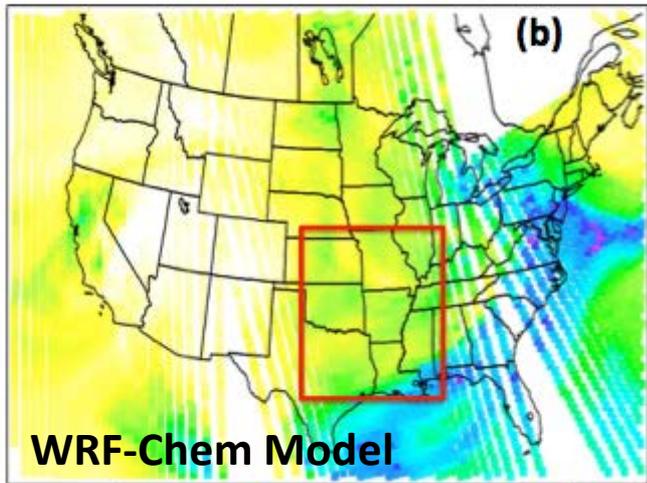
Model

Comparing Average Power Spectra: NUCAPS and Model

Total precipitable water (TPW) data, 6/10/13

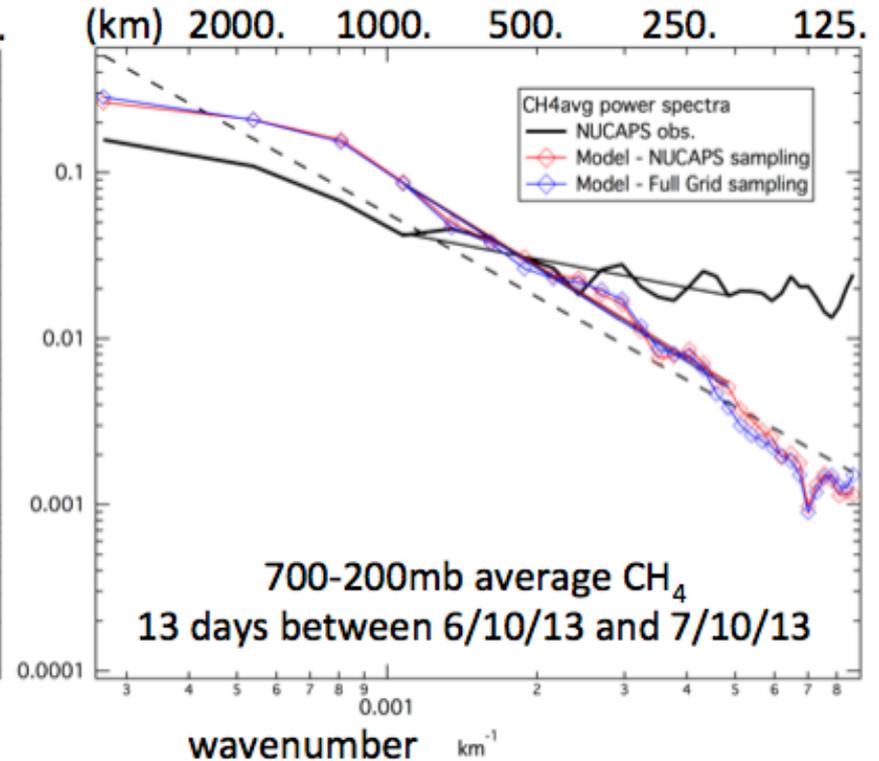
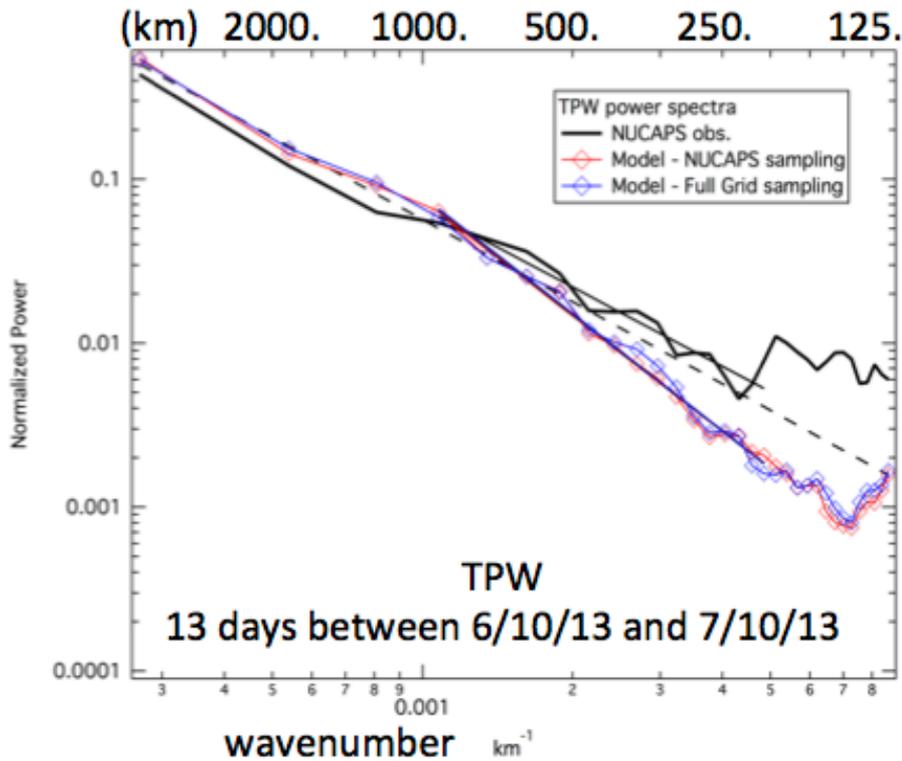


6/10/13, 15:56:59-21:02:00, integrated TPW



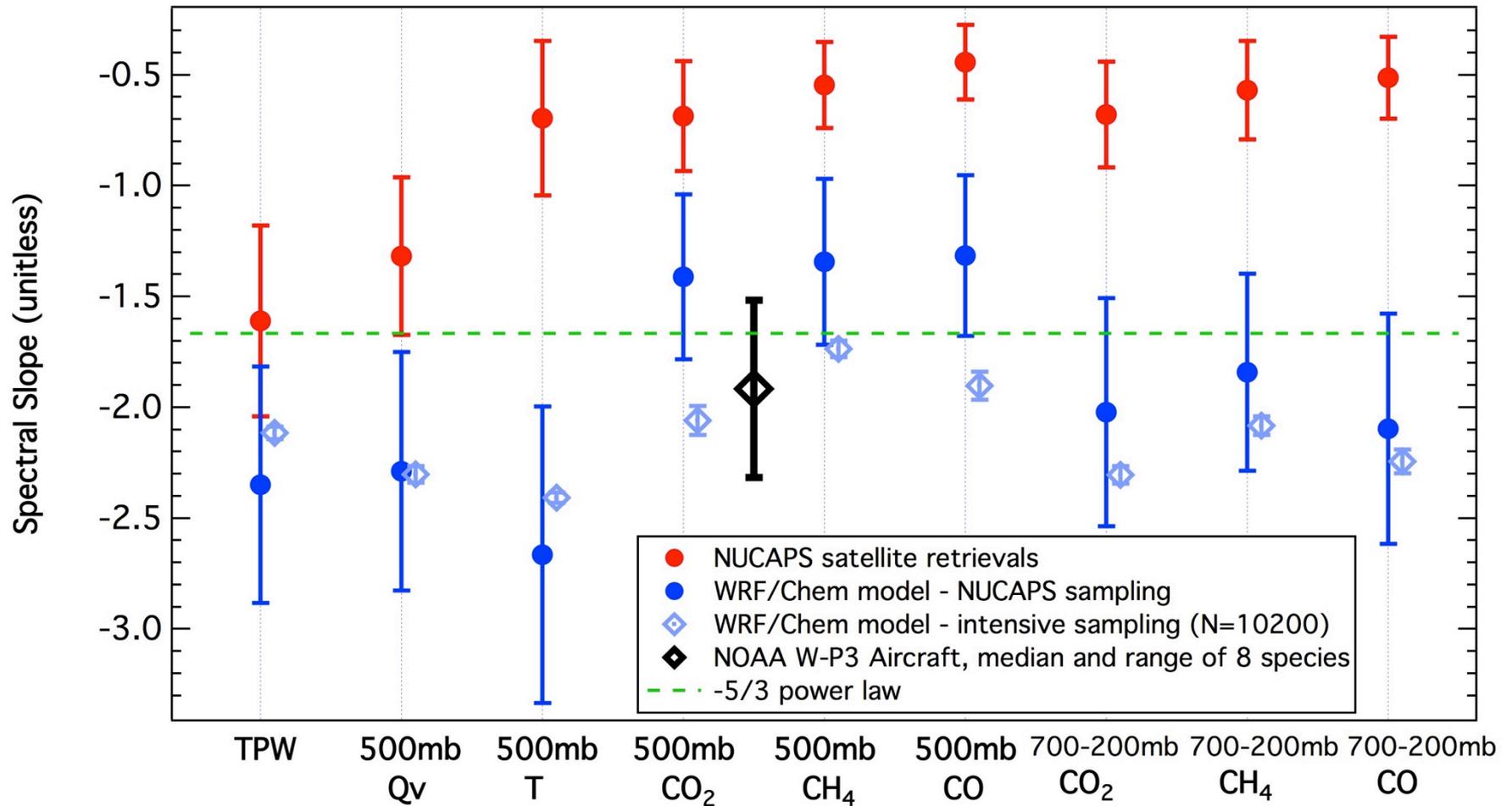
Comparing Average Power Spectra: NUCAPS and Model

TPW and CH₄ data, 13 days between 6/10/13-7/10/13



Comparing Average Power Spectra: NUCAPS and Model

6/10/13-7/10/13



Some Next Steps

- Use averaging kernels to scale model vertical sensitivity to match CrIS
- Incorporate updated NUCAPS data from science code processing and filter with revised quality control flags
- Examine alternative scale variance approaches beyond Fourier analysis to evaluate NUCAPS data
- Examine NUCAPS CH₄ and CO during other recent aircraft field experiments (2015 and beyond)



A Surface-to-Space Atmospheric Carbon Observing System for Decision Support

Arlyn Andrews

NOAA Earth System Research Laboratory



STAR JPSS 2016 Annual Science Team Meeting
8-12 August 2016

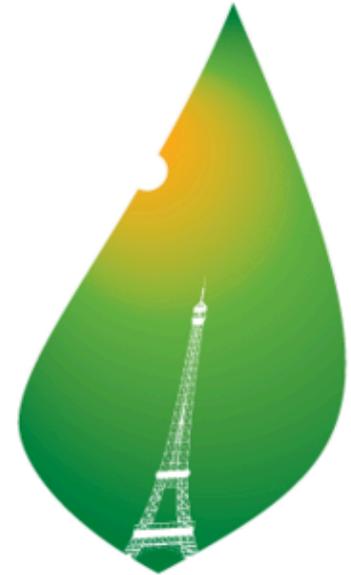
Outline

- Current and planned surface, aircraft, and satellite measurements of atmospheric CO₂ and CH₄
- Magnitude of important carbon emissions and sink signatures
- A vision for a future observing system to provide decision support services

Focus here is on CO₂, but story for CH₄ is similar.

There is broad and growing consensus that rising atmospheric CO₂ is a planetary emergency:

- The Paris Agreement at the 21st Conference of the Parties of the UNFCCC was negotiated by representatives of 195 countries.
- The agreement opens for signature on Earth Day, 22 April 2016. Some 120 countries, including the US and China, are expected to sign.



PARIS2015
CONFÉRENCE DES NATIONS UNIES
SUR LES CHANGEMENTS CLIMATIQUES
COP21·CMP11



United Nations
Framework Convention on
Climate Change

Data Transparency: New Dynamic at COP-21 in Paris

Posted by Angel Hsu, Andrew Moffat and Kaiyang Xu on Dec 22, 2015

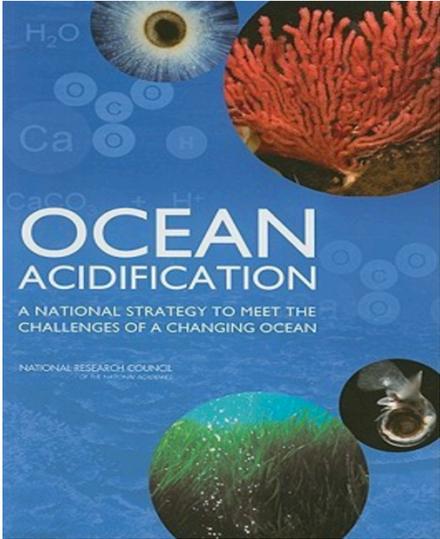
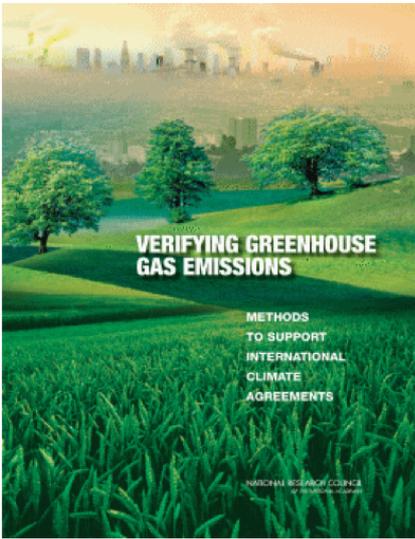
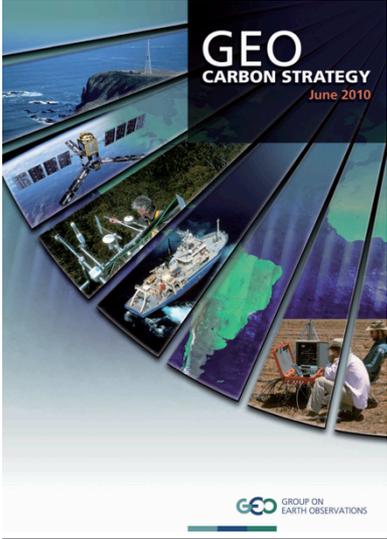
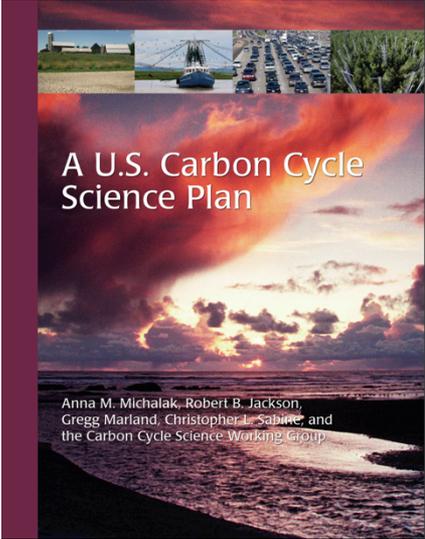


From the Paris Climate Negotiations

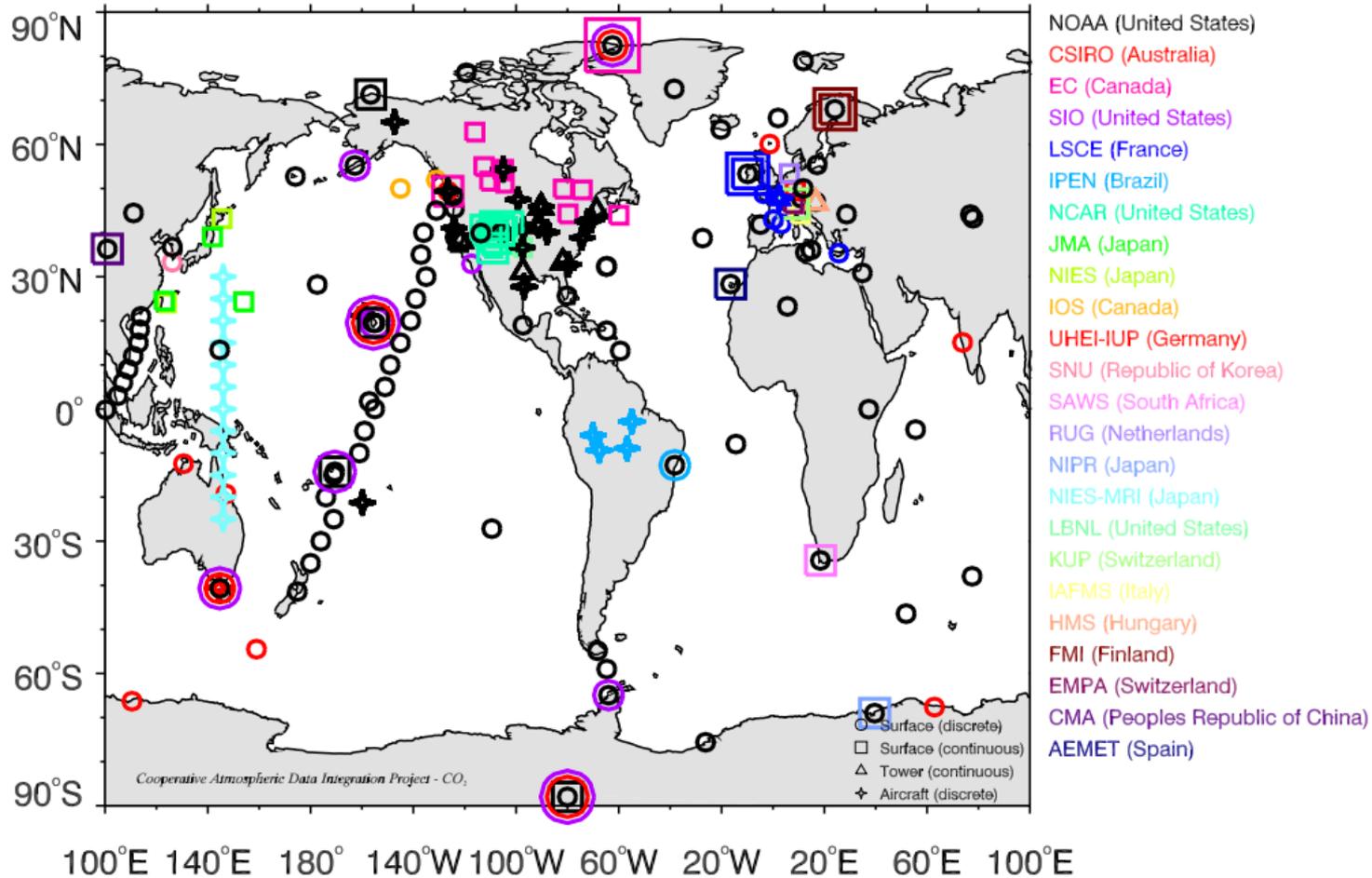
The **Paris Agreement and decision** together mention “transparency” 30 times. Language is often open to interpretation, yet **the Agreement’s mandate is clear**: each country is to regularly provide standardized national GHG emissions inventories and “information necessary to track progress made in implementing and achieving its nationally determined contribution” (Article 13). This provision, part of an agreement signed by all Parties including the U.S. and China, marks a step forward toward gaining clarity on what the world is doing to address climate change.

There is an urgent need to transition carbon research efforts into a state-of-the-science greenhouse gas information system for decision support. Long-term monitoring of atmospheric CO₂ and CH₄ will be an essential component of this system.

Several recent reports describe measurement requirements for carbon observations to advance science and to support policy:



GLOBALVIEW-CO2, 2013

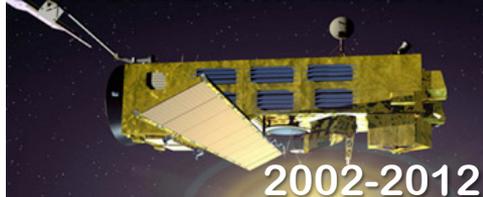


- Current knowledge of global CO₂ and CH₄ budgets is based primarily on in situ measurements, with satellite data products becoming available during the past decade.

The Evolving Near-Infrared Atmospheric Carbon Measurement Capabilities

PAST

EnviSat SCHIAMACHY



2002-2012

If carefully coordinated, these missions can be integrated into an ad hoc constellation and their measurements can be combined to produce a continuous data record.

PRESENT

GOSAT



2009 ...

OCO-2



2014 ...

However, none of these missions provides the capabilities needed to identify carbon/climate tipping points

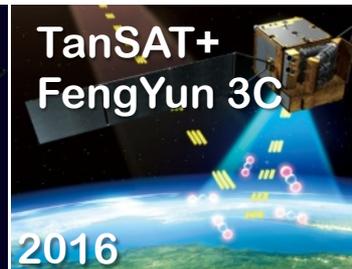
NEAR FUTURE

Sentinel 5p



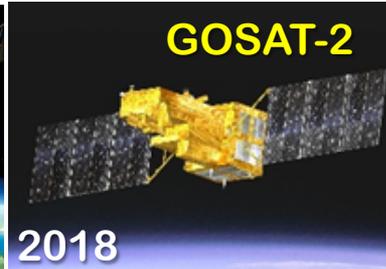
2016

**TanSAT+
FengYun 3C**



2016

GOSAT-2



2018

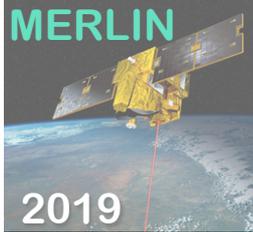
OCO-3/ISS



2018

LATER

MERLIN



2019

MicroCarb



202X

GOSAT-3



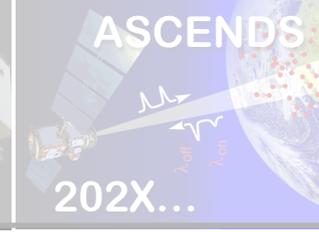
2023

Sentinel #



202X

ASCENDS



202X...

**GEO
Carbon**



202X...



Slide courtesy of Dave Crisp, NASA JPL

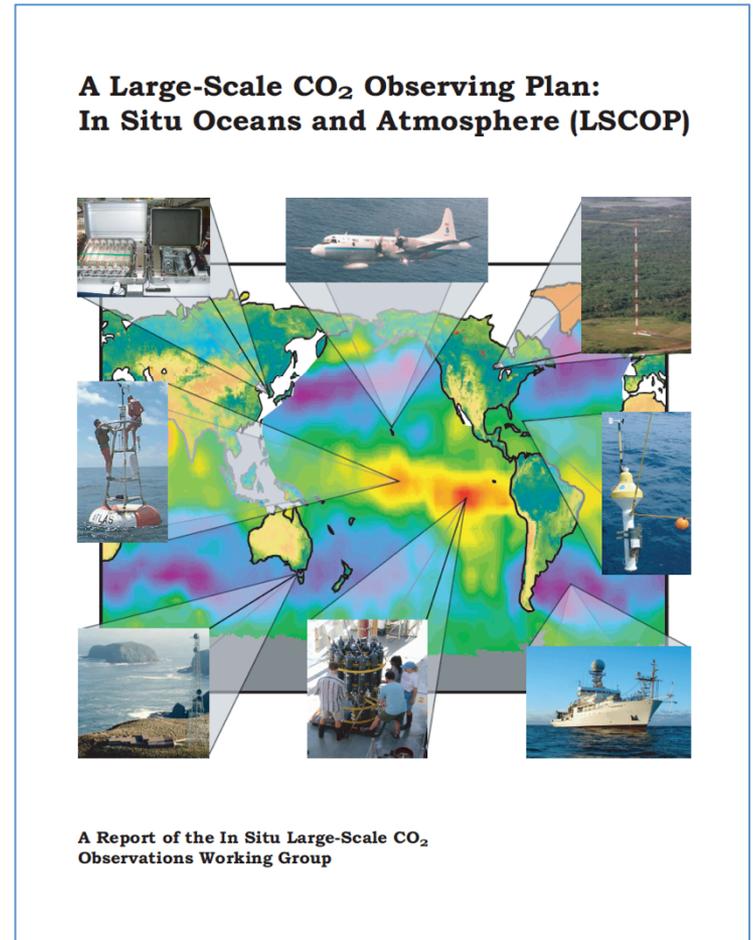
Tracking emissions and sink changes with atmospheric data:
A very hard problem

Tracking emissions and sink changes with atmospheric data: A very hard problem

In Situ Large-Scale CO₂ Observations Working
Group:

Bender, M., S. Doney, R.A. Feely, I. Fung, N.
Gruber, D.E. Harrison, R. Keeling, J.K. Moore,
J. Sarmiento, E. Sarachik, B. Stephens, T.
Takahashi, P. Tans, and R. Wanninkhof

Note: the report covers oceanic and
atmospheric observations, but for this talk
focus is on atmospheric measurements.



A contribution to the implementation of the
U.S. Carbon Cycle Science Plan, April 2002

Our future observing system should have the following characteristics:

- Regional spatial resolution, down to 10^6 km² on the continents and 10^7 km² over the oceans, with an accuracy of 0.1 Gt C/yr. This resolution will enable meaningful quantification of processes regulating surface carbon exchange. An ability to see the effects on atmospheric CO₂ of specific processes and mechanisms on these spatial scales will allow a marked increase of confidence in our understanding and predictive capability.
- Integration of satellite observations. The in situ measurements should be able to stand on their own, but will be merged with satellite CO₂ data if and when these become available, providing crucial accuracy to the latter. Space-based observations of the CO₂ mole fraction in the atmospheric column are expected to have nearly complete spatial coverage, but lower chemical resolution and accuracy.
- Assimilation of all available data. Data assimilation models must be an integral part of the observing system. The models should assimilate weather and CO₂ observations, and remotely sensed indicators of primary productivity. They should be high resolution in time and space, dynamically consistent, and include carbon processes.

Magnitude of atmospheric signature of various carbon fluxes:

Table 2-1: Rate of change in integrated vertical column abundance for specific CO₂ sources and sinks.

Source	Assumptions	ppm/day
Los Angeles Basin	12×10^6 people, 4,000 km ² , 1100 mol C/person/day	+10
Netherlands	16×10^6 people, 40,000 km ² , 500 mol C/person/day	+0.6
Germany	83×10^6 people, 350,000 km ² , 580 mol C/person/day	+0.4
Photosynthetic Uptake	Harvard Forest, July	-1.2
U.S. Carbon Sink	1 Gt C/yr, constant in time, uniform over the lower 48 states	-0.08
Southern Oceans	$\Delta p\text{CO}_2 = -30 \mu\text{atm}$, wind 15 m/s	-0.06
Eastern Equatorial Pacific	$\Delta p\text{CO}_2 = 100 \mu\text{atm}$, wind 7 m/s	+0.04

If residence time of air over Los Angeles Basin is ~3 hours, then column signal downwind would be 1.25ppm.

Signal comparisons and measurement requirements for continental-scale fluxes

Source or Sink	Emission Rate (GT C / year)	Column CO ₂ signal downwind of continent (ppm)
US fossil fuel emissions	1.4	0.7
20% emissions reduction	0.28	0.14
Biological Uptake during July	5.8	2.9
Climate Induced terrestrial anomalies	0.2	0.1

Detection of subtle signals resulting from changes in emissions and from climate-induced biological flux anomalies will require sensitivity of ~0.1 ppm in X_{CO_2} maintained over many years.

Space-based observations of megacity carbon dioxide

Eric A. Kort,^{1,2} Christian Frankenberg,² Charles E. Miller,² and Tom Oda^{3,4}

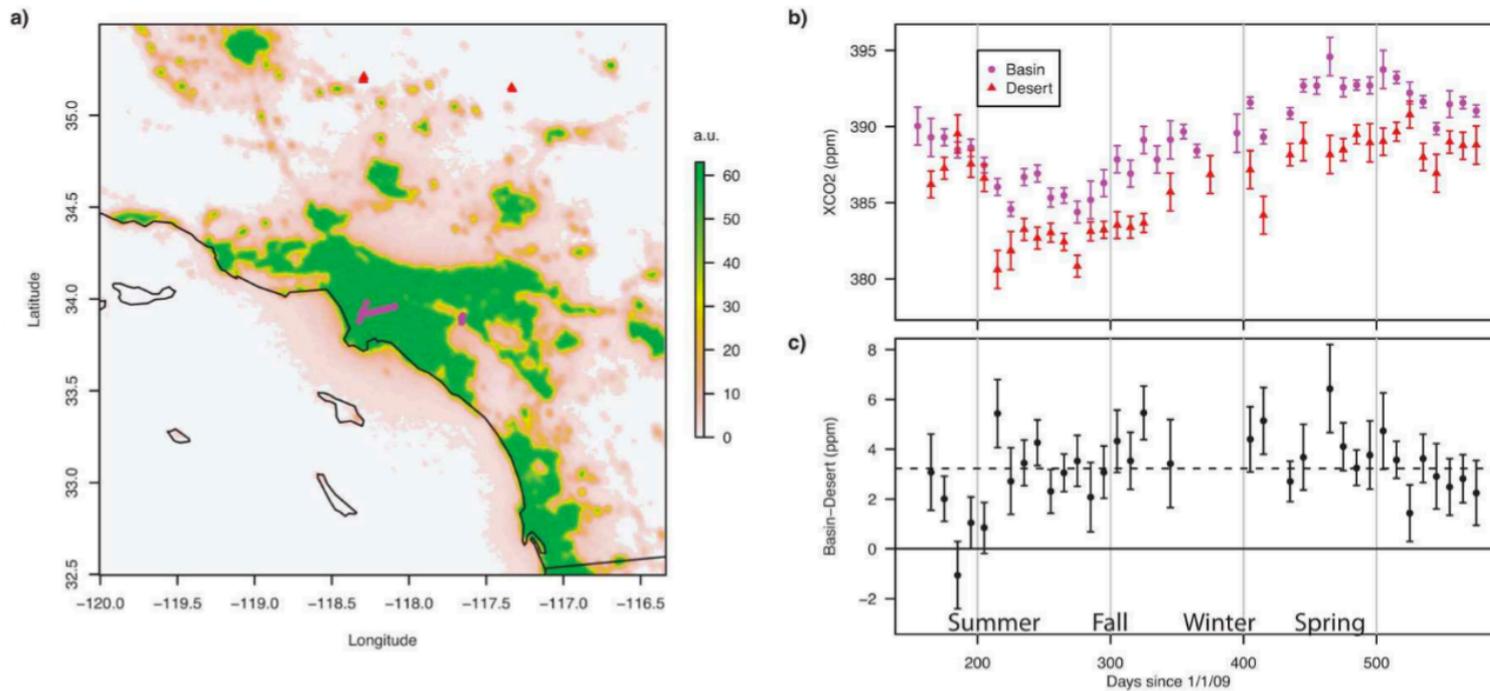
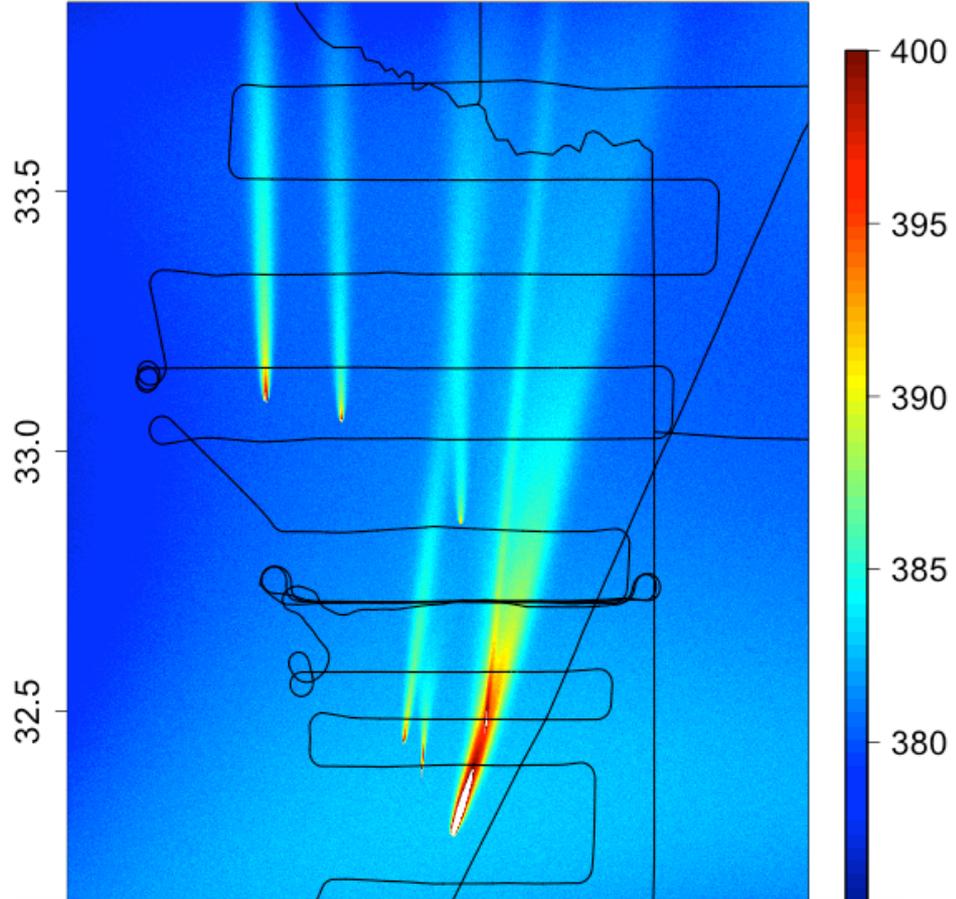
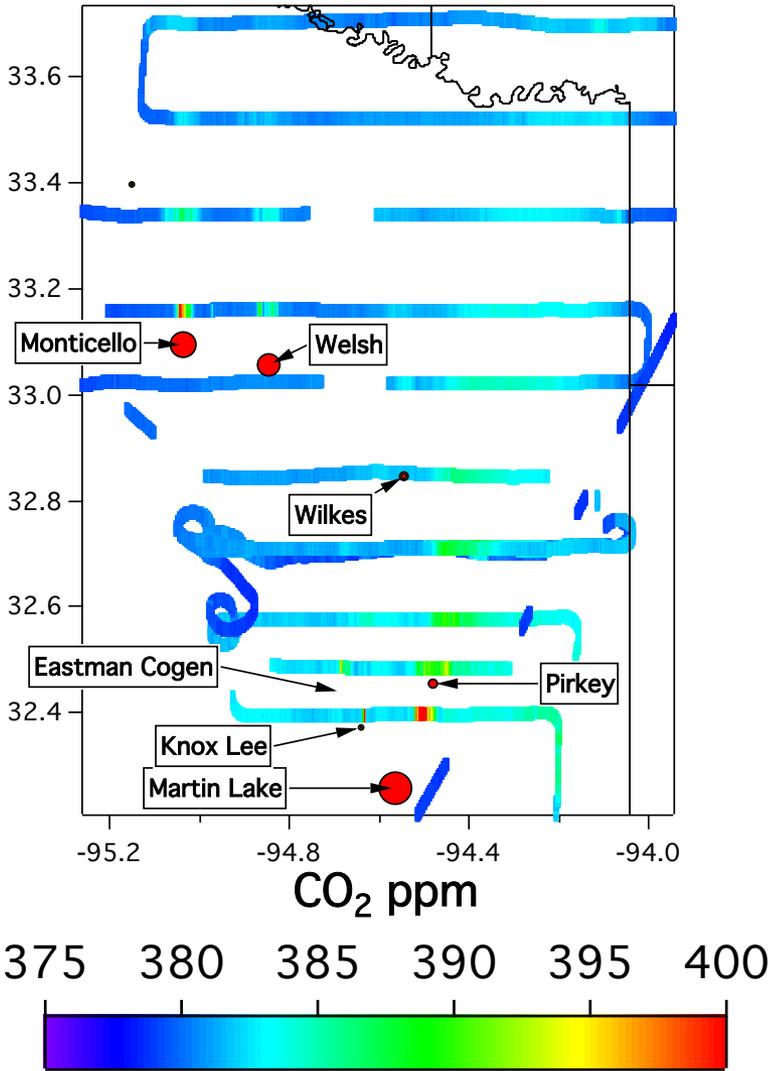


Figure 1. Observed X_{CO_2} urban dome of Los Angeles from June 2009 to August 2010. (a) Nightlights map of the Los Angeles megacity and surroundings. Selected GOSAT observations within the basin (pink circles near 34°N, 118°W) and in the desert (red triangles near 35°N, 117–118°W). (b) Time-series for basin and desert observations averaged in 10-day bins. (c) The difference between 10-day block averages of basin and desert observations. The dashed black line shows the average difference (3.2 ± 1.5 ppm). All error bars plotted are one-sigma. Note Bakersfield is located near 35.4°N, 119.0°W.

Power Plant Plume Sampling by the NOAA WP-3D Aircraft

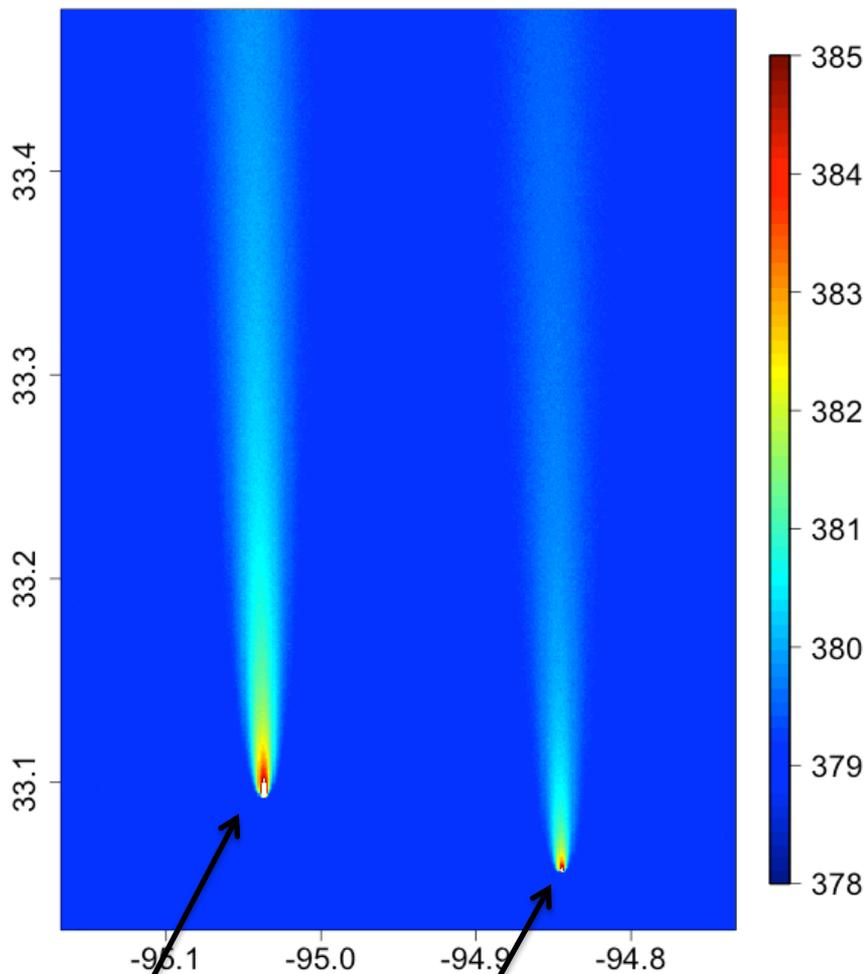
Texas: 16 Sept 2006



Use a simple plume model to create a 2D field representing the PBL integrated CO₂.

Total Column: XCO₂

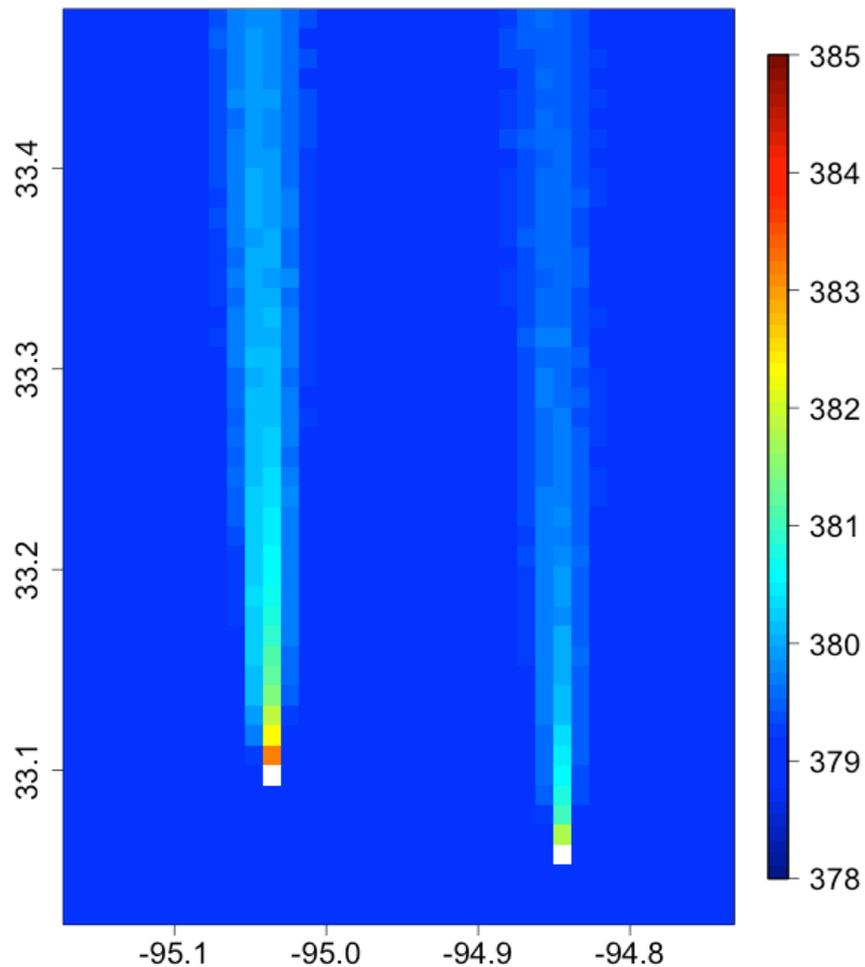
100m x 100m



Monticello

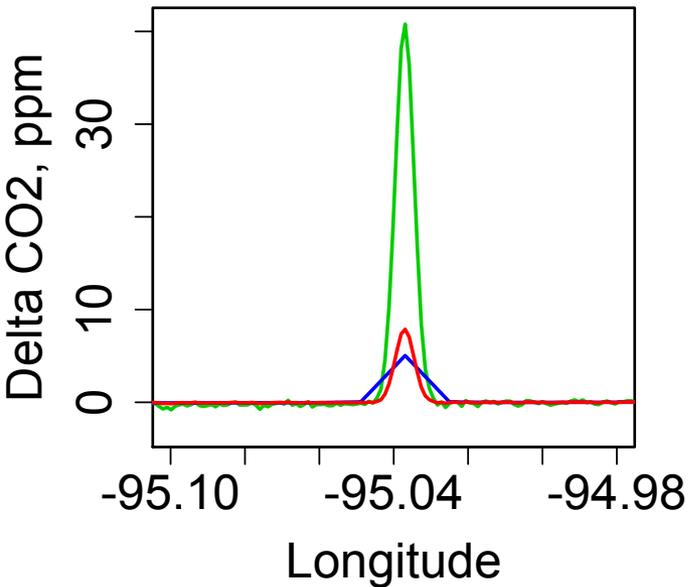
Welsh

1km x 1km



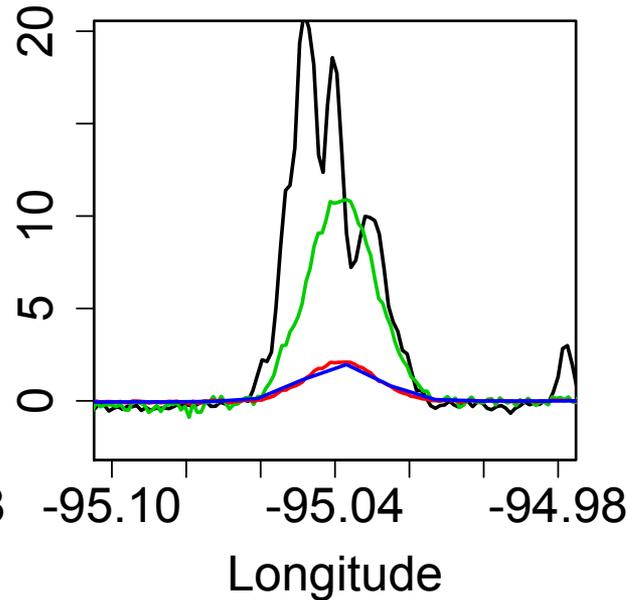
Monticello (18.3 MTon CO₂/yr, 1.98 GW)

0.5 km Downwind



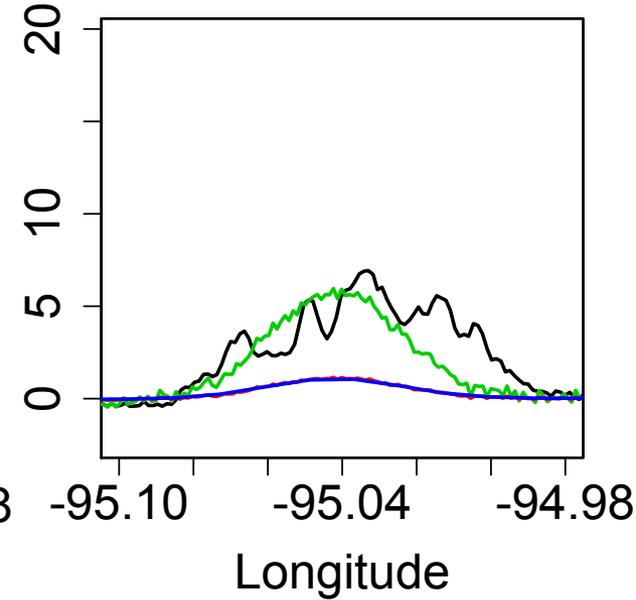
PBL: 40.8 ppm
XCO₂ 100m: 7.9 ppm
XCO₂ 1km: 5.0 ppm
No Obs

7.6 km Downwind



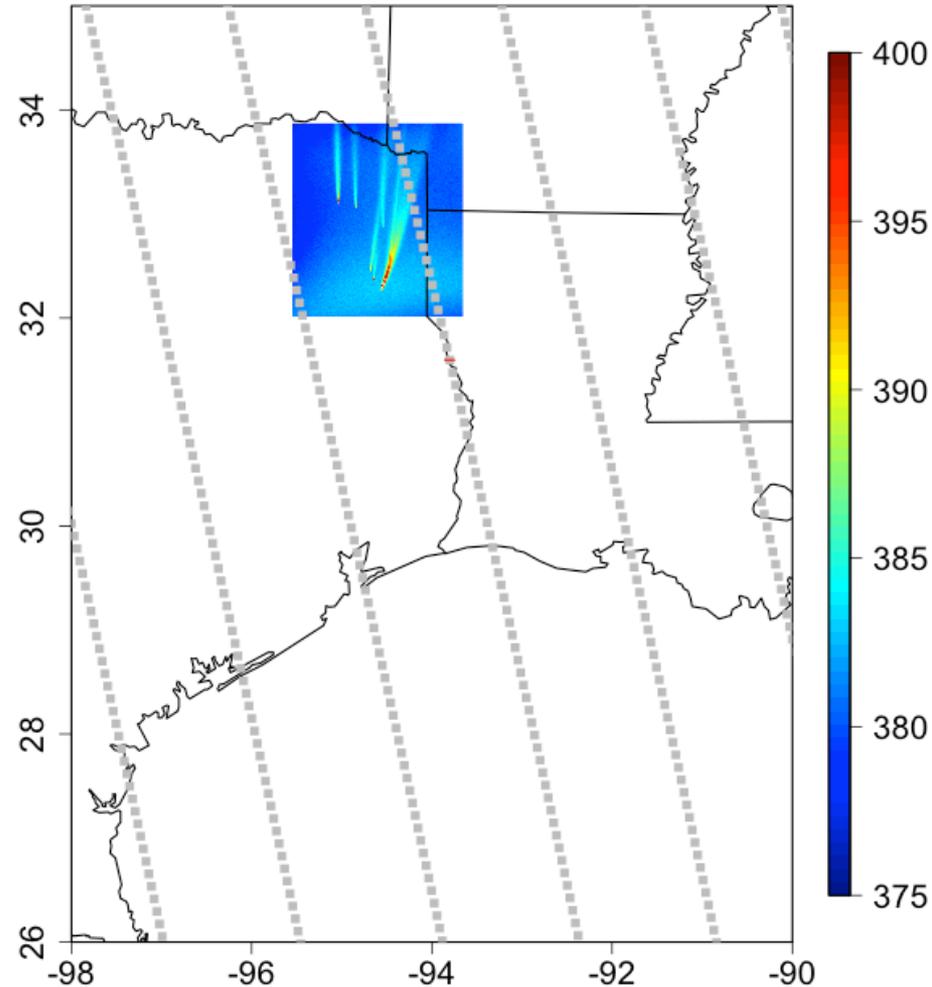
PBL: 10.9 ppm
XCO₂ 100m: 2.1 ppm
XCO₂ 1km: 1.97ppm
Obs: 600 magl

27.4 km Downwind



PBL: 6.0 ppm
XCO₂ 100m: 1.1 ppm
XCO₂ 1km: 1.0ppm
Obs: 600 magl

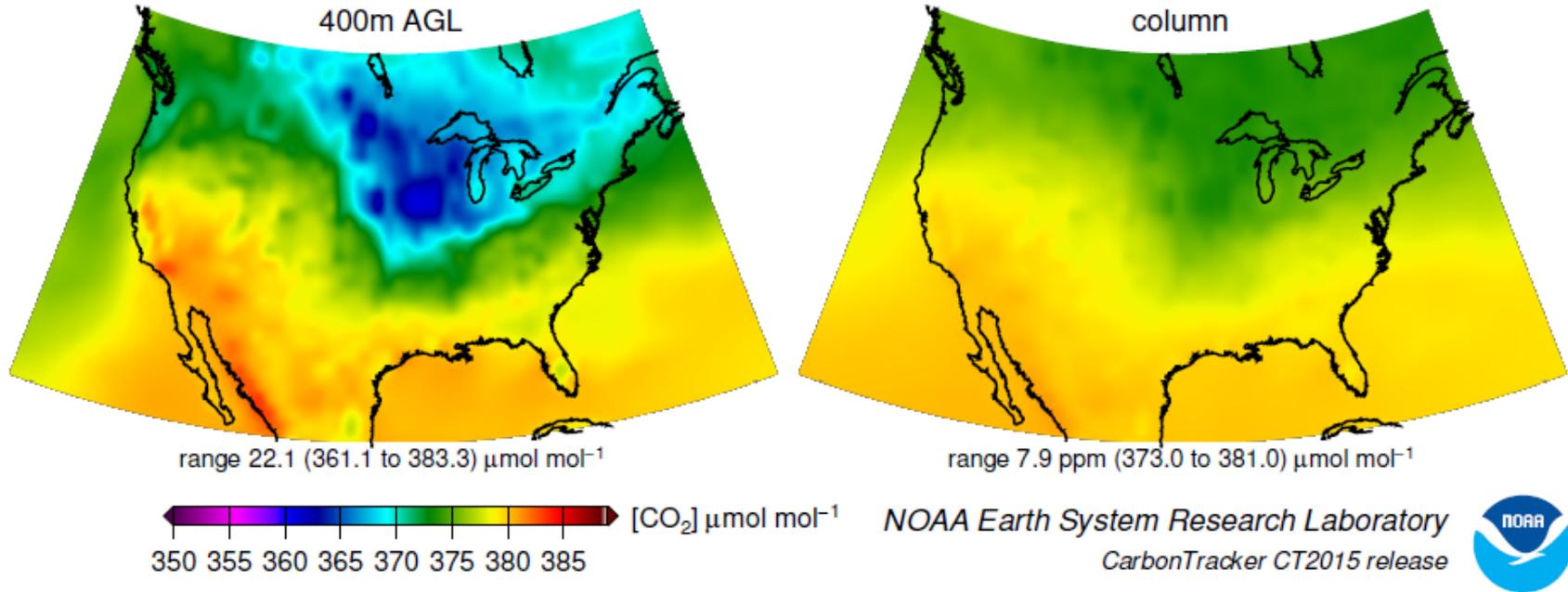
- Current and planned satellite CO₂ sensors do not have large enough field of view for emissions monitoring.
- Geostationary or Low Earth Orbiting mapping satellites have been proposed to monitor emissions from large point sources and urban areas.



OCO-2 swath width is ~10km. Figure shows A-train afternoon orbit with 10x10 km pixel size.

Boundary Layer versus Column CO₂:

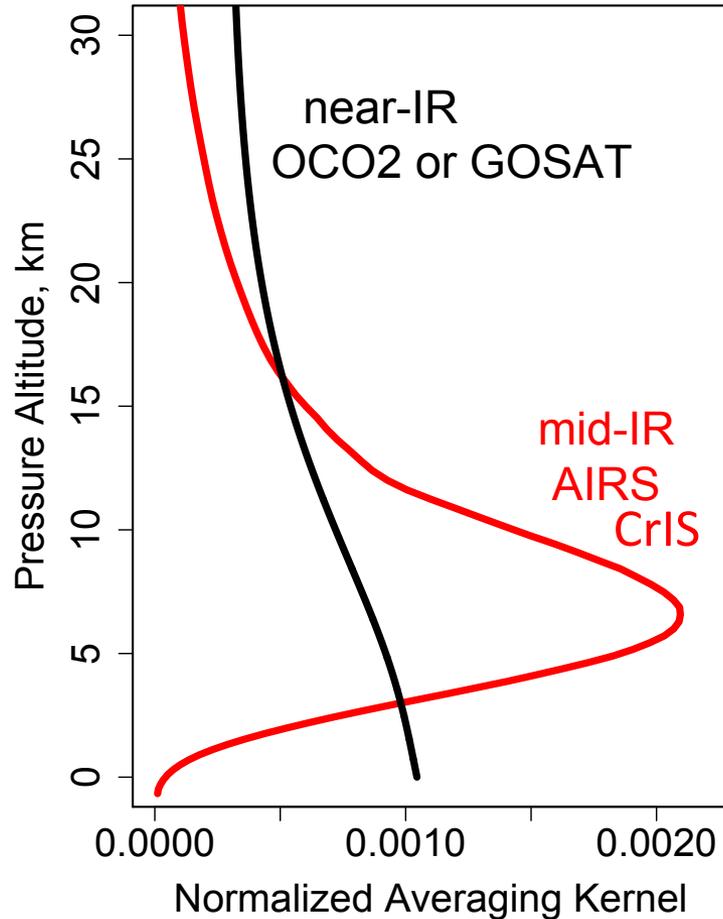
CarbonTracker July 2005 (mean) CO₂ sampled at 13:30 LST



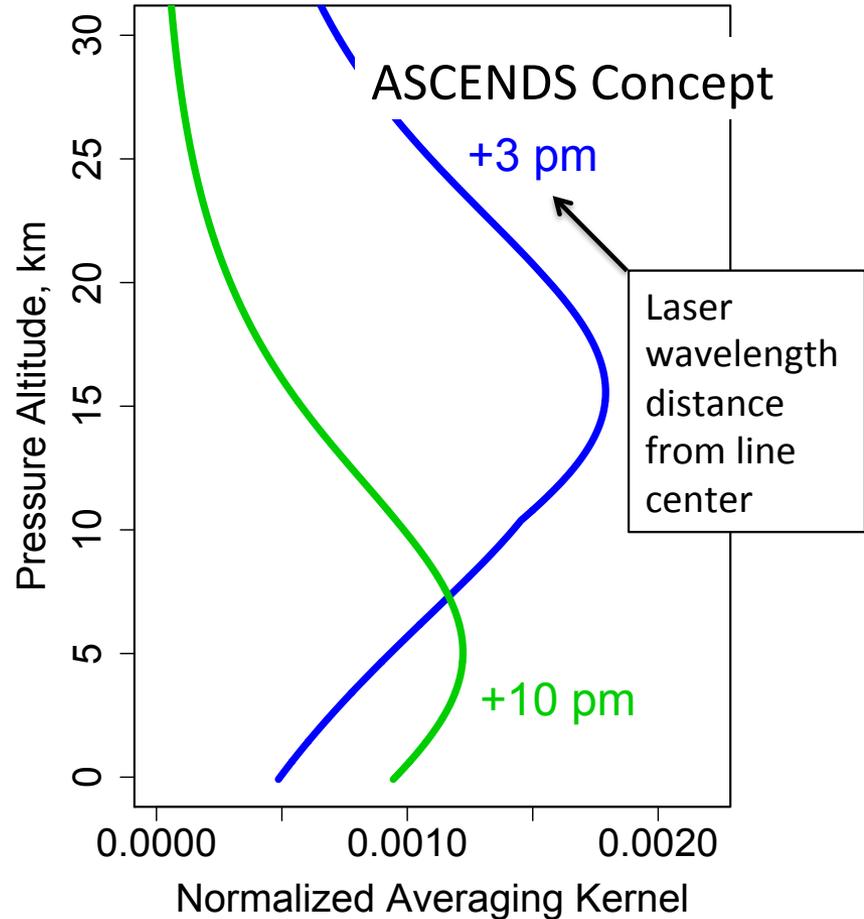
- Relevant signatures of CO₂ and CH₄ emissions are very small in the column -- detection with satellites will be extremely challenging.
- In situ measurements can be made very precisely, but measurements are sparse and variability in proximity to sources is large.

Satellite Sensor Averaging Kernels

PASSIVE



ACTIVE (Laser)



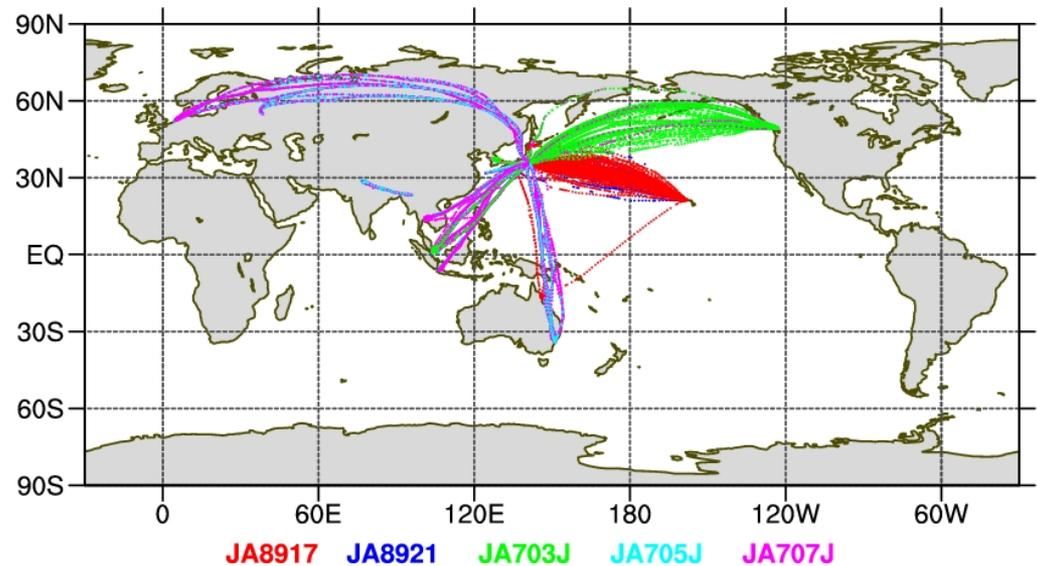
Combination of thermal-IR and near-IR satellite measurements should enable separation of boundary layer versus free-troposphere signals with rigorous data assimilation techniques.

Commercial aircraft are an underutilized platform for atmospheric sampling and could provide critical data for evaluating satellite retrievals and for flux estimation:

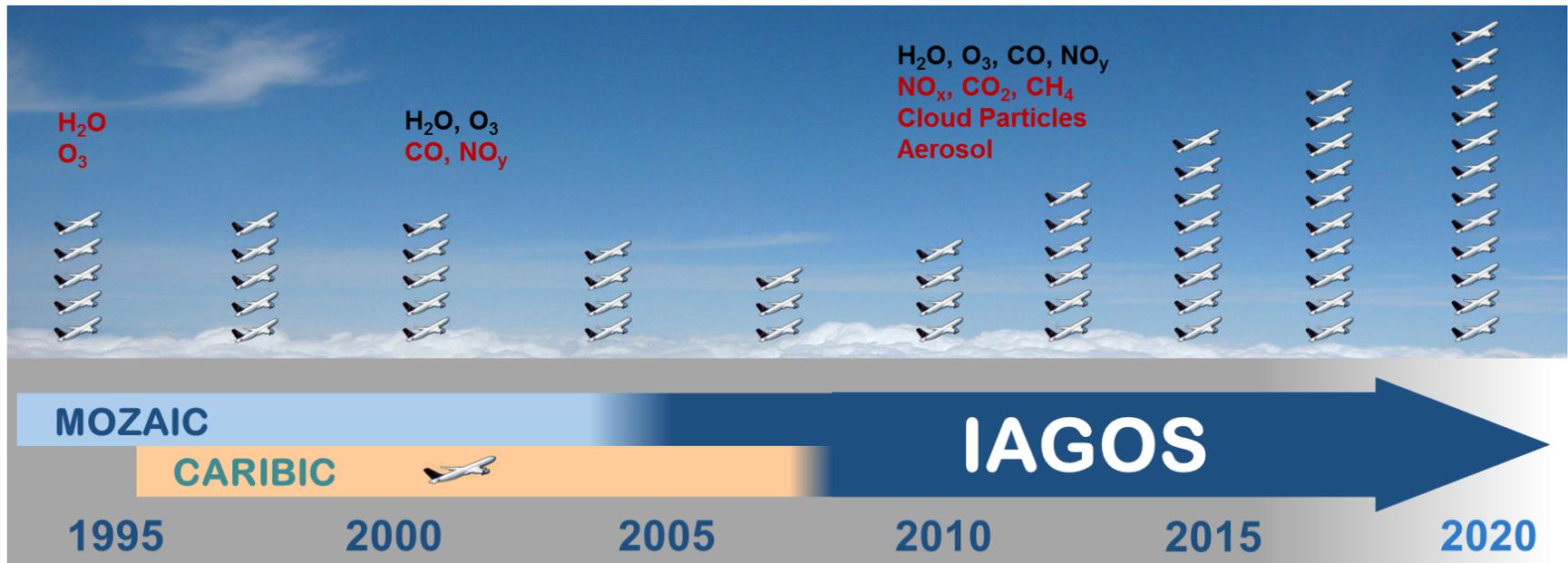
Japanese CONTRAIL program has been making continuous CO₂ measurements on Japan Airlines flights since 2005:



- Five aircraft
- 20 Airports
- >2000 vertical profiles



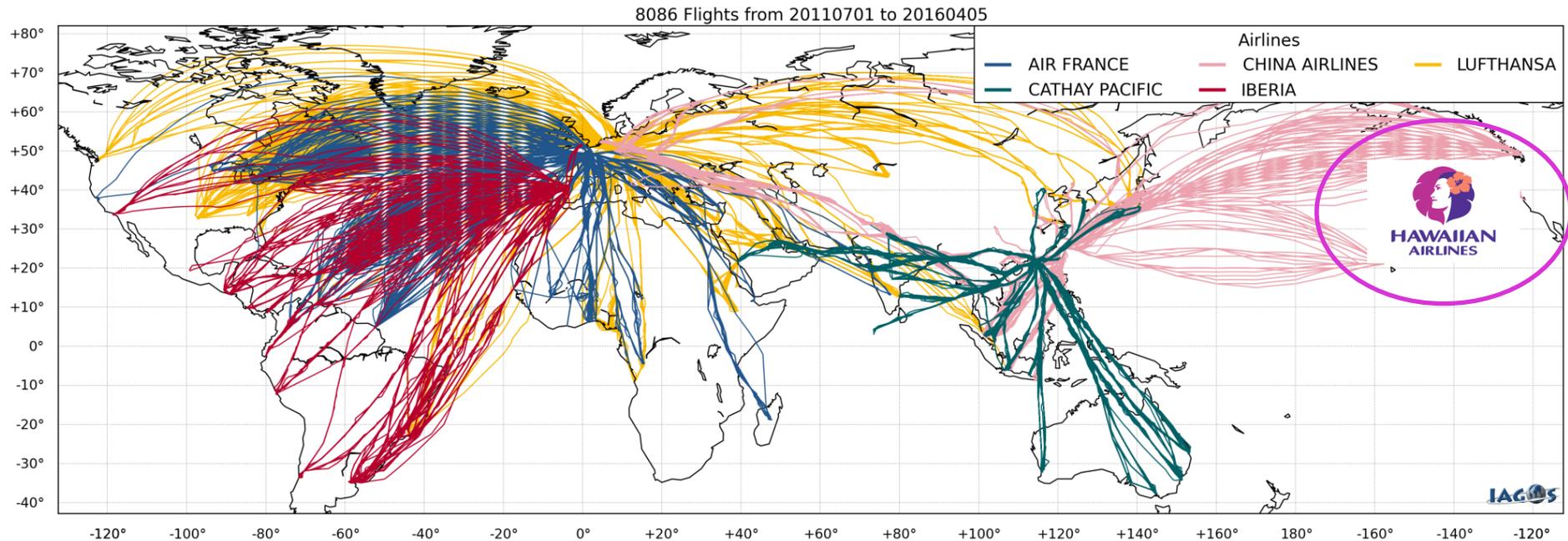
European In-service Aircraft for a Global Observing System (IAGOS)



Plans to add CO_2 and CH_4 as soon as certification is finalized.

IAGOS-CORE Flight Routes

> 8300 flights July 2011 - May 2016



NOAA already has the WVSS-2 commercial aircraft program for measuring water vapor from more than 100 commercial aircraft:

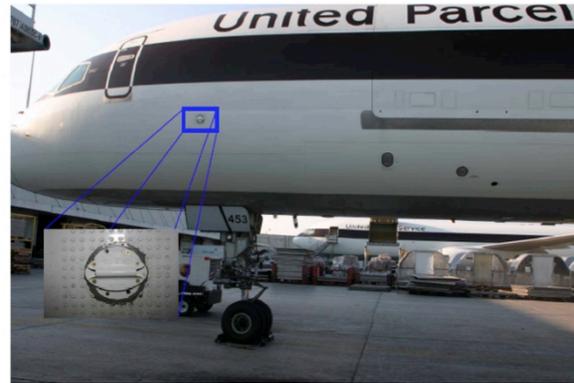
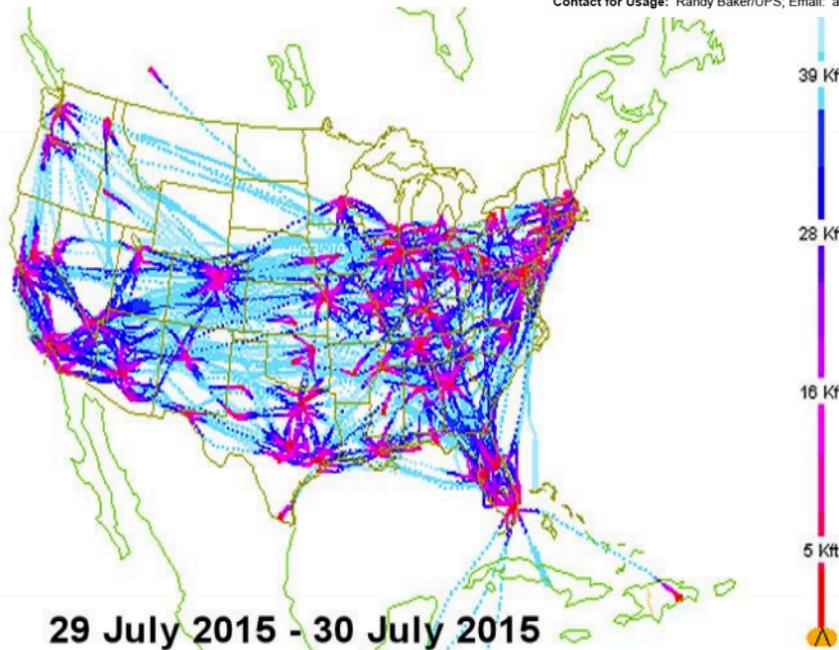


Photo Credit: UPS Dispatch
Contact for Usage: Randy Baker/UPS, Email: air1rtb@ups.com



29 July 2015 - 30 July 2015

29-Jul-2015 15:00:00 -- 30-Jul-2015 14:59:59 (71535 obs loaded, 69563 in range, 20643 shown)

Final Points

New investment and coordination of existing resources will be required to realize a global greenhouse gas information system for decision support.

- Sophisticated data assimilation systems are needed that can utilize in situ, near-IR and thermal-IR measurements.
- A thorough and coordinated approach is needed to evaluate retrievals from current and future greenhouse gas missions and to establish continuity across missions.
- Careful observing system design experiments are needed to evaluate cost, risk, and information content of proposed new measurements.



Quantifying Lower Tropospheric Methane Using Total Column (NIR) and Tropospheric (TIR) measurements

Authors

John R. Worden¹, Alex J. Turner², Anthony Bloom¹, Susan S. Kulawik³, Robert Parker⁴, and Vivienne H. Payne¹

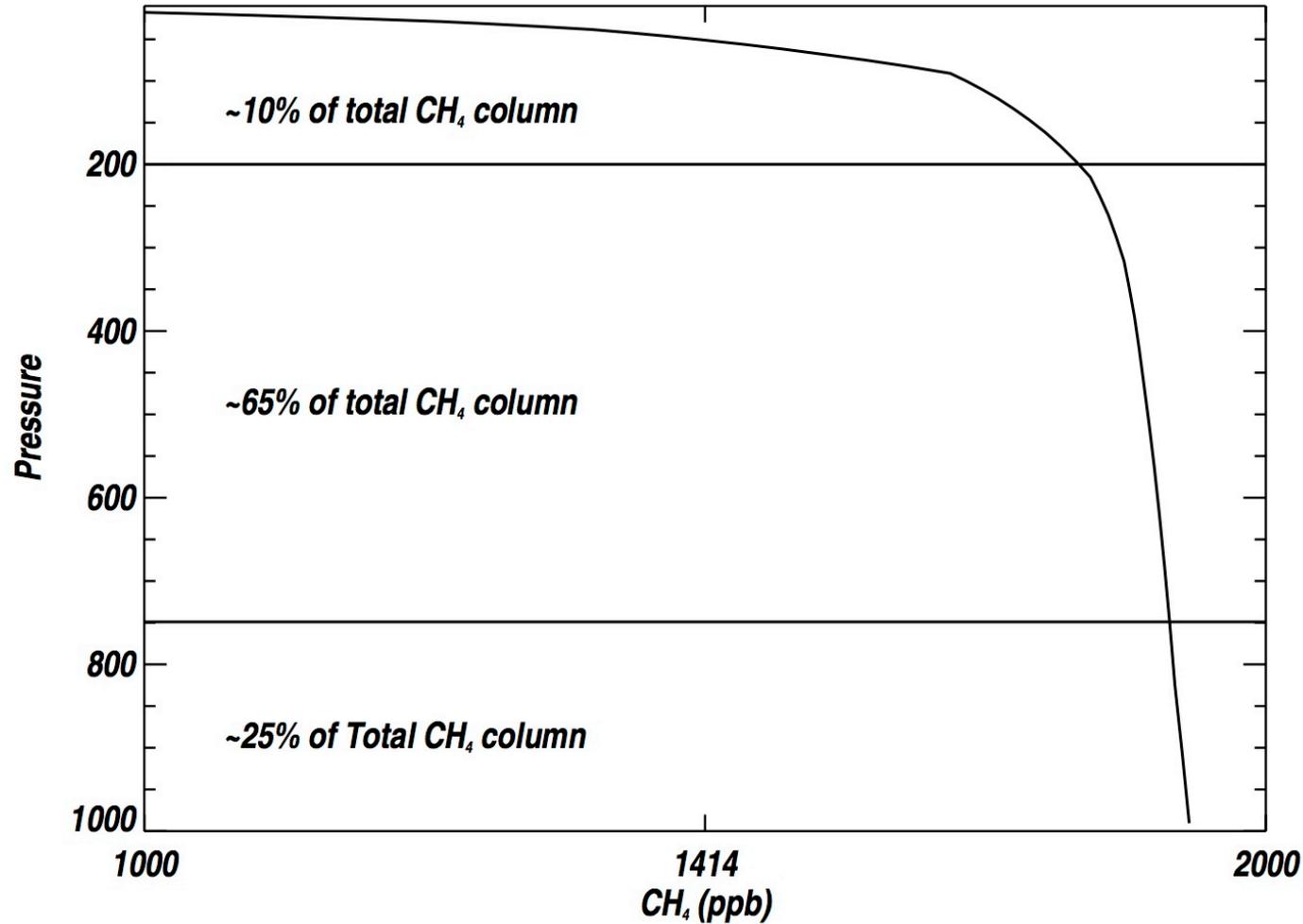
1. Earth Sciences Section, Jet Propulsion Laboratory / CalTech,
Pasadena USA

2. School of Engineering and Applied Sciences, Harvard
University, Cambridge MA, USA

3. Bay Area Environmental Research Institute, Mountain View CA,
USA

4. Dept. of Physics and Astronomy, University of Leicester,
Leicester, UK

Methane profile at ~55 N in July 2006

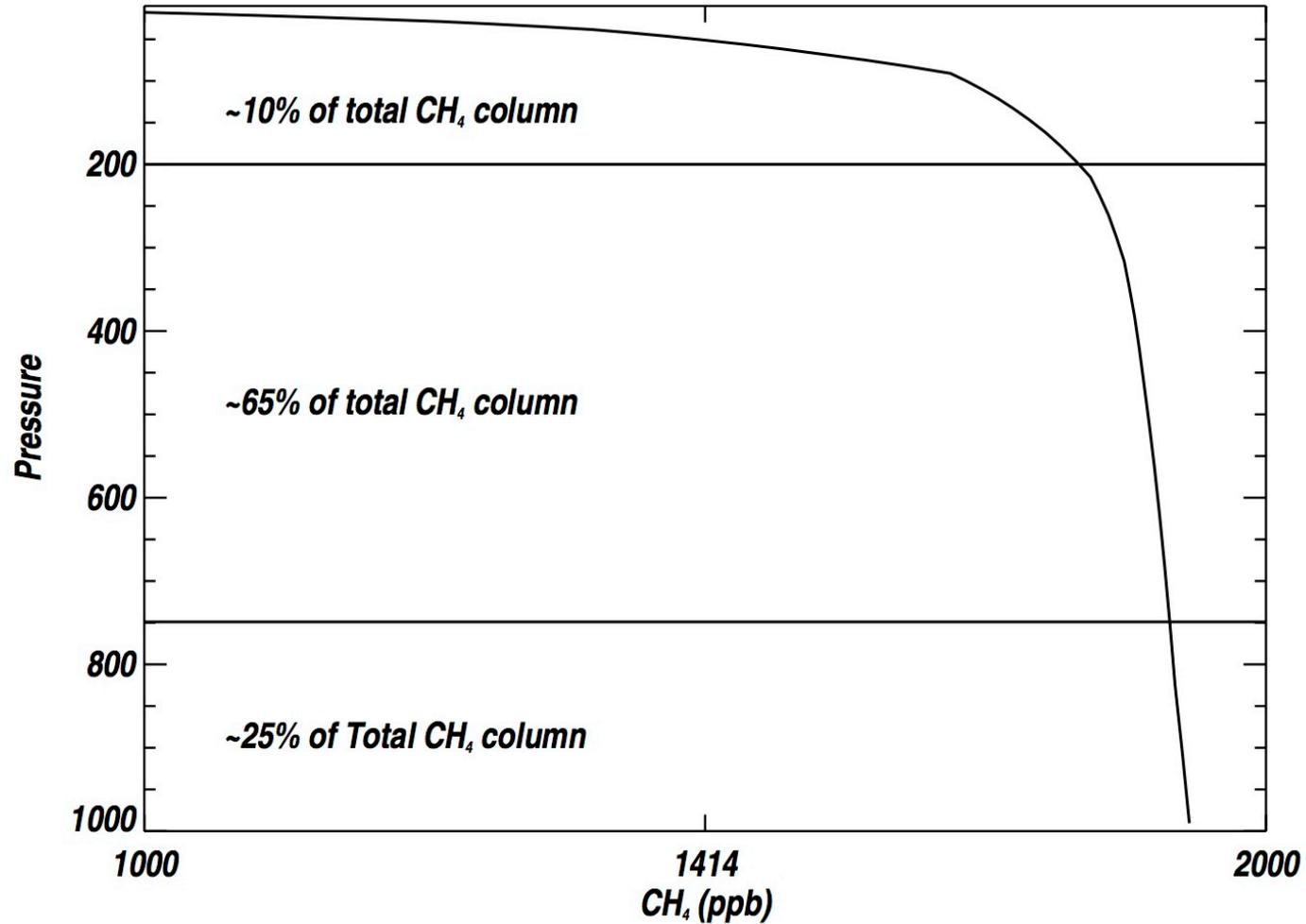


Primarily sensitive to sources really really far away from measurement

Primarily sensitive to sources ~1000's of km away

Primarily sensitive to sources ~100's of km away from measurement

Methane profile at ~55 N in July 2006

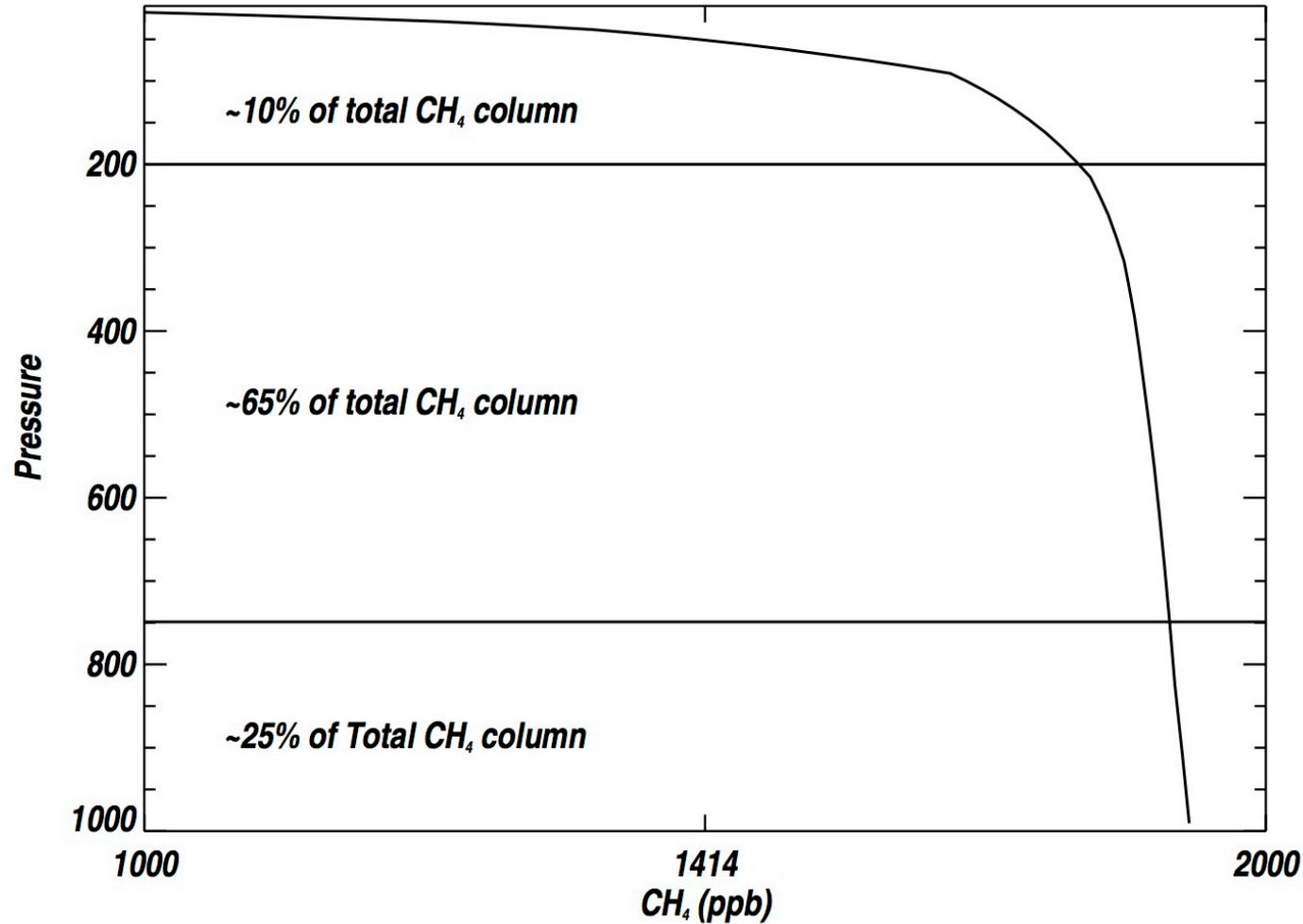


Chemistry, transport, and tropopause height

Transport and Chemistry

Boundary layer height, transport, and chemistry

Estimating Fluxes Using Surface Network

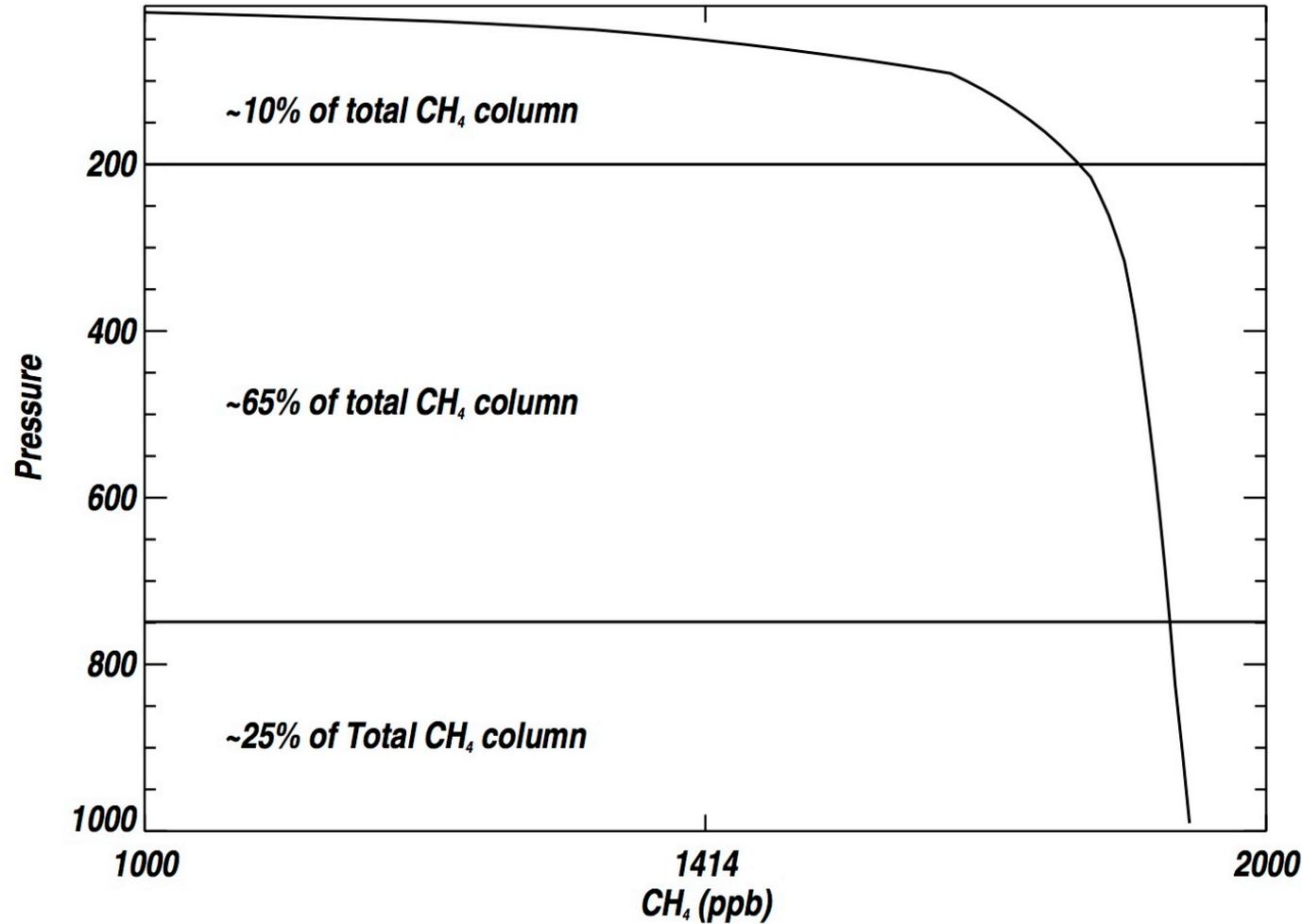


Transport and Chemistry

Boundary layer height,

Transport, and chemistry

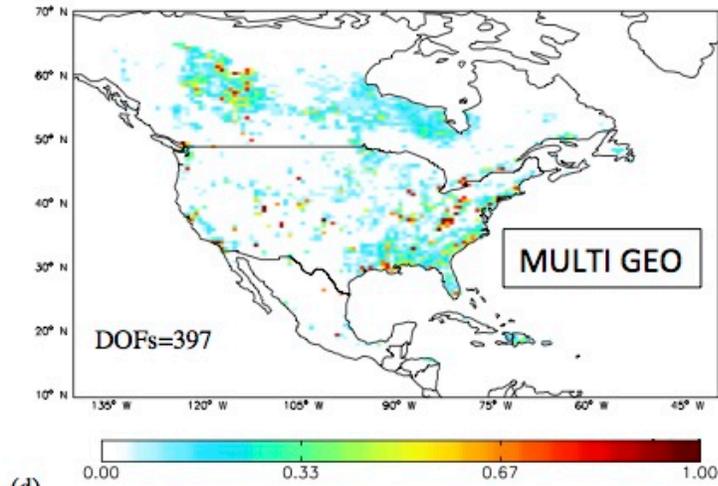
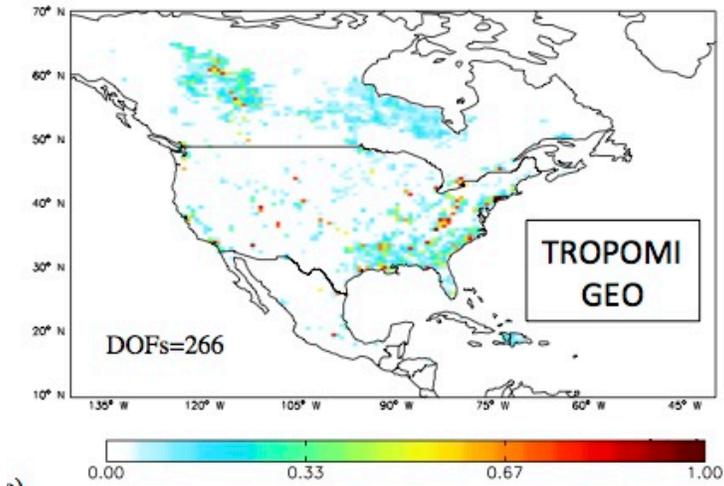
Estimating Fluxes Using Total Column Data



Need accurate model calculations of transport and chemistry over very long length scales (~1000's of km)

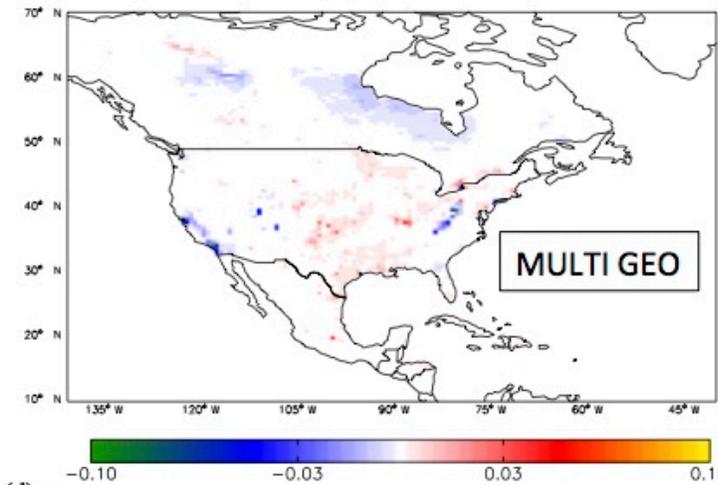
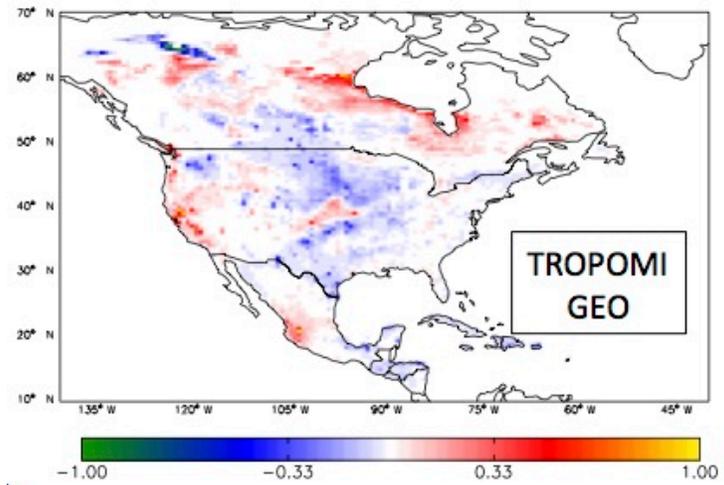
Estimating Fluxes Using Methane Total Column and Profiles from a GEO Orbit

Bousserez et al., ACP 2016



c)

d)



a)

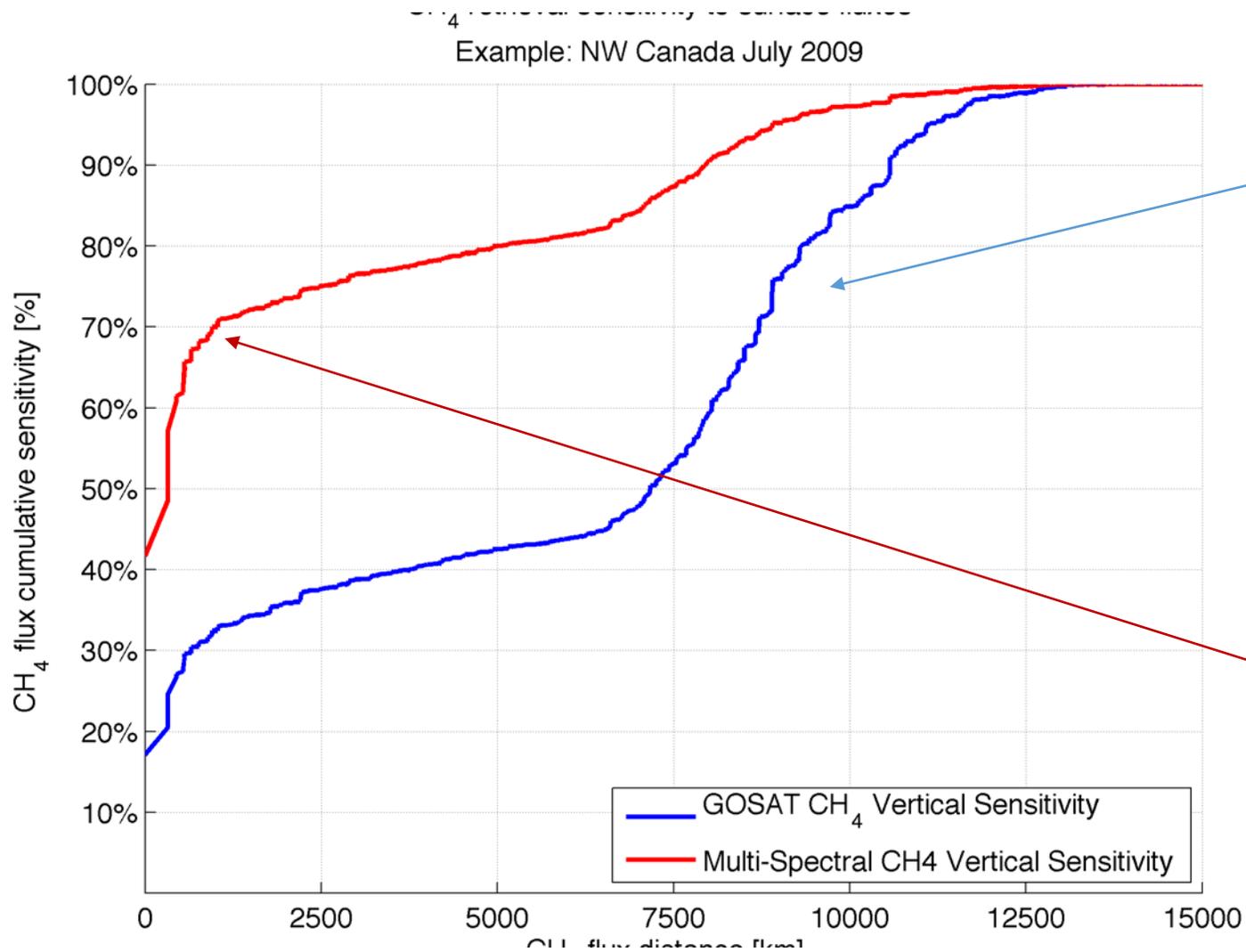
b)

Use of Thermal IR and Near IR radiances allows for profiling of methane that can resolve the boundary layer.

Use of profiles (instead of columns) to quantify fluxes results in a: ~50% increase in sensitivity to surface fluxes

Substantial reduction in sensitivity to background errors (e.g. transport and chemistry)

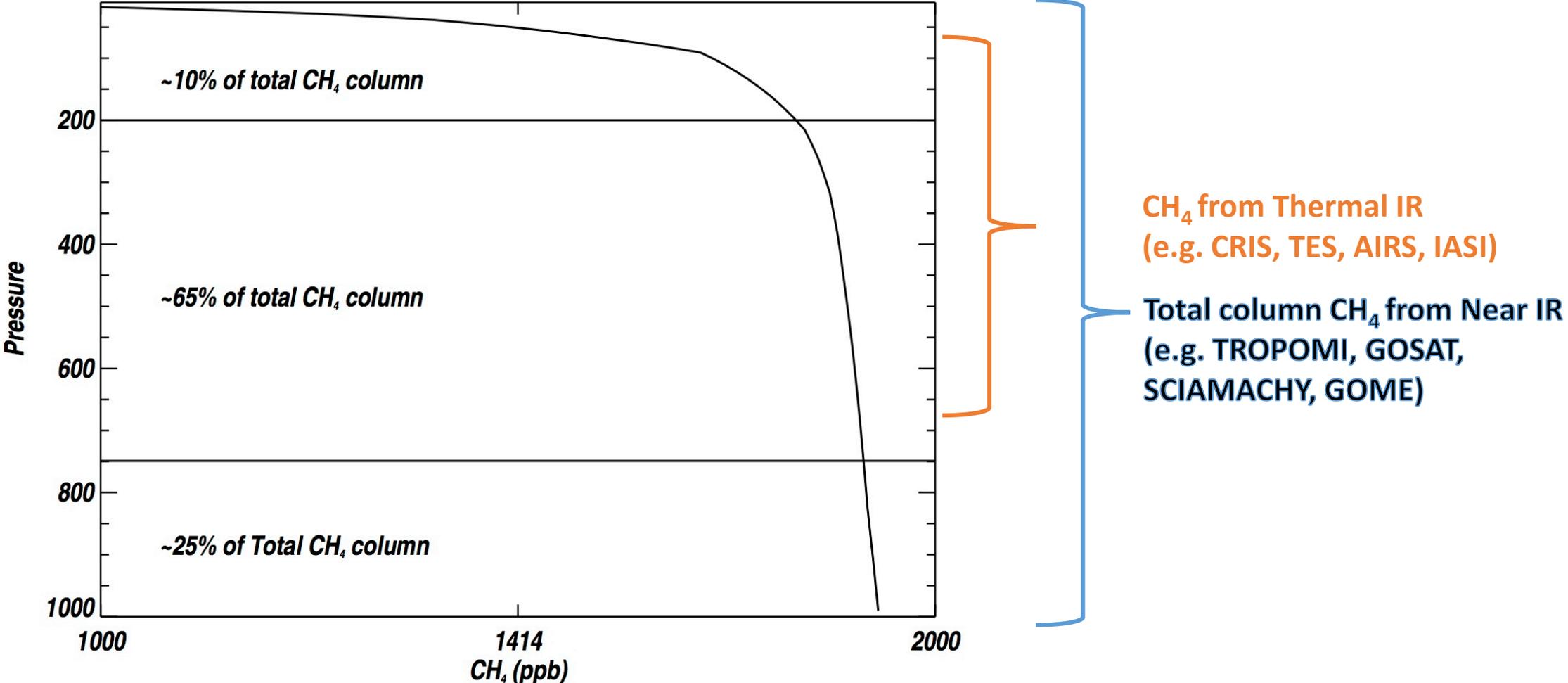
Sensitivity of Total Column and Lower-Tropospheric Methane (at high latitudes) to Methane Fluxes Using the Adjoint of the GEOS-Chem Model



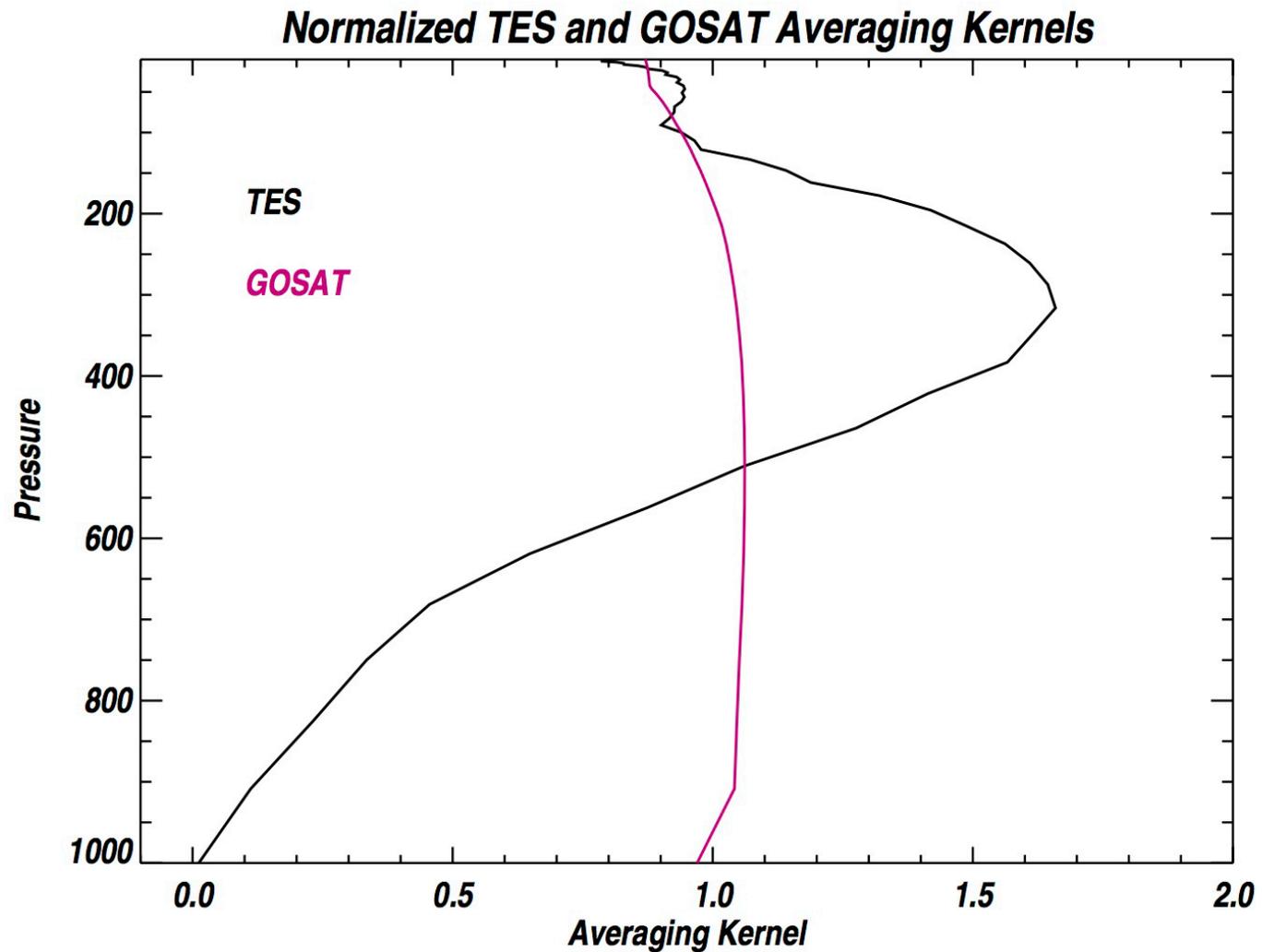
Total Column Methane primarily sensitive to fluxes ~8000 km away

Lower-Tropospheric Methane primarily sensitive to fluxes ~1000 km away

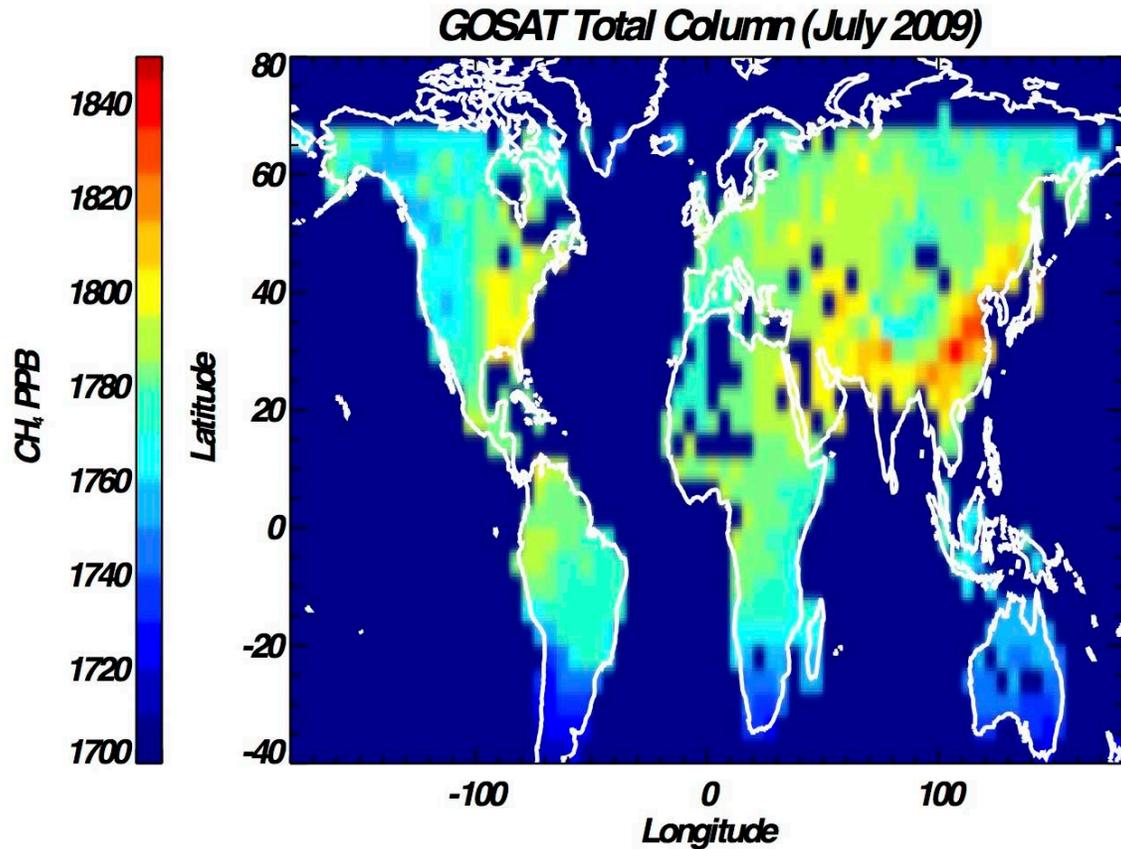
Estimating Fluxes Using Profile (or Lower Tropospheric Methane Measurements)



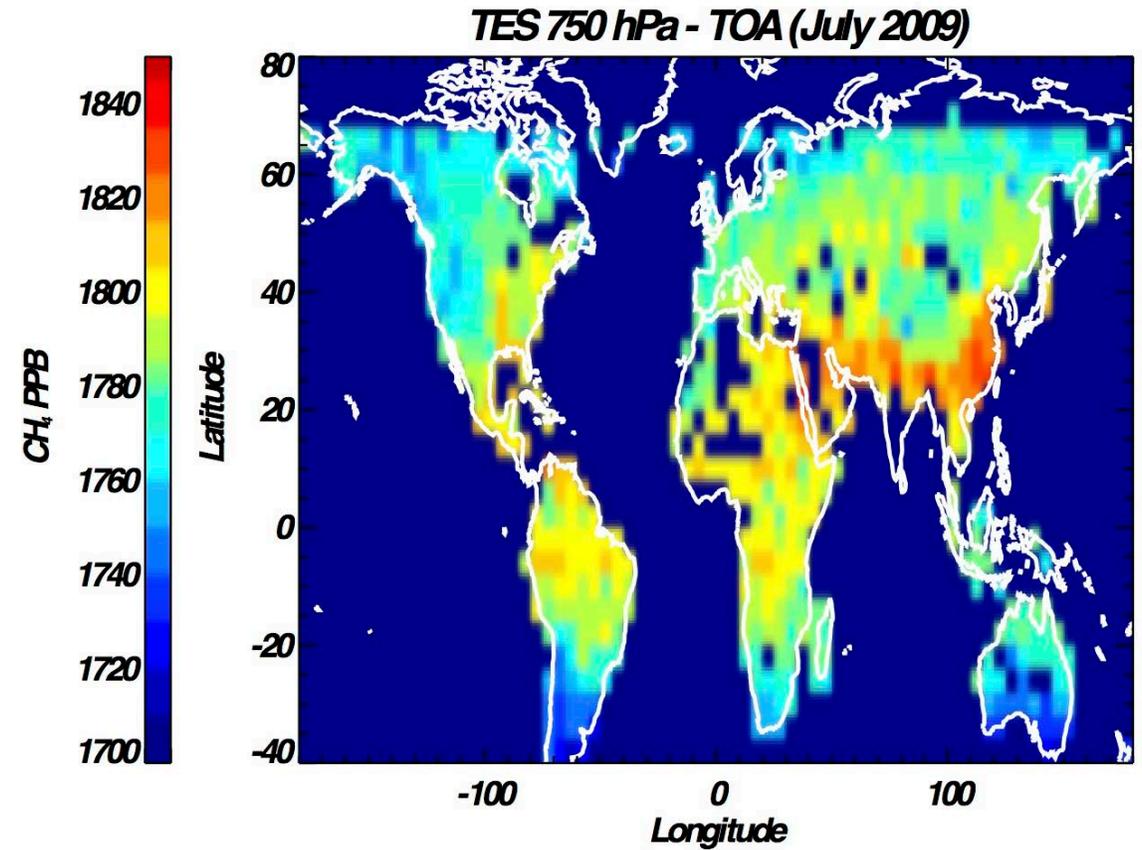
Example of Lower-Tropospheric Methane from GOSAT and TES: GOSAT and TES Total Column Averaging Kernels



Comparison of GOSAT Total Column and Aura TES FT/Strat Column (~850 hPa to TOA)



Precision ~15 ppb
Bias ~-17 to 2ppb
Parker et al., GRL 2011



Precision ~15 ppb
Bias ~26 ppb
Worden et al., AMT 2012; Alvarado et al., 2015

Both data sets use optimal estimation → a priori, vertical sensitivity (averaging kernels), and a posteriori uncertainties for noise and interferences are provide in the product files

Some Math: Derivation of Averaging Kernel and Uncertainties

$$\hat{C} = C^a + C_{air} h^T A(x - x^a) + C_{air} \sum_i h^T \delta_i$$

$$\hat{C}_L = \hat{C}_{tot} - \hat{C}_U$$

$$\hat{C}_L = C_L^a + C_{air} \mathbf{b}_L(x_L - x_L^a) + C_{air}(\mathbf{b}_u - \mathbf{h}_u \mathbf{A}_{UU}^{TES})(x_u - x_u^a) + C_{air} \sum_i h \delta_i$$

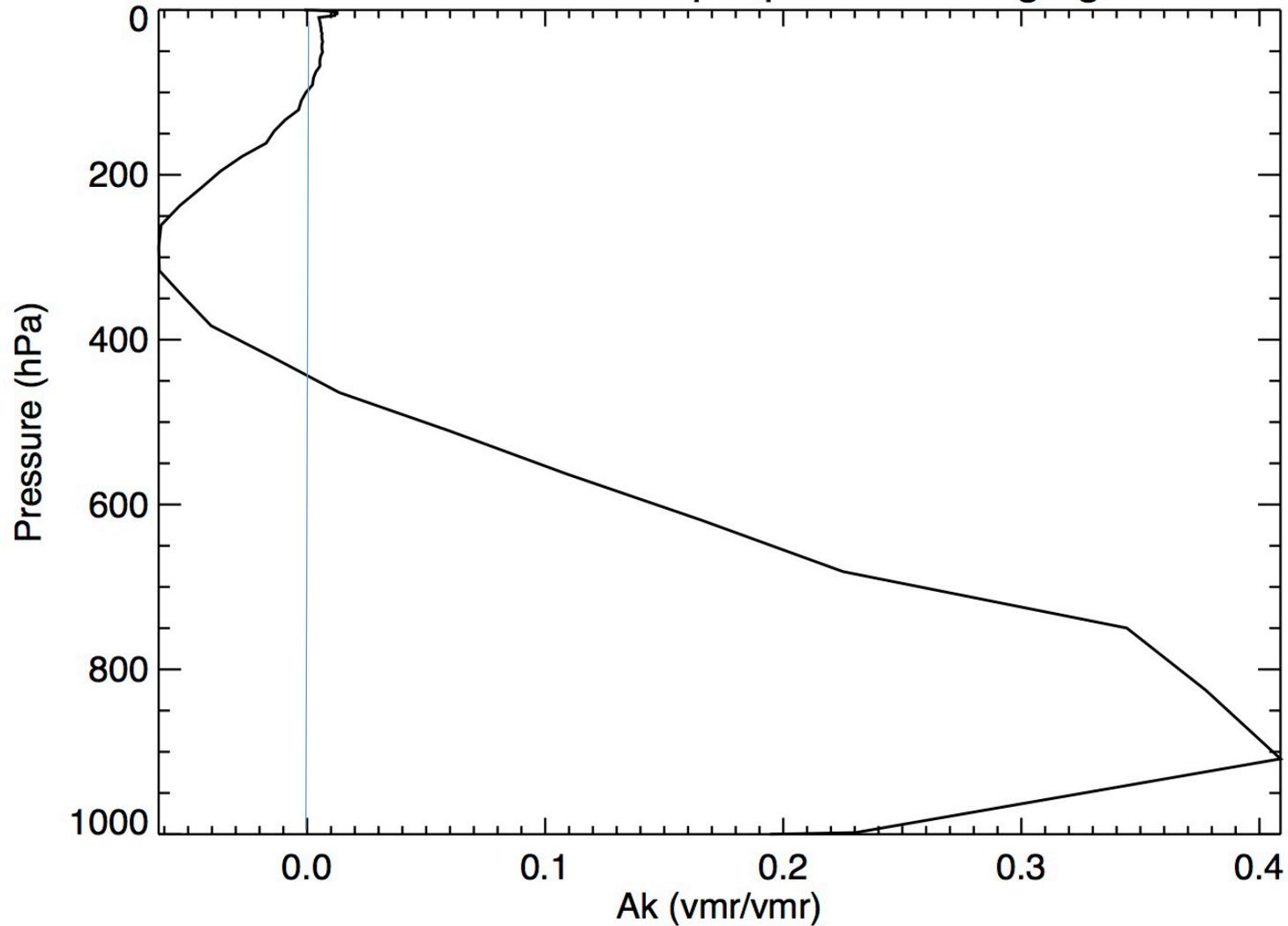
Divide above equation by the column of dry air in the lower troposphere and re-arrange and combine terms and we get:

$$\hat{X}_L = X_L^a + a^T(x - x^a) + C_{air}/C_L^{air} \sum_i h \delta_i$$

Now we have an equation that is similar to that described in Rodgers (2000).

Note amplification of uncertainties by about a factor of 4 due to C_{air}/C_L^{air} term

GOSAT / TES Lower Tropospheric Averaging Kernel

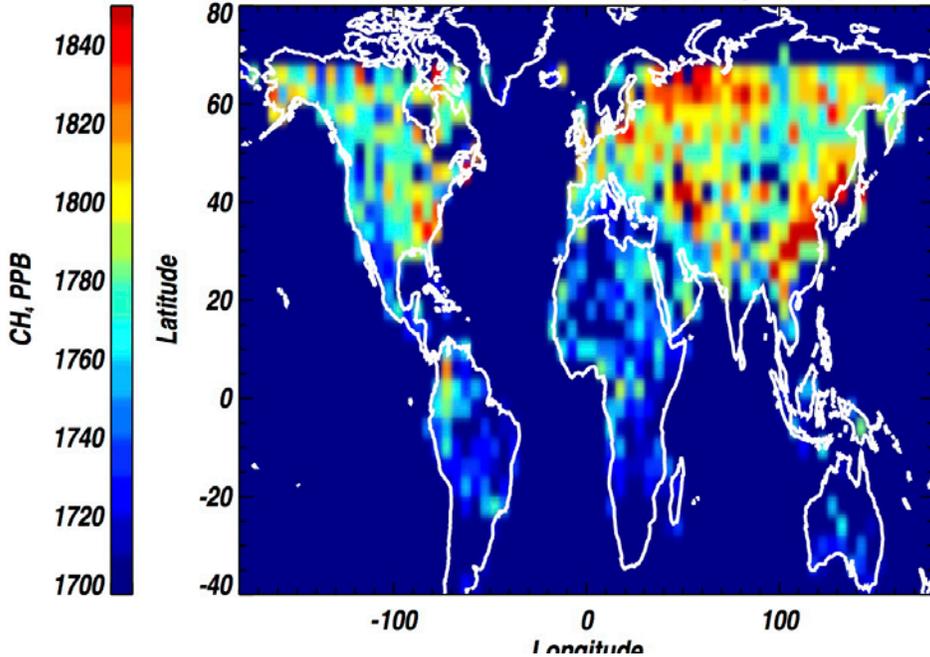


Reduced sensitivity of lower tropospheric estimate to stratosphere and upper troposphere → Reduced uncertainties due to transport and chemistry

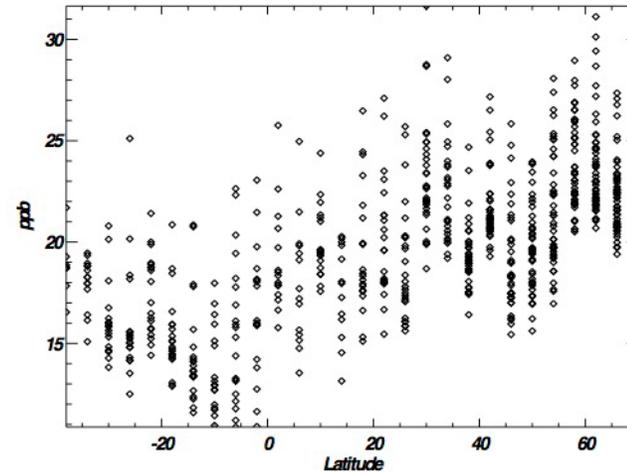
Typical Averaging Lower Trop “column” averaging kernel peaks at 900 hPa → Greater sensitivity to nearby methane sources

Lower Tropospheric CH₄ Estimates are for a Monthly Average on a 4x5 degree bin

GOSAT - TES Lower Trop (July 2009)

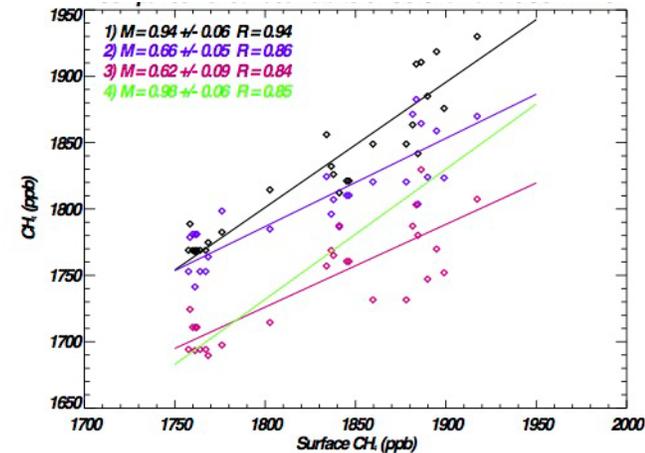


Precision



Precision depends on (1) noise, (2) sampling differences between GOSAT and TES, (3) cross-state error in TES free-tropospheric methane

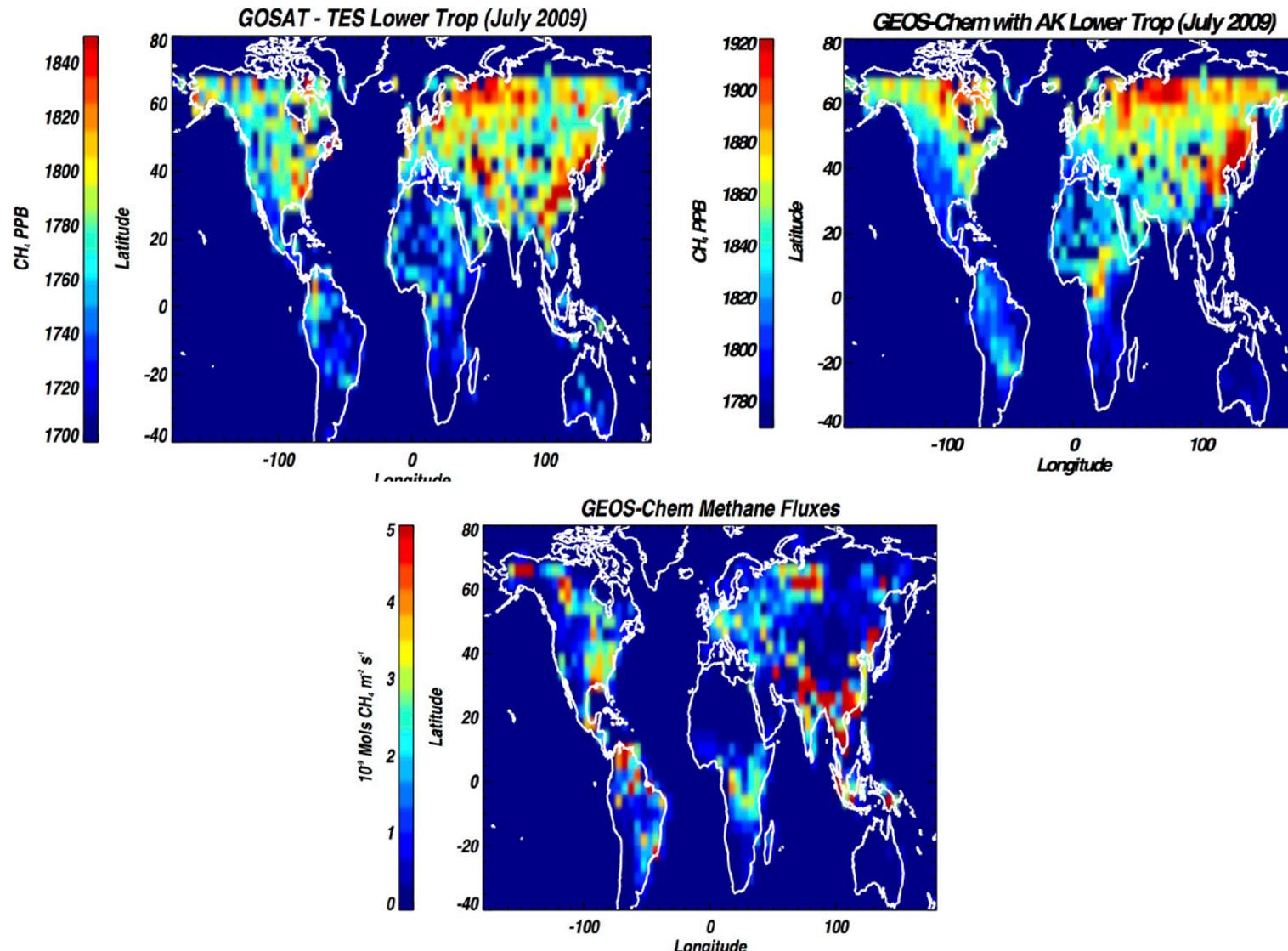
Comparison to Surface Network



Comparison to surface data (via GEOS-Chem model) suggests that data are biased low by ~65 ppb)

Comparison between data and model (using averaging kernel and a priori constraints) reveal regional enhancements over methane sources

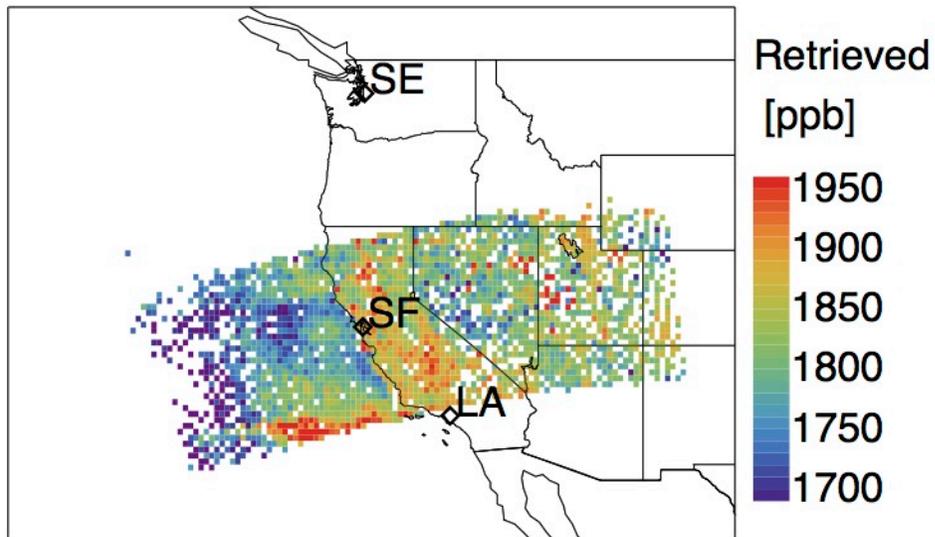
$$\hat{X}_L = X_L^a + a^T(x - x^a)$$



Lower Tropospheric Estimates from CRIS and TROPOMI

- TROPOMI ~1000X soundings relative to GOSAT ~same precision and accuracy as GOSAT
- CRIS ~ 10000X soundings relative to TES ~same accuracy and better precision than TES
- Precision of GOSAT/TES estimate ~30 ppb so precision of TROPOMI/CRIS estimate ~< 1 ppb
- Greatly increased precision and sampling allows us to better diagnose accuracy using surface network and aircraft data

CRIS Methane Retrievals Based on Aura TES Optimal Estimation Composition Retrieval Algorithm



Summary

Lower tropospheric estimates based on CRIS/TROPOMI measurements can quantify boundary layer methane with ~1ppb precision or better at 100 km length scales

These data could potentially provide fluxes with greatly reduced uncertainty (~10x reduction) due to transport and chemistry error, one of the limiting errors for using satellite-derived estimates of methane fluxes to evaluate the processes controlling the global methane cycle.

Key to this effort is an optimal estimation based methane retrieval algorithm in order to quantify and characterize lower-tropospheric methane → subtraction approach depends on knowledge of vertical resolution, a priori constraints, and a posteriori uncertainties of both TIR and NIR based methane estimates.

A New Global HCHO Retrieval Technique based on Principal Component Analysis of Satellite Radiance Data: Implementation with OMPS and Preliminary Results

Can Li

NASA GSFC Code 614 & ESSIC, UMD

Email: can.li@nasa.gov

Joanna Joiner, Nick Krotkov, Laura Dunlap

Trace Gas Session

3rd Annual JPSS Meeting

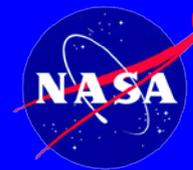
August 11, 2016

College Park, MD



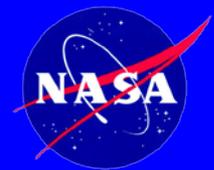
Why Formaldehyde (HCHO)?

- Intermediate oxidation product of volatile organic compounds (VOCs)
 - Small global background from oxidation of methane
 - Relatively large regional sources (NMVOCs emitted from biogenic, anthropogenic, and biomass burning sources)
- Short-lived (lifetime: hours) - **used to provide constraints on NMVOCs** [e.g., Barkley et al., 2008; Fu et al., 2007; Palmer et al., 2003; Zhu et al., 2014]
- Why NMVOCs? – **precursors of tropospheric ozone and organic aerosols** (e.g., isoprene)



Space-based Detection of HCHO

- Absorption of UV in $\sim 325\text{-}360$ nm
- Weak signals, various interferences (BrO, O₃, NO₂, rotational Raman scattering or RRS, *aka* the Ring effect)
- DOAS-type algorithms using hyperspectral measurements to separate HCHO signals from interferences
- First demonstrated for **GOME** [*Chance et al.*, 2000]
- Products available from **OMI** [*e.g.*, *De Smedt et al.*, 2015; *González Abad et al.*, 2015], **GOME-2** [*e.g.*, *De Smedt et al.*, 2012], **SCIAMACHY** [*e.g.*, *Wittrock et al.*, 2006]
- **Still fairly large differences between satellites and/or algorithms** [*e.g.*, *Zhu et al.*, 2016]

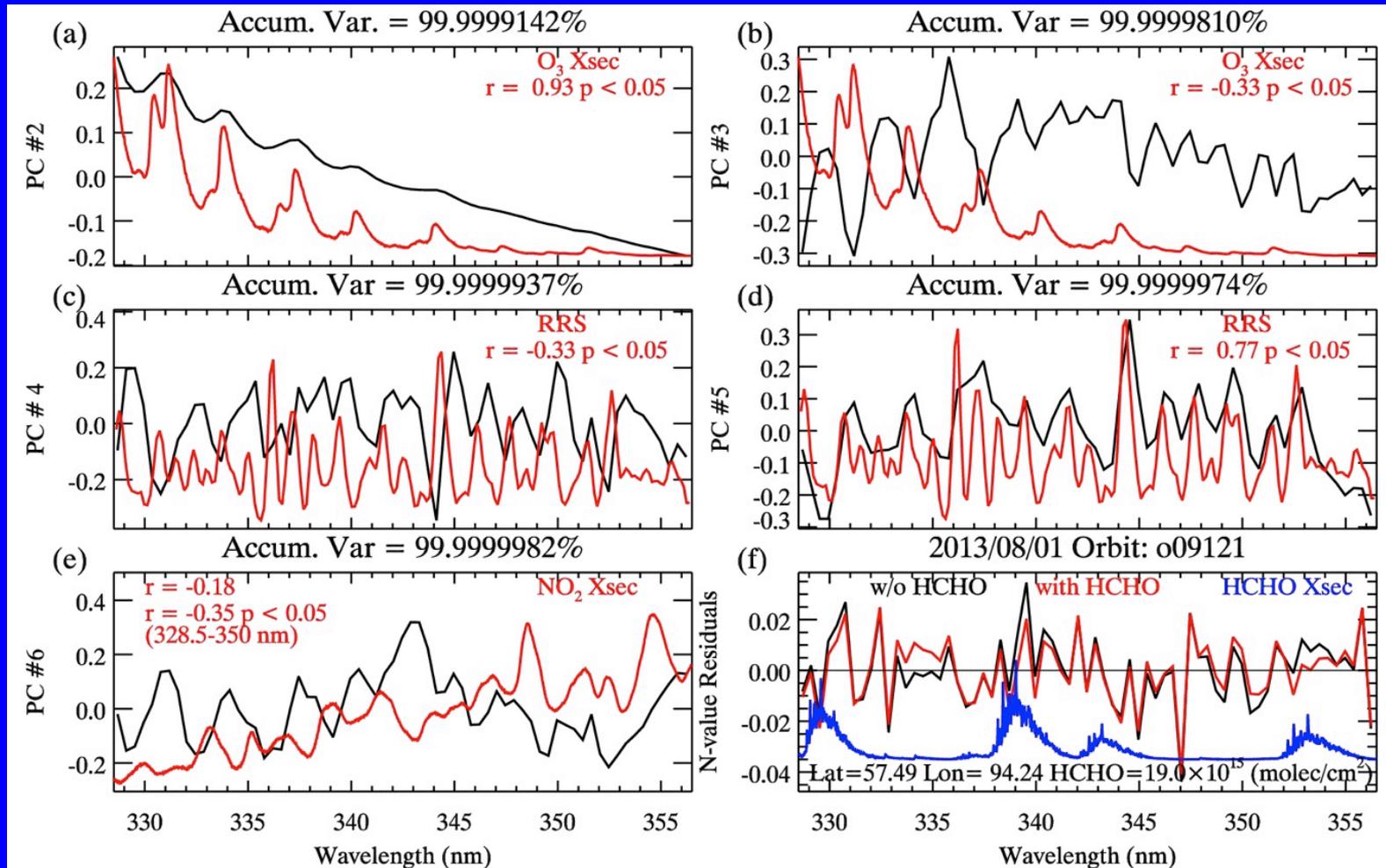


PCA-based Approach

- Based on successful PCA SO₂ algorithms
- Extract spectral features directly from satellite radiance data
- Use these features in spectral fitting to minimize interferences
- Preliminary implementation with OMPS :
 - PCs from each row, each orbit
 - Window: 328.5-356.5 nm
 - 8 PCs in fitting (no strong dependence on # of PCs)
 - Additional reference spectrum: BrO cross section
 - *A priori* profiles from GMI simulated climatology
 - A table lookup approach for Jacobians for each pixel: O₃ and cloud from NASA OMPS products



Principle Components and Residuals



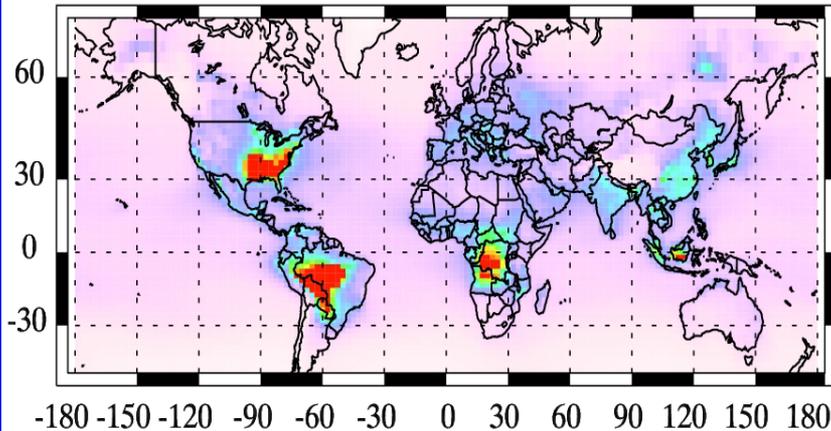
Example PCs from **entire row** # 20, Orbit 9121 reveal clear, known physical features

[Li et al., GRL, 2015]

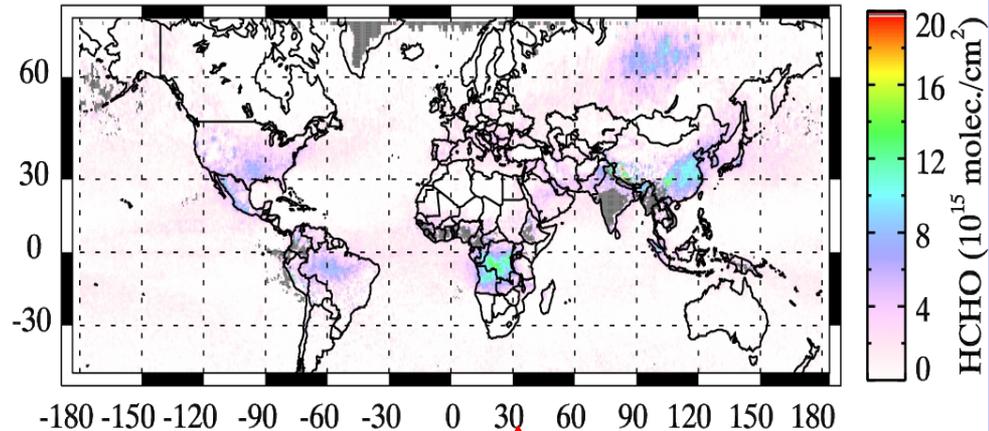


OMPS Capable of Detecting HCHO Signals

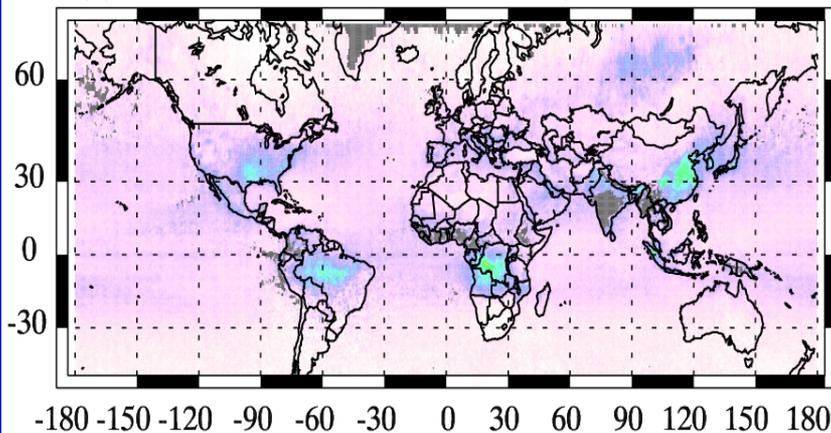
(a) GMI HCHO Month: 08



(b) OMPS HCHO (PBL Profile) 2013/08



(c) OMPS HCHO (GMI Profile), 2013/08



The same *a priori* profile everywhere, independent from model

Model *a priori* profiles + adding model column amounts from Pacific to all longitudes

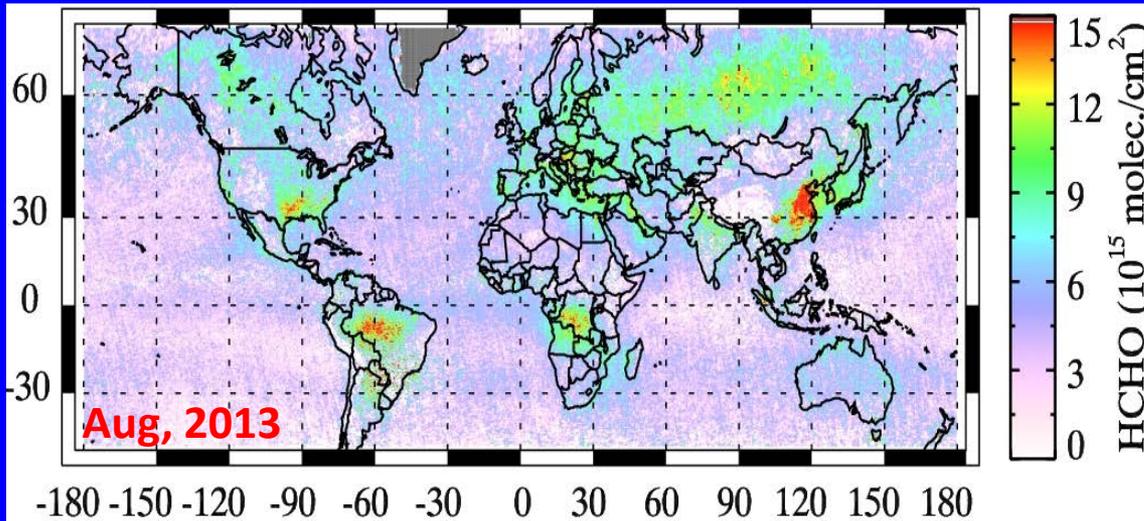


[Li et al., GRL, 2015]

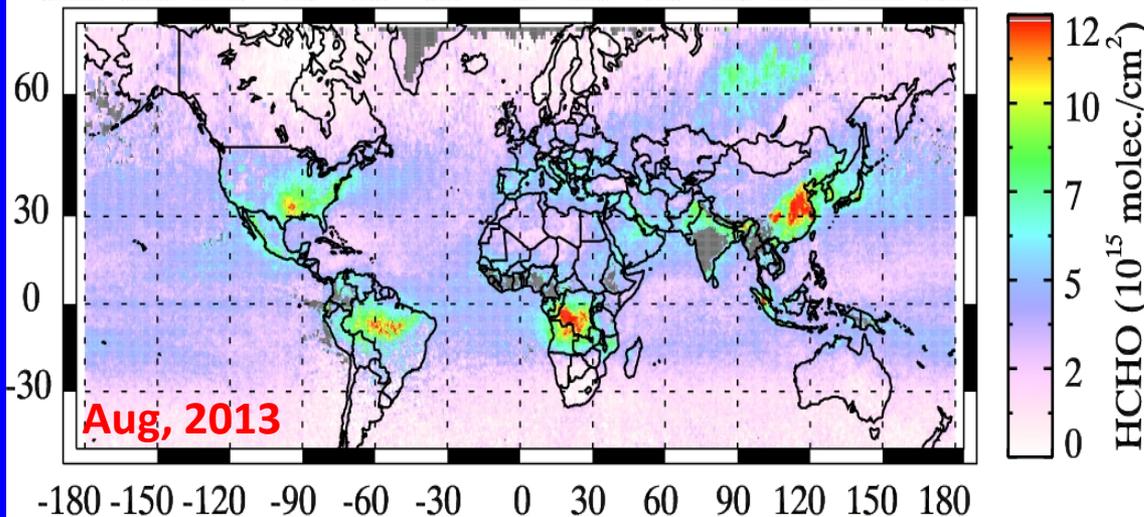


Comparison with OMI DOAS HCHO

OMI
DOAS
(BIRA)

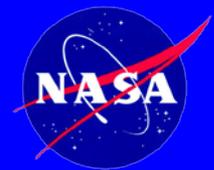


OMPS
PCA
(GSFC)



Two independent retrievals show fairly consistent spatial patterns in HCHO.

OMPS HCHO ~15-20% smaller than OMI, probably due to several instrumental and algorithmic factors (e.g., *a priori* profiles etc.).

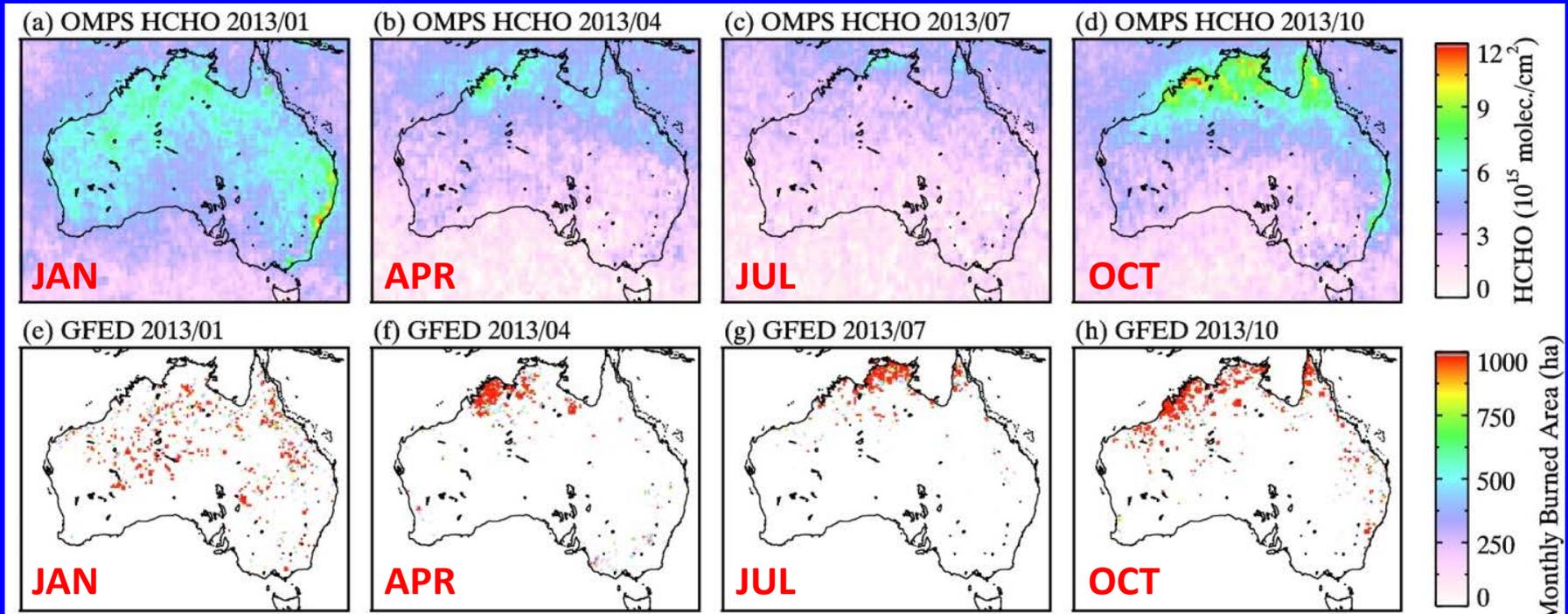


[Li et al., GRL, 2015]



Seasonal Pattern: OMPS HCHO vs. Global Fire Emission Database - Australia

OMPS PCA HCHO Retrievals for 2013



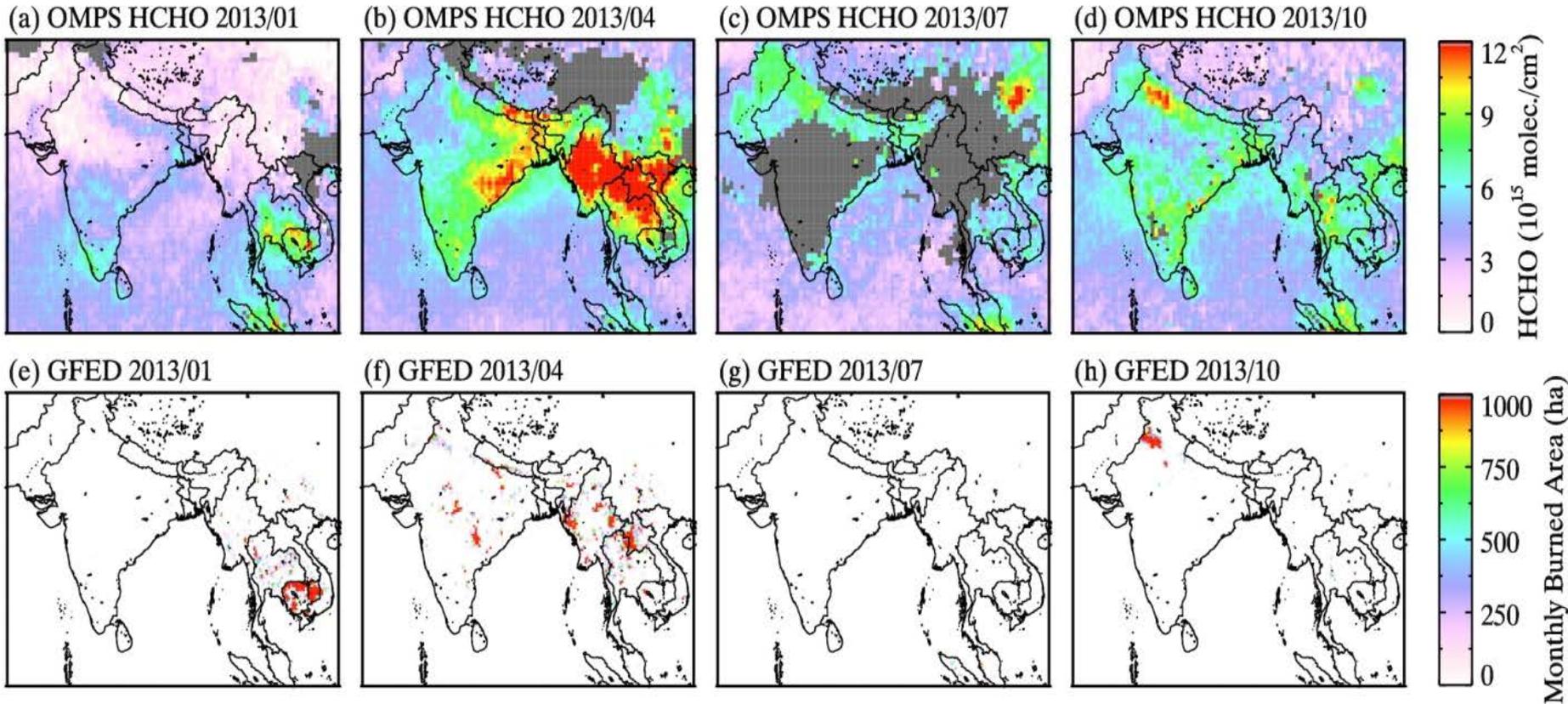
GFED Monthly Burnt Area (indicator of fires)

OMPS PCA HCHO retrievals show consistent spatial and seasonal patterns with fires in regions where seasonal biomass burning emissions dominate sources of NMVOCs (and HCHO). Biogenic emissions also contribute in the growing season (January).

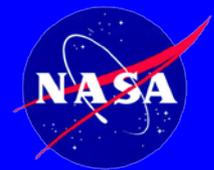


Seasonal Pattern: OMPS HCHO vs. Global Fire Emission Database – South & Southeast Asia

OMPS PCA HCHO Retrievals for 2013



GFED Monthly Burnt Area (indicator of fires)



Work Underway

- OMPS PCA retrievals biased low – more detailed comparison has been planned in collaboration with BIRA
- Algorithm also implemented with OMI and will be implemented with TROPOMI
- Airborne HCHO measurements regularly taken over and near the San Francisco Bay Area (the Alpha Jet and COFFEE¹ payload)

¹Compact Formaldehyde Fluorescence Experiment (Hanisco et al @NASA GSFC & Marrero et al @NASA Ames)



Conclusions

- The good news: **OMPS provides an unplanned opportunity to continue the OMI HCHO data record** (also demonstrated by *González Abad et al. [2016]*).
- A long-term data record will be crucial for investigating how biogenic emissions respond in a changing climate.
- More development underway.
- Inter-instrument consistency still an issue, but the PCA approach may offer a way to mitigate the issue.





Applications of satellite NO₂ observations in US National Air Quality Forecasting Capability

Pius Lee¹, Daniel Tong^{1,2,3*}, Lok Lamsal^{4,5}, Li Pan^{1,2}, Charles Ding^{1,6}, Hyuncheol Kim^{1,2}, Tianfeng Chai^{1,2}, Kenneth E. Pickering⁵, Shobha Kondragunta⁷, and Ivanka Stajner⁷, Barry Baker^{1,9}

1) NOAA ARL; 2) UMD CICS; 3) GMU CSISS; 4) USRA;
5) NASA GSFC; 6) UC-Berkeley; 7) NOAA/NESDIS/STAR; 8) NOAA NWS
9) NRC



The Great Recession

- ❖ **Starting – Ending time: December 2007 – October 2009;**
- ❖ **Cause: Bursting of the housing bubble in 2007, followed by a subprime mortgage crisis in 2008;**
- ❖ **Impacts:**
 - **Unemployment rate: 4.7% in Nov 2007 → 10.1% in Oct 2009.**
 - **Income level: dropped to 1996 level after inflation adjustment;**
 - **Poverty rate: 12% → 16% (50 millions);**
 - **GDP: contract by 5.1%;**
- ❖ **Worst economic recession since the Great Depression**

Question: What does it mean to Air Quality (and Emissions)?



Methodology

❖ Emission Indicator – Urban NO_x in Summer

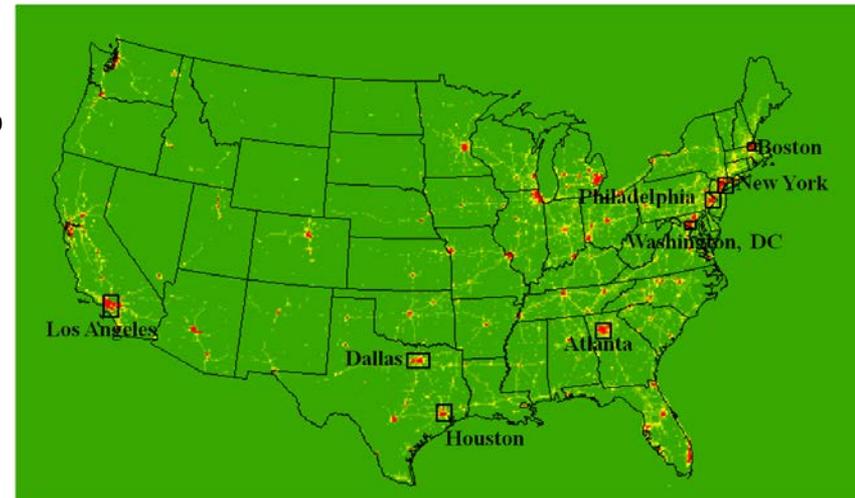
- Short lifetime → proximity to emission sources
- Urban NO₂ dominated by local sources;
- High emission density → low noise/signal ratio;

❖ NO_x Data sources

- Satellite remote sensing (OMI-Aura NO₂).
- Ground monitoring (EPA AQS NO_x);
- Emission data (NOAA National Air Quality Forecast Capability operational emissions);

❖ Deriving the trend: $(Y2 - Y1) / Y1 \times 100\%$

❖ Selection of urban areas



NO_x Regulatory Actions Since 2005

- **2003 – 2008: NO_x Budget Trading Program (SIP Call)**
 - Summer time power plant emission reductions in 20 states
 - Point sources can pay for reductions at other facilities (trading)
 - 2500 large combustion units affected.
- **2005: Clean Air Interstate Rule (CAIR)**
 - NO_x reductions of 53% by 2009 (2003 baseline). Affects 28 states
 - Thrown out by courts in 2008.
- **State-specific rules beyond Federal CAIR have led to further NO_x reductions in some states.**
- **2011: Cross-State Air Pollution Rule (CSAPR)**
 - Replacement of CAIR
 - Add five additional mid-West states to reduce NO_x during ozone season.
- **Tier II Tailpipe NO_x Emission Standards – 5% reduction in fleet emissions per year over 2002 to 2010.**

Ozone Monitoring Instrument (OMI)

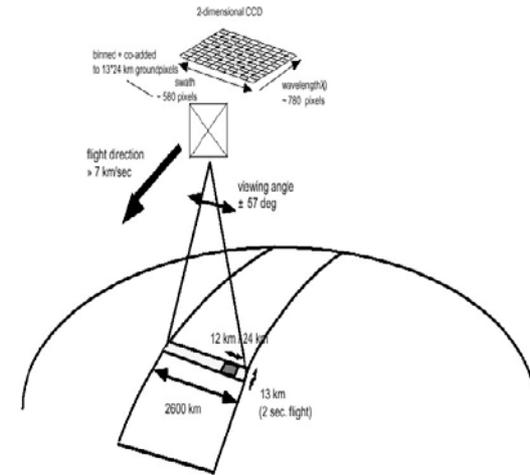
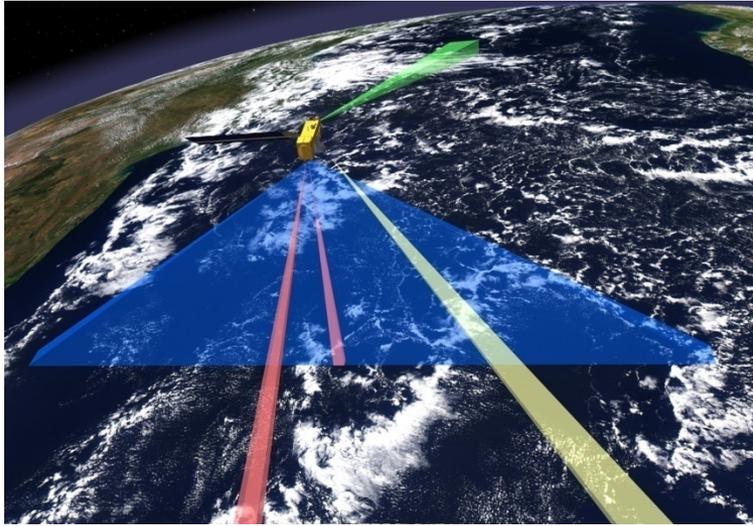


Figure 2.1 Measurement principle of OMI.

Courtesy of Fokker Space

One of four sensors on the EOS-Aura platform (OMI, MLS, TES, HIRDLS)

Courtesy of OMAR Torres

Launched on 07-15-04

Instrument Characteristics

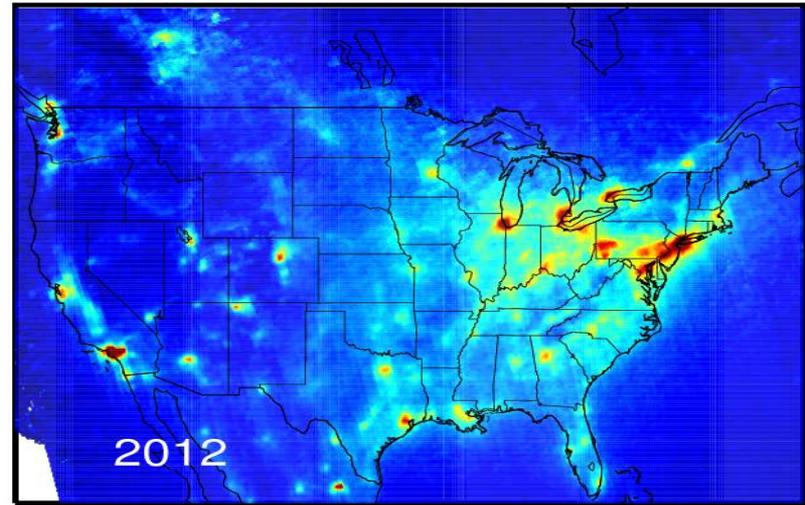
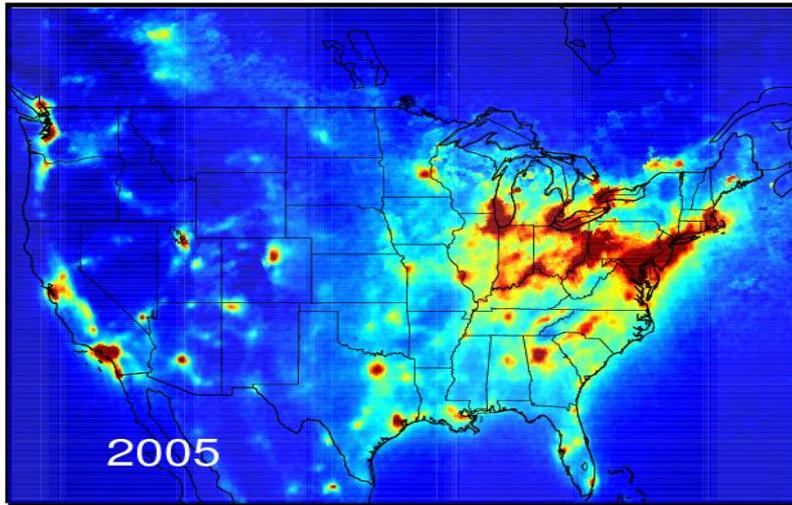
- Nadir solar backscatter spectrometer
- Spectral range 270-500 nm (resolution~0.6 nm)
- Spatial resolution: 13X24 km footprint
- Swath width: 2600 km (global daily coverage)
- 13:45 (+/- 15 min) Local equator crossing time (ascending node)

Data Quality Control

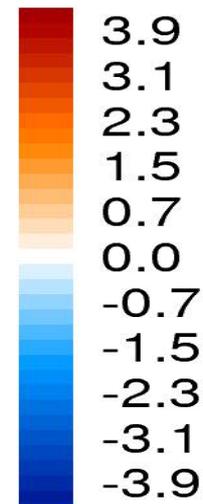
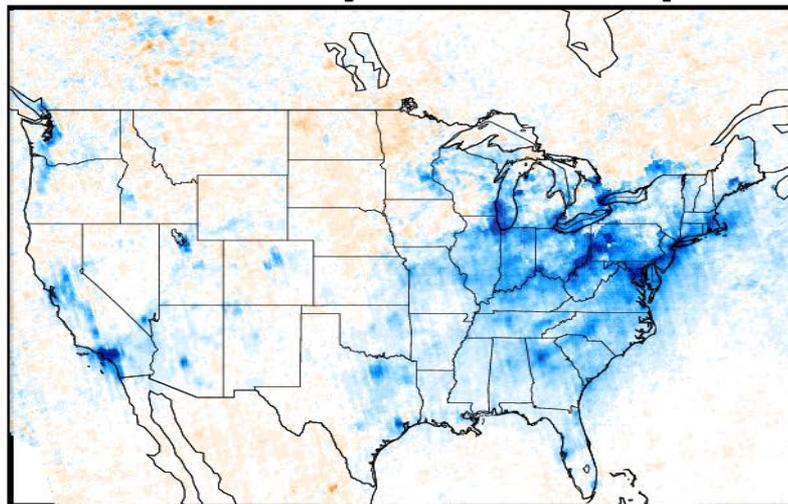
- VCD quality flag;
- Cloud fraction;
- Row Anomaly;
- Outliners (5% at each end)

OMI Observed NOx Change (July)

Tropospheric NO₂ [10^{15} molec cm⁻²]

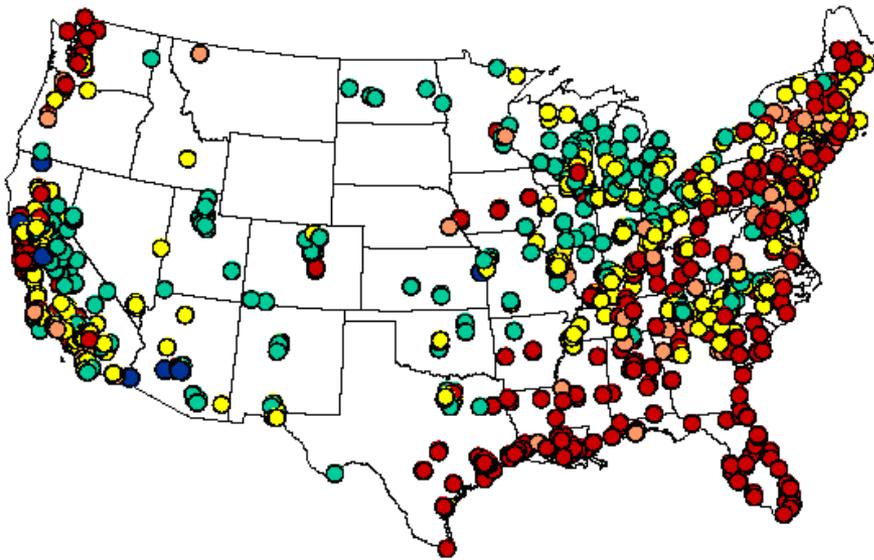


difference [10^{15} molec cm⁻²]

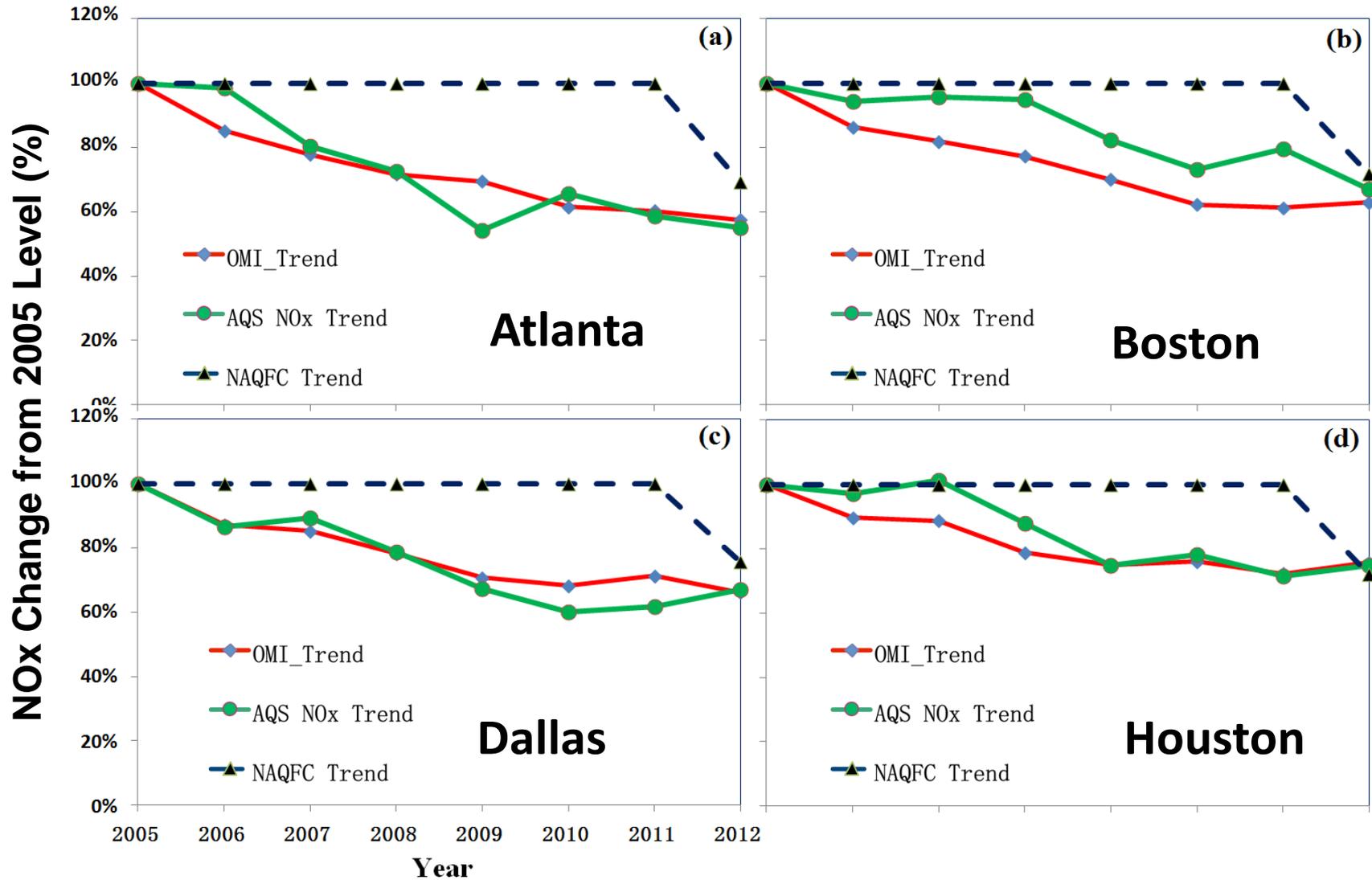


AQS: EPA Ambient NO₂ Monitoring

- ❖ **Method: Chemiluminescence**
 - Interferences with PAN, O₃ and alkyl nitrates
 - Uncertainty higher at lower end
- ❖ **Select early morning rush hours (6-9AM): higher values and less photochemistry**

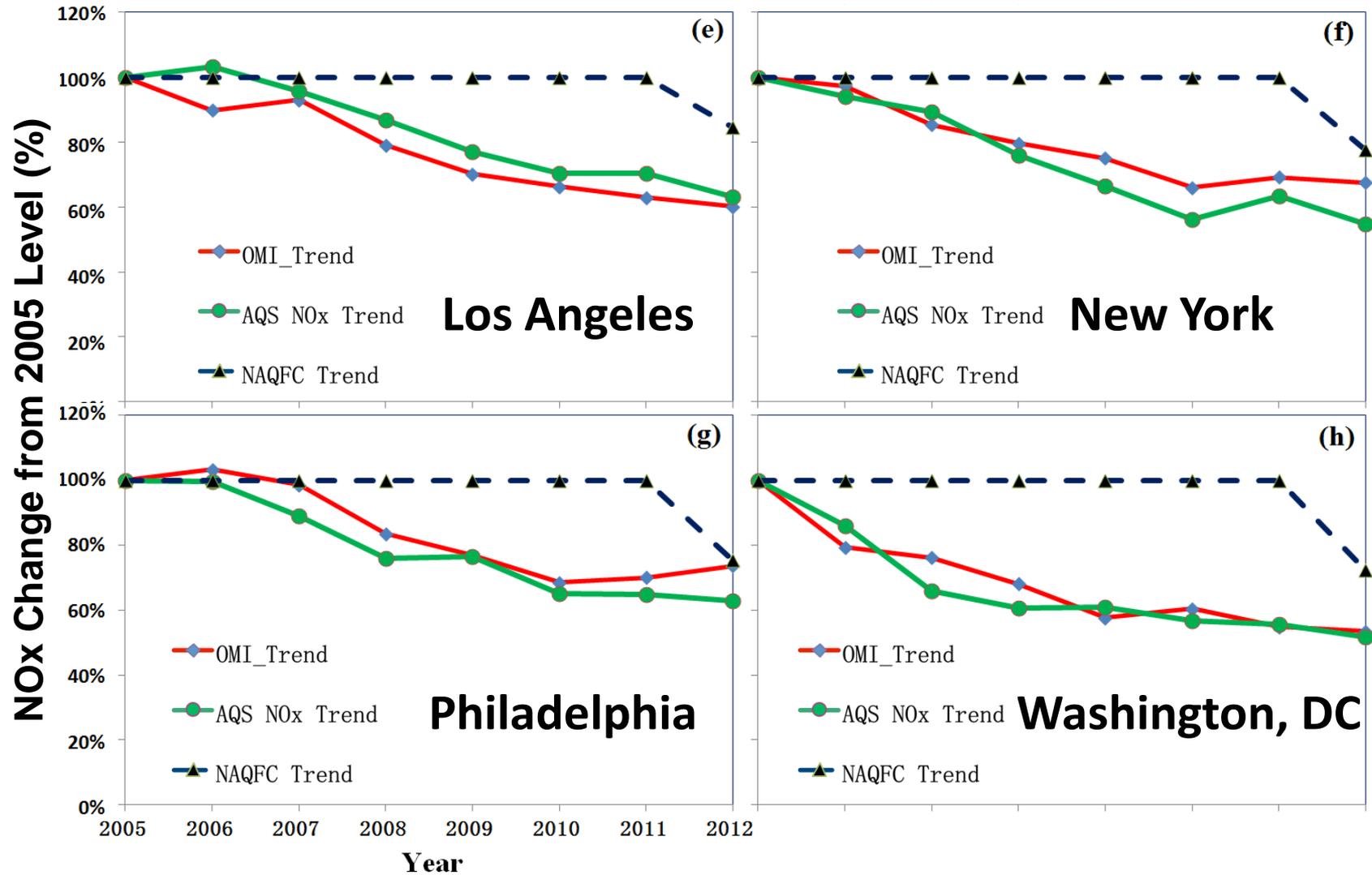


Inter-Comparison of OMI, AQS and NAQFC



(Source: Tong et al., 2015)

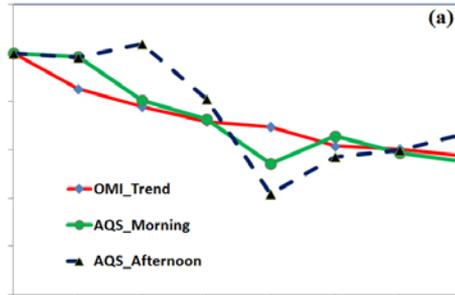
Inter-Comparison of OMI, AQS and NAQFC (Continued)



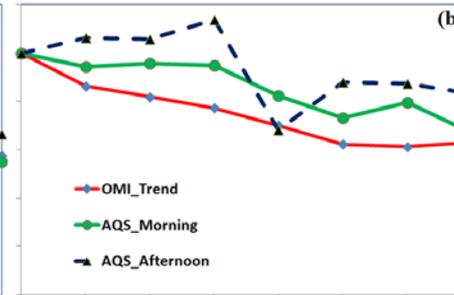
(Source: Tong et al., 2015)

Morning Rush Hours vs Early Afternoon

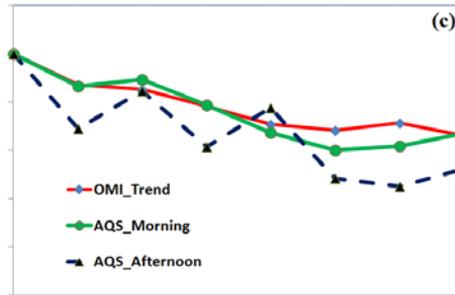
Atlanta



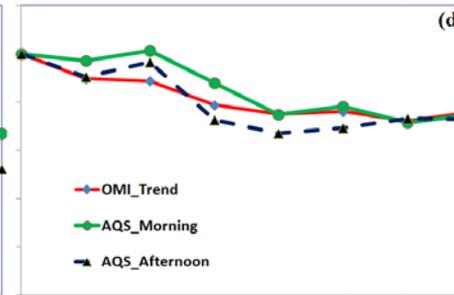
Boston



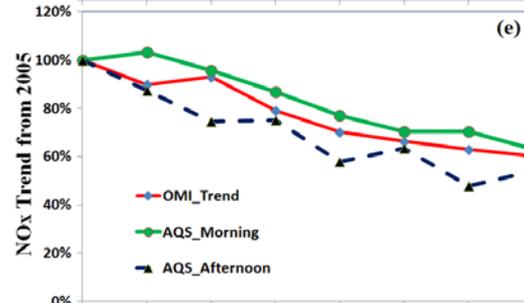
Dallas



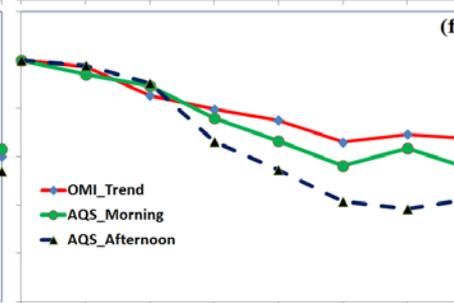
Houston



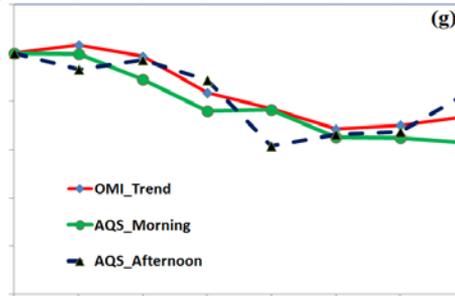
Los Angeles



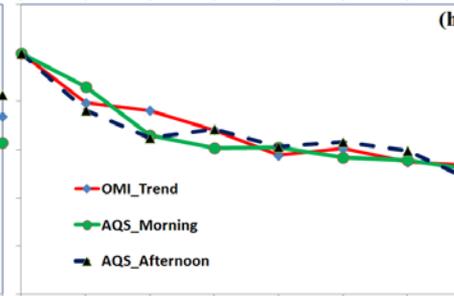
New York



Philadelphia



Washington, DC



Year

(Source: Tong et al., 2015)

Seven-year NOx Changes

City	Atlanta	Boston	Dallas	Houston	Los Angeles	New York	Philadelphia	Washington, DC	Mean
OMI	-42%	-37%	-34%	-24%	-40%	-32%	-26%	-47%	-35%
AQS	-45%	-33%	-33%	-25%	-37%	-45%	-37%	-48%	-38%
NAQFC	-31%	-28%	-24%	-28%	-15%	-22%	-25%	-28%	-25%

- ❖ Both observations (OMI and AQS) revealed -5%/yr reduction rate;
- ❖ NAQFC adopted change corresponds to -3.5%/yr;

NOx Changes

Prior to, during and after the Recession

Stage	Sources	Atlanta	Boston	Dallas	Houston	Los Angeles	New York	Philadelphia	Washington, DC	Mean
Before	OMI SP	-11.7	-9.4	-7.5	-5.7	-3.3	-7.5	-0.6	-12.3	-7.3
	AQS	-9.9	-2.1	-5.2	0.7	-2.0	-5.5	-5.5	-18.7	-6.0
During	OMI SP	-5.5	-7.5	-8.9	-7.9	-13.1	-6.2	-11.7	-13.0	-9.2
	AQS	-17.5	-7.0	-13.0	-14.0	-10.3	-13.6	-7.0	-3.7	-10.8
After	OMI SP	-6.0	-3.3	-2.1	0.4	-5.0	-3.2	-1.2	-2.3	-2.8
	AQS	1.4	-6.1	0.1	0.2	-6.4	-5.4	-6.1	-5.3	-3.4

- ❖ **Distinct regional difference;**
- ❖ **Average NOx changes are consistent for OMI and AQS data;**
- ❖ **-6%/yr - -7%/yr prior to Recession;**
- ❖ **-9%/yr - -11%/yr during Recession;**
- ❖ **-3%/yr after Recession (Recovery?).**

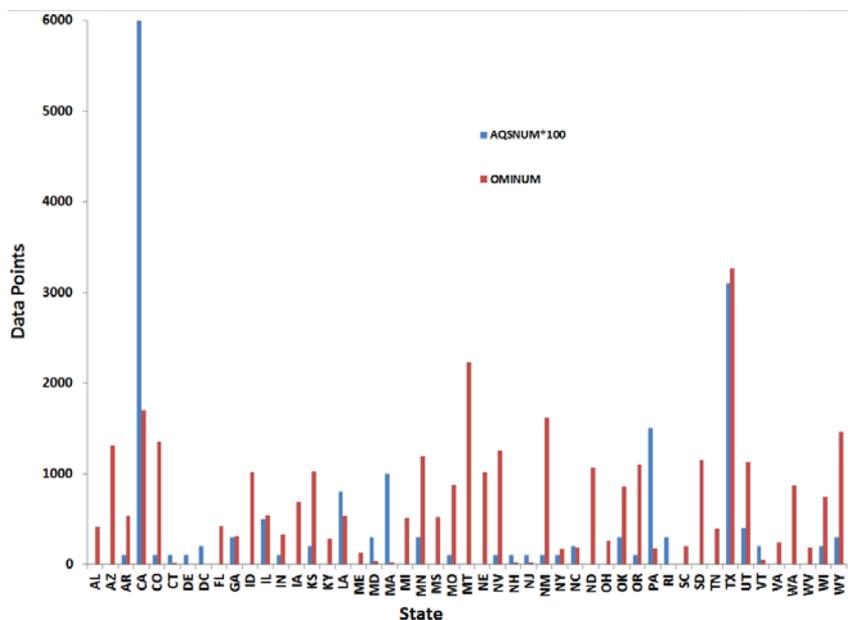
(Source: Tong et al., 2015)

Rapid Refresh of NO_x Emissions

Question: Can satellite and ground data be used to rapidly refresh NO_x emissions?

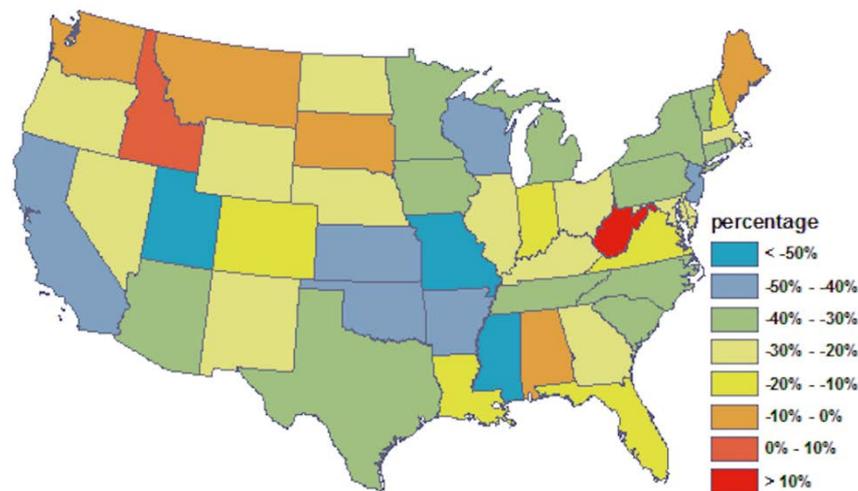
Fusing AQS & OMI

$$AF = \frac{\Delta S \times N_S \times f_S + \Delta G \times N_G \times f_G}{N_S \times f_S + N_G \times f_G}$$



Comparison of OMI and AQS (x100) Samples

State-level Projection



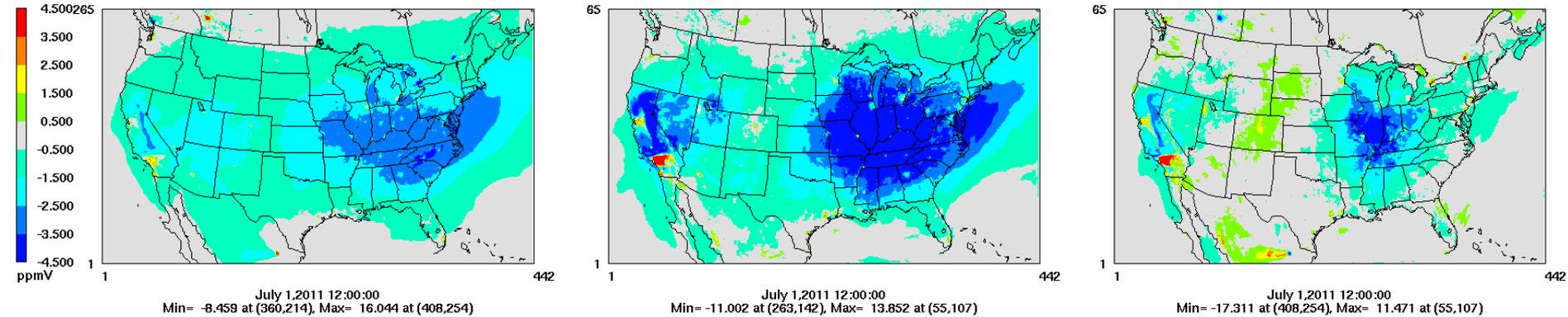
(2005 to 2012)

Effect on O₃ Forecast

Effect of Using EPA Projection

Effect of Using Fused Obs.

Difference



Performance Metrics (July 2011 over CONUS)

	MB (ppbv)		NMB (%)		RMSE (ppbv)	
	Hourly	Max8	Hourly	Max8	Hourly	Max8
Op. NAQFC	11.9	9.9	29.7	20.3	23.1	21.5
Fused Obs	11.5	9.7	28.7	20.1	22.7	21.4

Summary

- ❖ Revealed consistent NO_x responses to the 2008 Economic Recession by OMI and AQS (-6%, -10%, and -3% reduction per year before, during and after the Recession);
- ❖ Demonstrated how to use space and ground observations to 1) evaluate emission updates; and 2) rapidly update NO_x emissions to support national air quality forecasting.

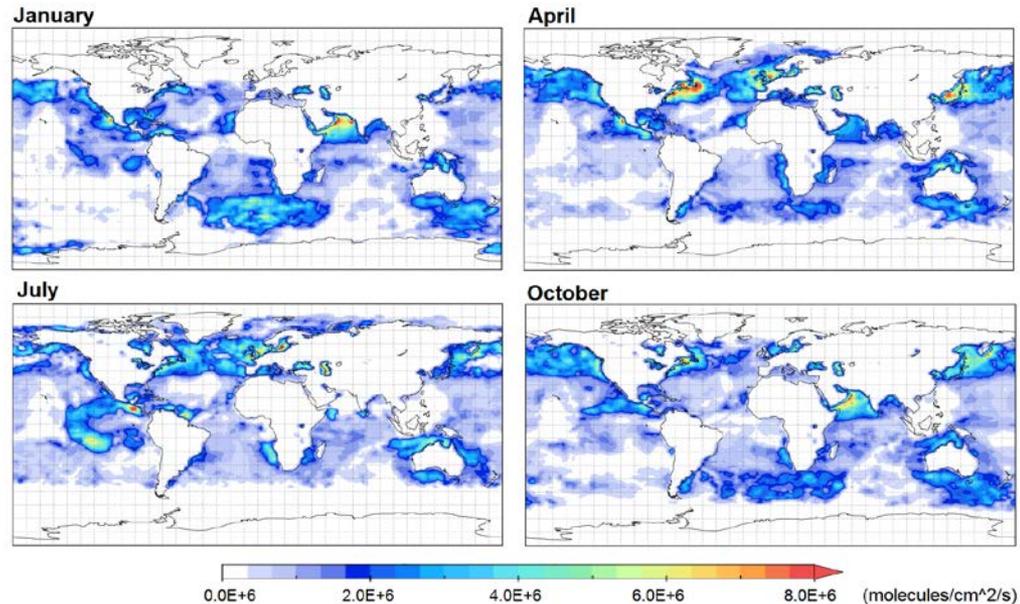
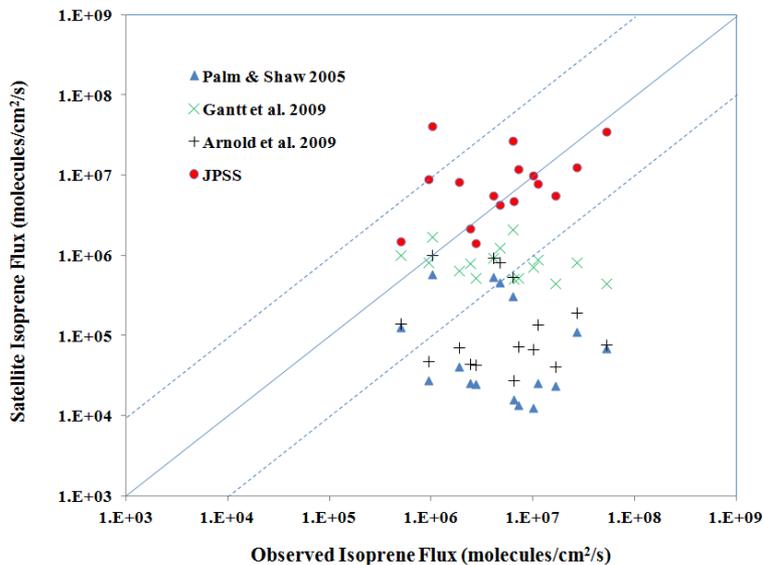
References:

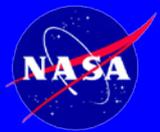
Tong, D.Q., L. Pan, W. Chen, L. Lamsal, P. Lee, Y. Tang, H. Kim, S. Kondragunta, I. Stajner, 2016. Impact of the 2008 Global Recession on air quality over the United States: Implications for surface ozone levels from changes in NO_x emissions. Geophysical Research Letter, Accepted.

Tong, D.Q., L. Lamsal, L. Pan, C. Ding, H. Kim, P. Lee, T. Chai, and K.E. Pickering, and I. Stajner, 2014. Long-term NO_x trends over large cities in the United States during the 2008 Recession: Intercomparison of satellite retrievals, ground observations, and emission inventories, Atmospheric Environment, 107,70-84, doi:10.1016/j.atmosenv.2015.01.035.

JPSS and Marine Isoprene

- SNPP-VIIRS, MODIS and SeaWiFS was used to produce marine isoprene emissions for use in NAQFC and other NOAA models





Continuation of Global Anthropogenic and Volcanic SO₂ Monitoring from OMI to OMPS

Nick Krotkov

NASA GSFC Code 614

Email: Nickolay.A.Krotkov@nasa.gov

Can Li, Yan Zhang, Simon Carn, Joanna Joiner, Rob Spurr

Trace Gas Session

3rd Annual JPSS Meeting

August 11, 2016

College Park, MD



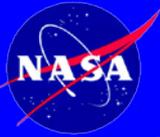
Outline

- Background and motivation
- PCA algorithm – data driven, straightforward to implement, small noise and artifacts
- Application to OMI – operational algorithms for new OMI PBL and volcanic SO₂ data
- Application to OMPS – implementation of OMI PCA algorithms with OMPS shows good consistency between two instruments



NASA SO₂ processing

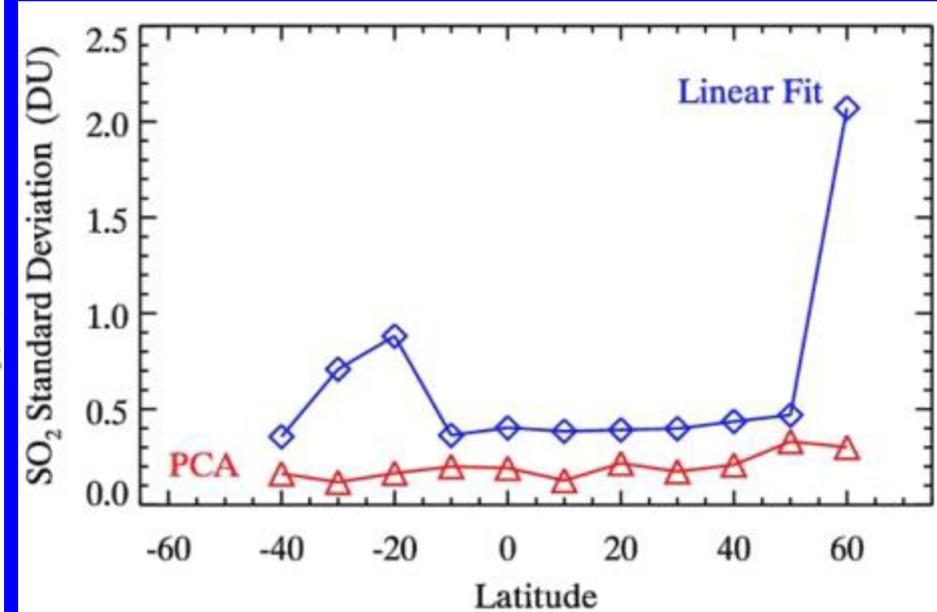
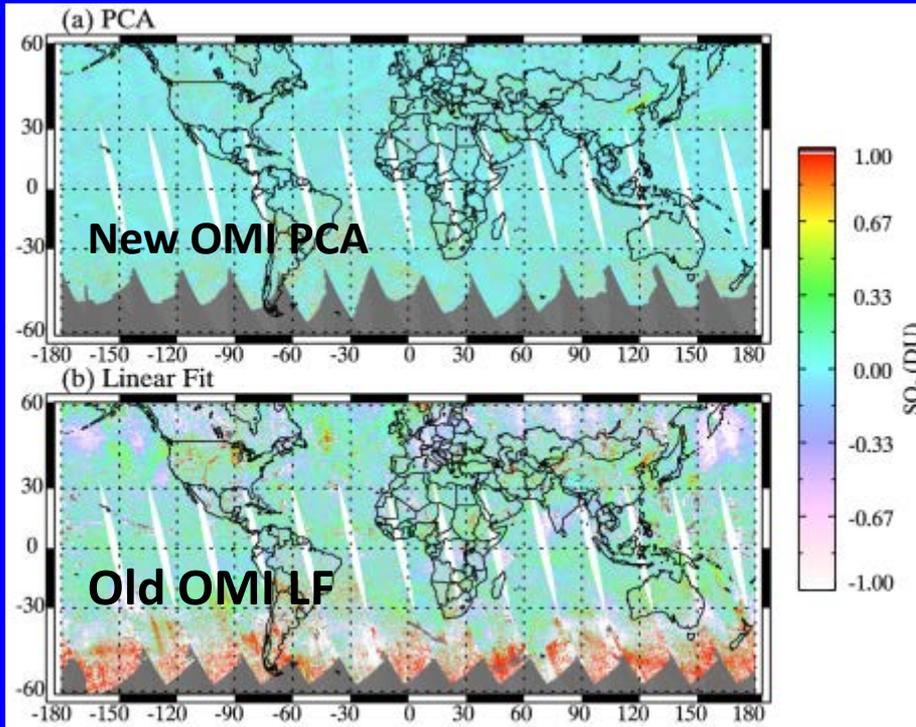
- Developed new PCA algorithm [Li et al., 2013]
 - data driven,
 - efficient,
 - smallest noise and artifacts
 - Does not require soft calibration => good consistency
- Application to OMI – operational algorithms for new OMI PBL and volcanic SO₂ data
- Application to OMPS – implementation of OMI PCA algorithms with OMPS shows good consistency between two instruments
- Data are available on our web site:
<http://so2.gsfc.nasa.gov>



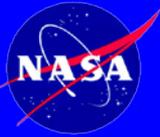
Execution Speed of the PCA SO₂ Algorithm

- ~4 min per OMI orbit (~70,000 pixels) using simplified SO₂ Jacobians LUT ;
- 5 days used for reprocessing 10-year OMI data for the current operational PBL product;
- ~65 min per OMI orbit using full LUT - can be reduced to ~10 min if cross-section is used in fitting for SCD and then converted to VCD using AMF;
- ~20 s per OMPS orbit (~10,000 pixels) using simplified SO₂ Jacobians LUT

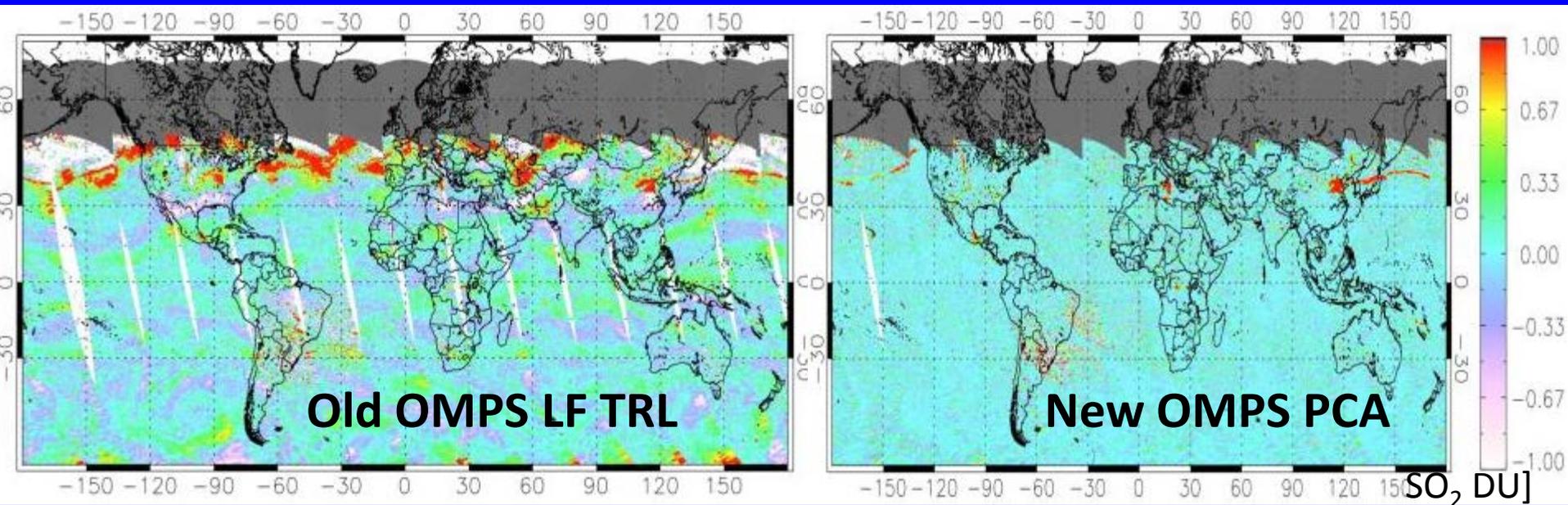
OMI: New Operational OMI Volcanic SO₂ Product Greatly Reduces Bias and Noise over Background Areas



Retrieval noise reduced by a factor of two



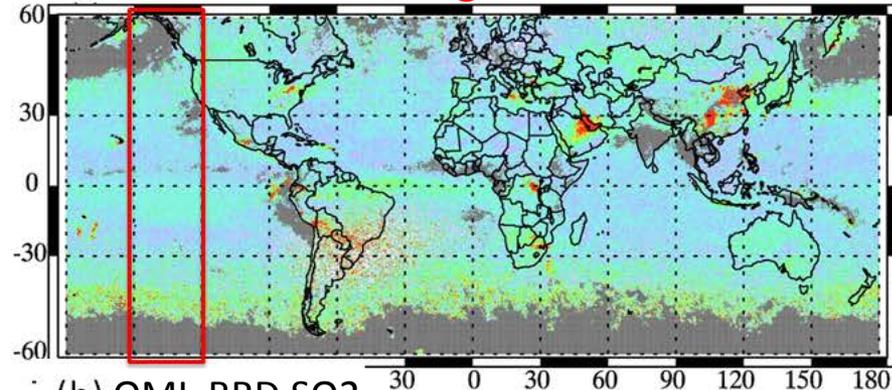
OMPS: Reduced Background noise and artifacts: volcanic SO₂



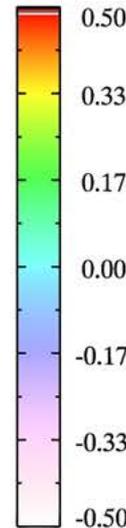
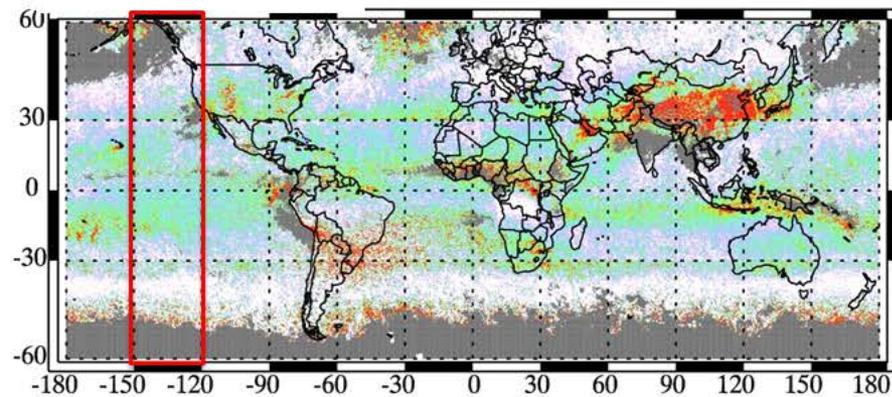
OMPS NRT LF TRL retrievals for 12/08/2015,
a few days after the December 3 2015
Mt. Etna eruption.

Reduced Background noise and artifacts: PBL SO₂

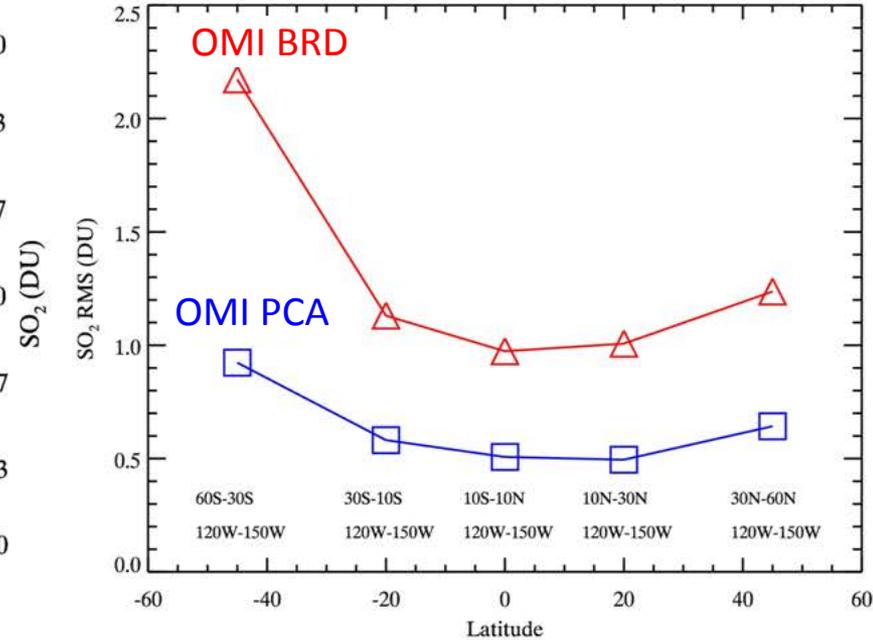
(a) OMI PCA SO₂ **August, 2006**



(b) OMI BRD SO₂

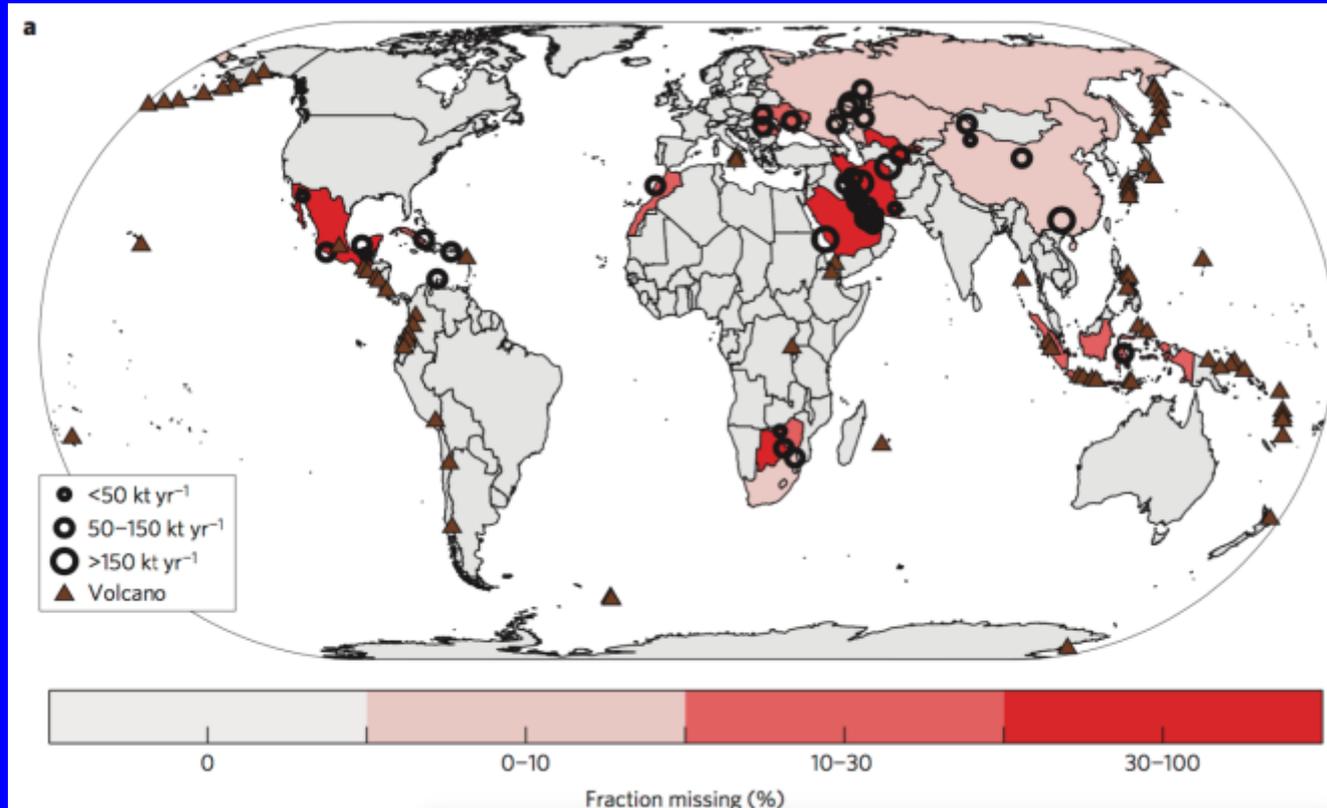


(c) RMS over the East Pacific (red box)



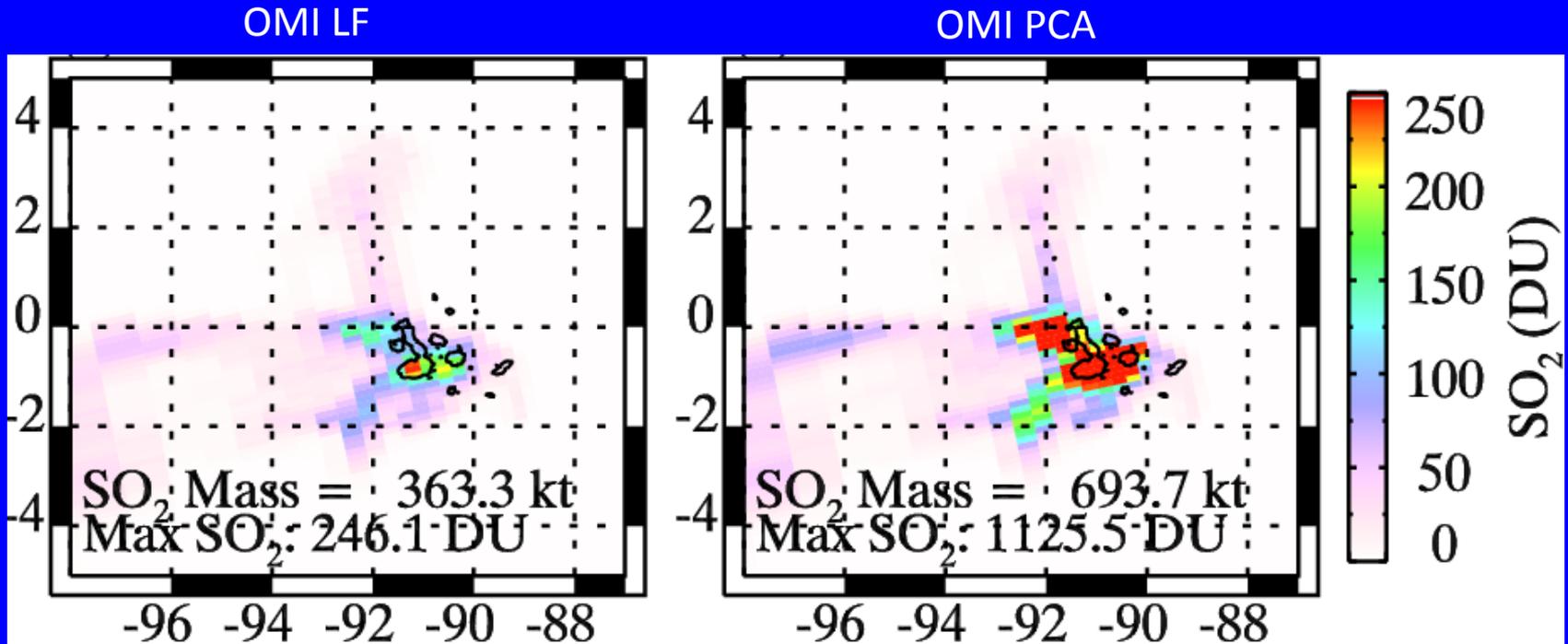
- PCA algorithm reduces retrieval noise by a factor of two as compared with the BRD algorithm
- SO₂ Jacobians for PCA algorithm calculated with the same assumptions as in the BRD algorithm

When combined with wind data and careful, innovative data analysis ...

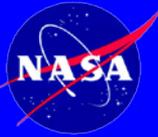


- An independent “top-down” global SO₂ emission inventory [McLinden et al., NG 2016];
- Annual emissions quantified for ~500 large sources, ~40 missing or unreported in “bottom-up” inventories, or ~6-12% of the total anthropogenic sources;
- Emissions quantified for 75 volcanoes – large differences between OMI measurements and the AeroCom database.

New OMI Operational PCA Volcanic SO₂ Greatly Reduces Low Bias in the old LF SO₂ for Large Eruptions



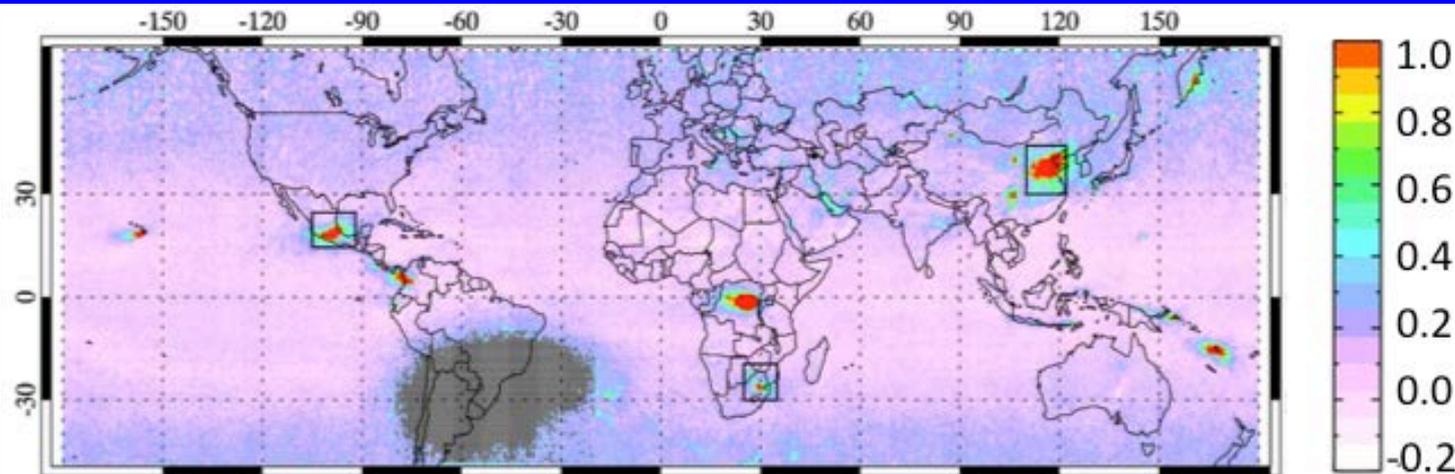
- Sierra Negra eruption in 2005, max SO₂ from new operational PCA algorithm ~1100 DU, in agreement with the offline ISF algorithm [Li et al., 2016]
- Kasatochi eruption in 2008: PCA total SO₂ ~1700 kt, consistent with ISF and OE algorithms for OMI and GOME-2, a factor of two more than LF with known low bias [Krotkov et al., 2010].



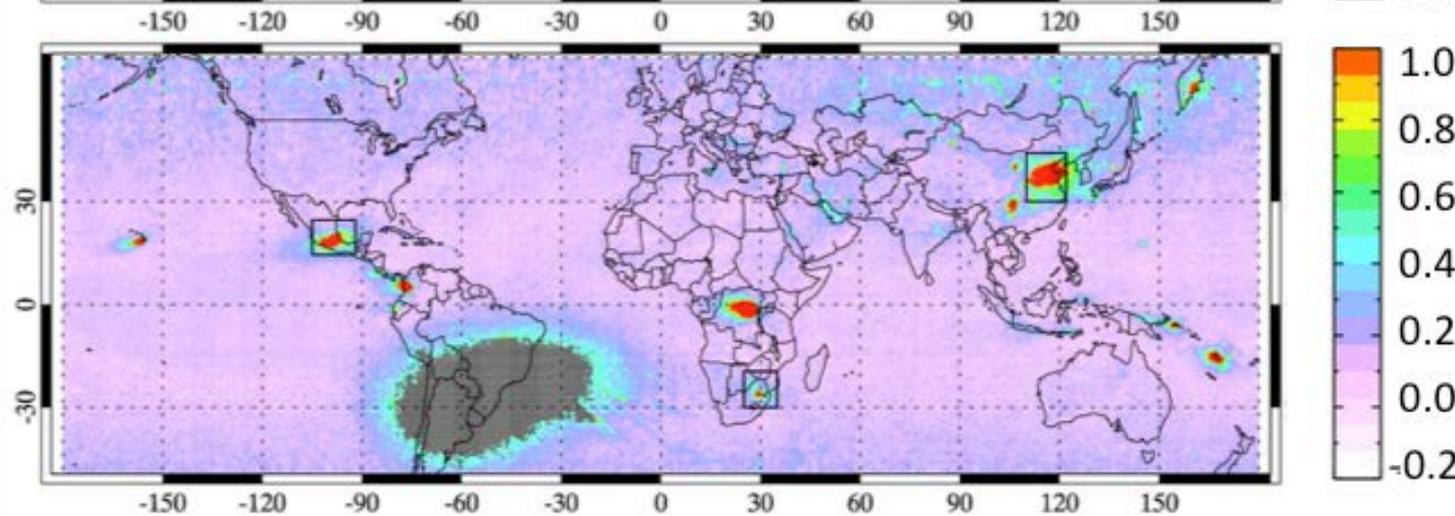
Good consistency between OMI and OMPS Annual Mean PBL SO₂ Retrievals for 2012



OMI



OMPS



No soft calibration or L2 correction

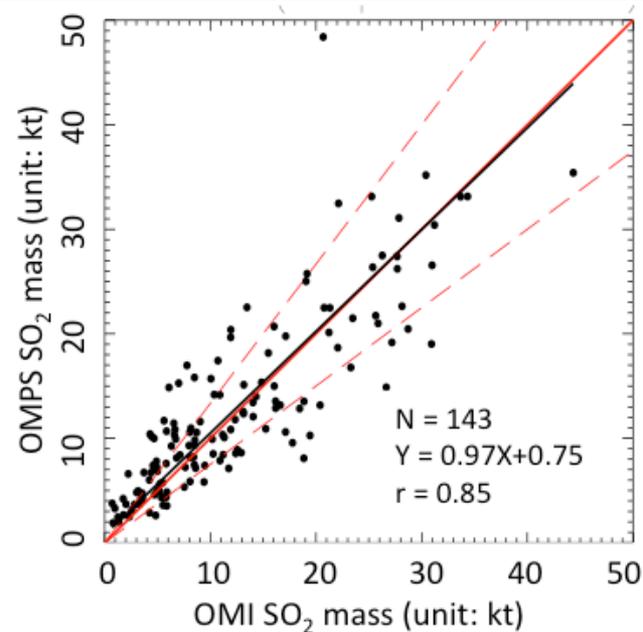
[Zhang et al., 2016]



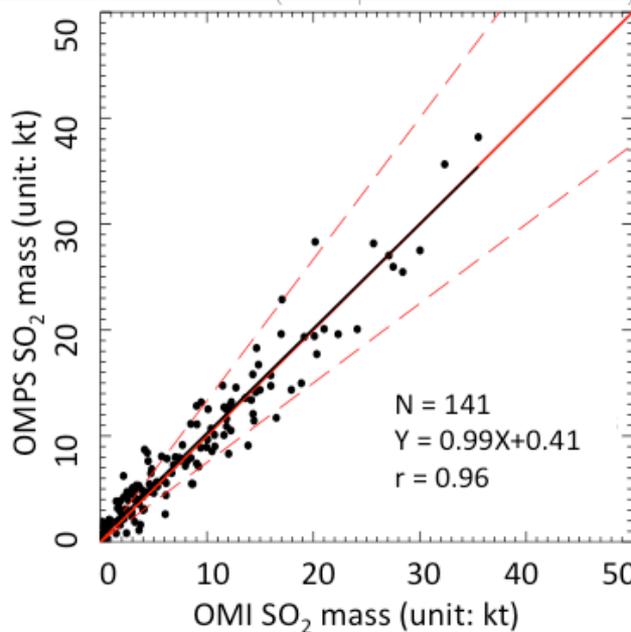
Daily regional SO₂ loading over the selected areas in 2012 (PBL retrievals)



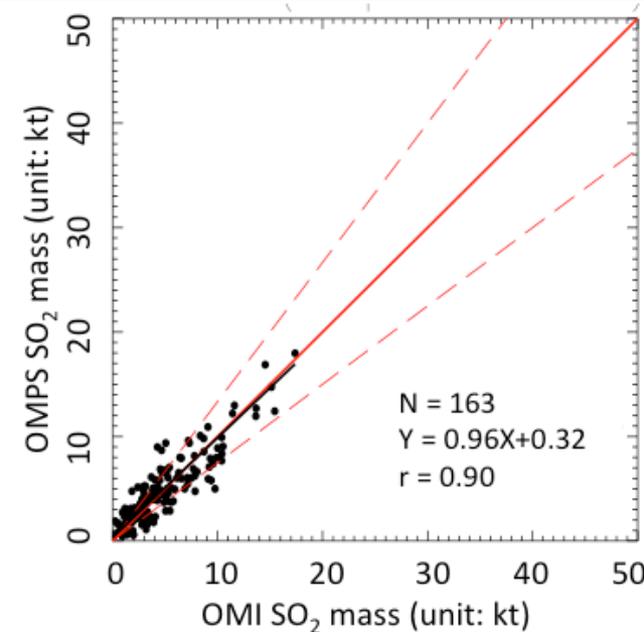
E China



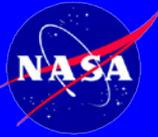
Mexico



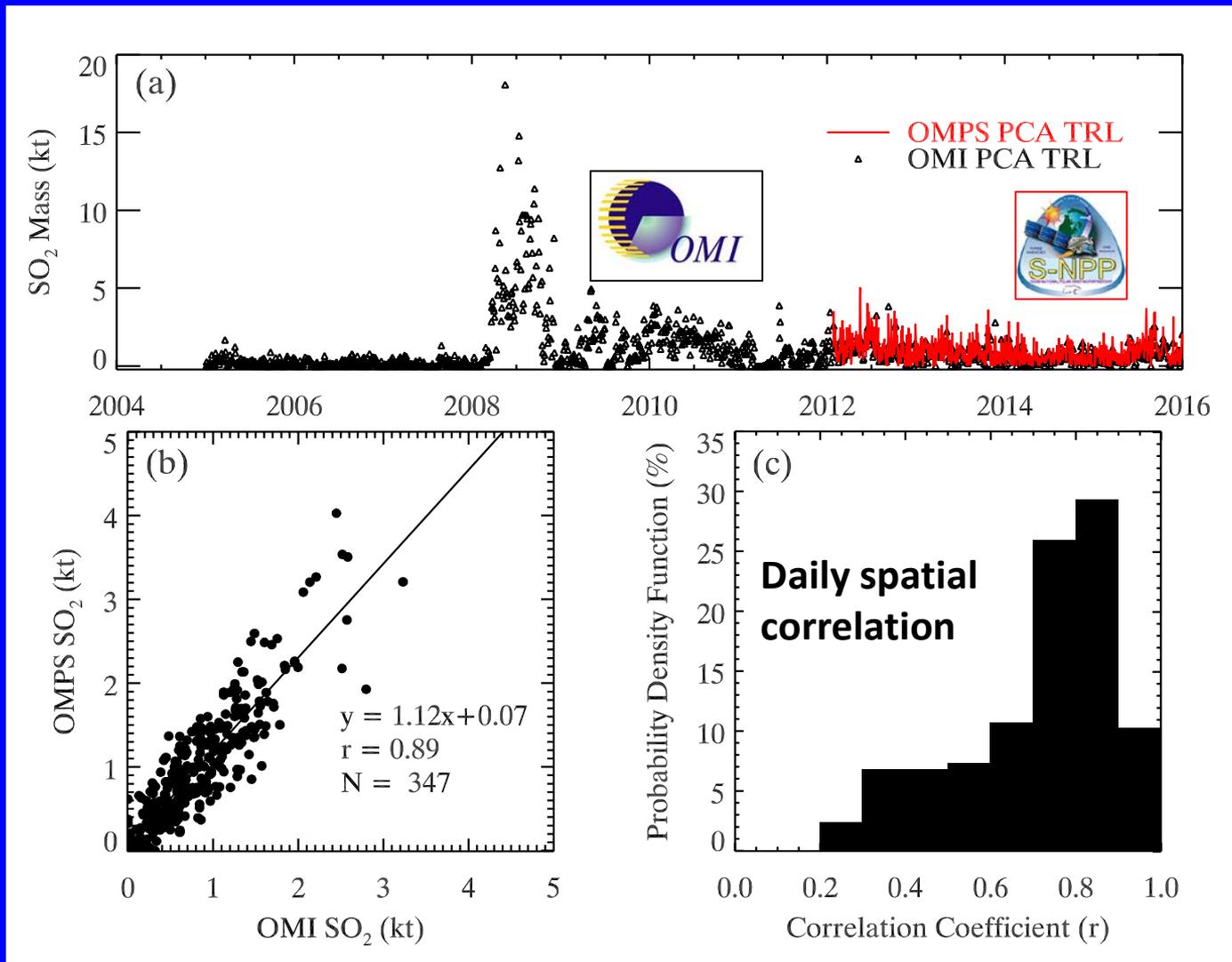
South Africa



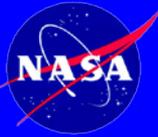
[Zhang et al., AMTD 2016]



Daily OMI/OMPS regional volcanic SO₂ loading Hawaii (PCA 3-km/TRL retrievals)

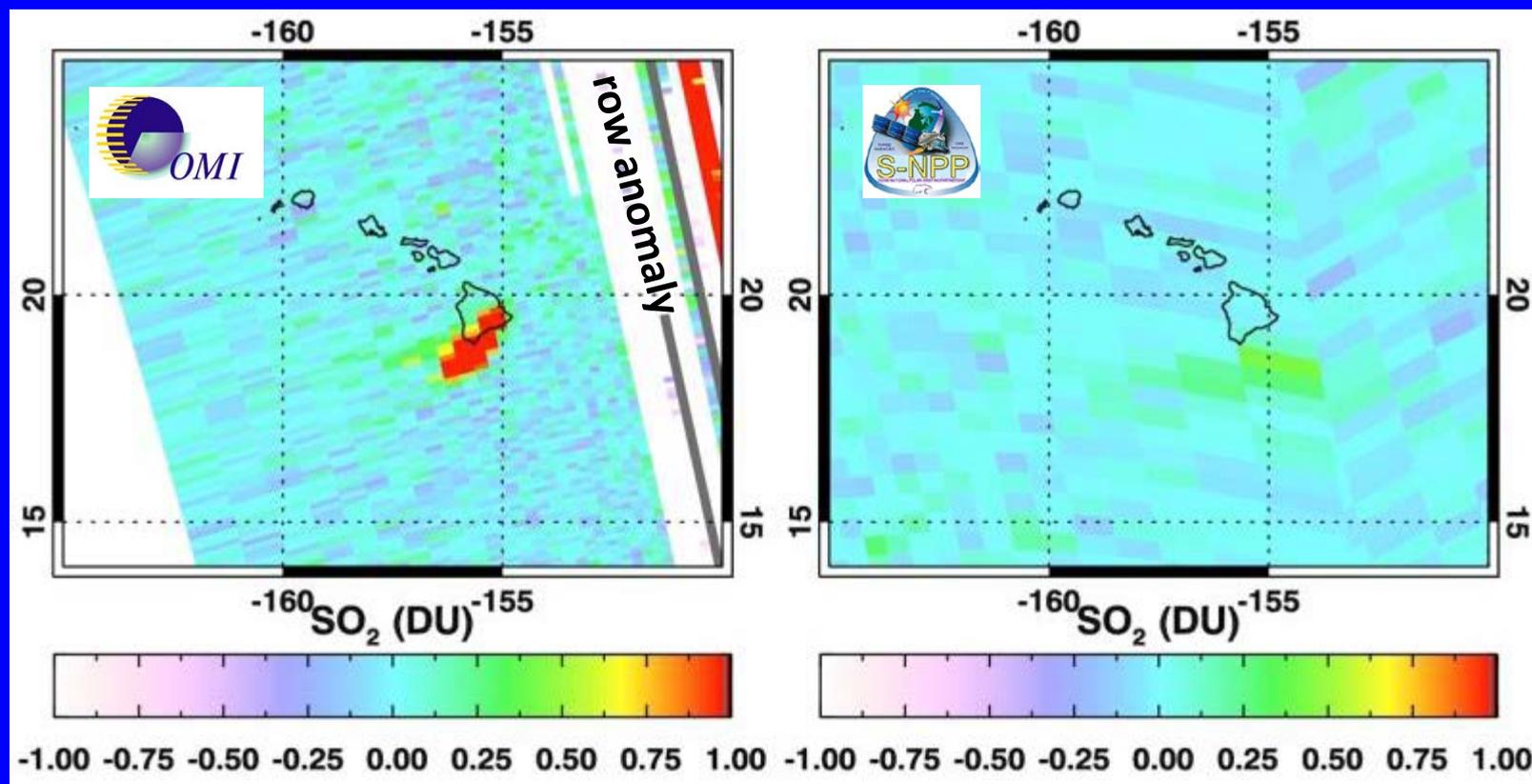


[Li et al., 2016]

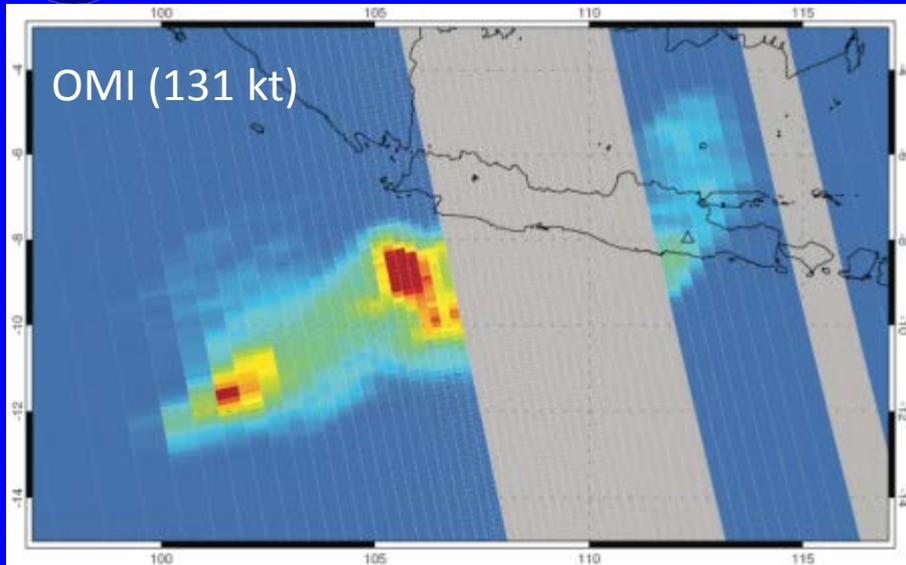


Five days with $r < 0.3$, why?

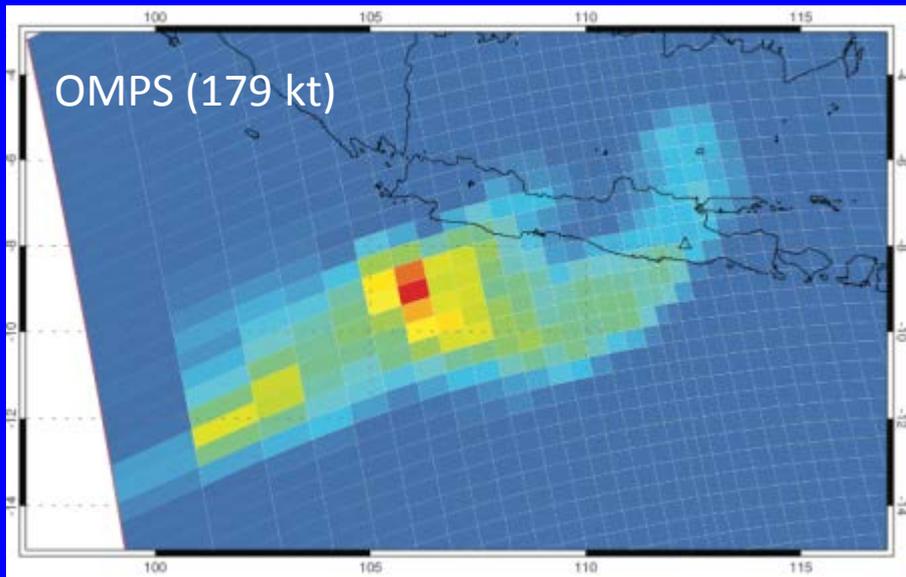
- ✓ Five days with $r < 0.3$: 02/05/2012, 10/02/2012, 05/14/2013, 11/06/2013, and 11/09/2014.
- ✓ For all five days, the plume was covered by OMI pixels near the nadir but by OMPS pixels near the edge of the swath.



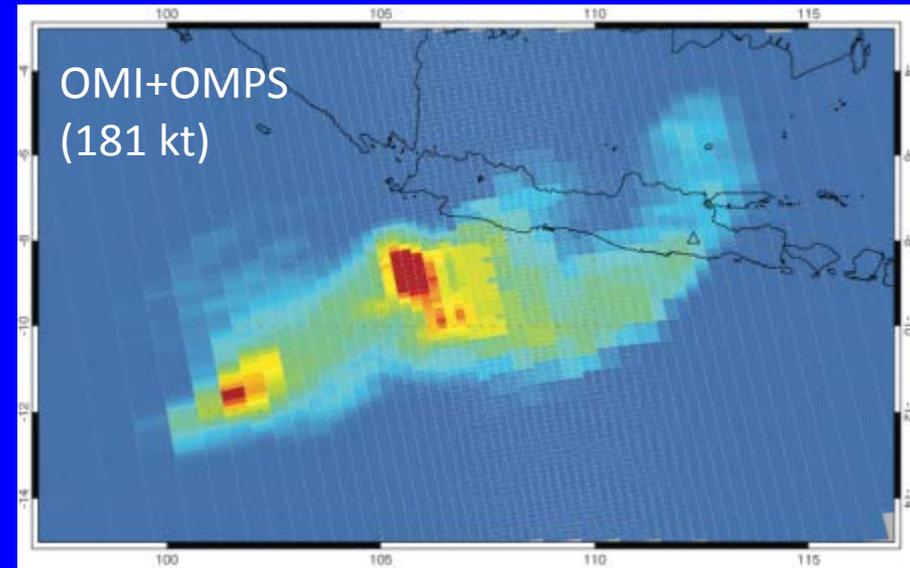
11/06/2013



+



=



- ✓ Merged OMI+OMPS provides full coverage and fine spatial detail
- ✓ Agrees with OMPS only SO₂ mass to within 3%

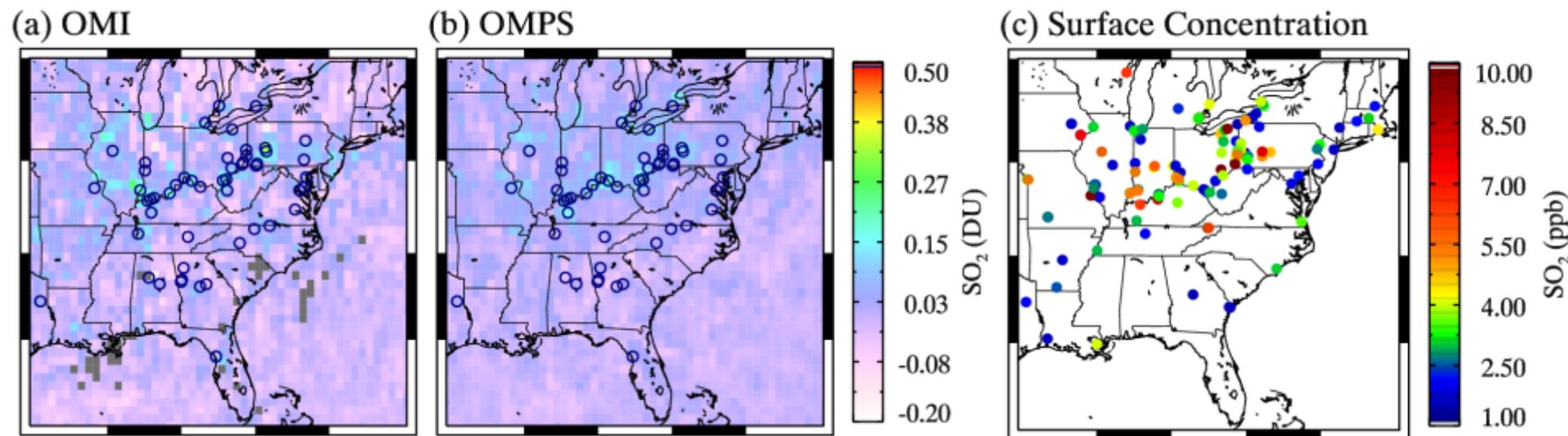


New OMI and OMPS anthropogenic SO₂ retrievals with comprehensive LUT for Jacobians

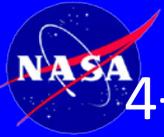


Monthly Mean, August 2012

Monthly Mean at 2 pm Local Time



- ✓ Preliminary new OMI and OMPS pollution SO₂ retrievals both reveal emission sources over the Ohio River valley (circles are sources with > 50 kt emissions in 2006).
- ✓ Surface monitoring stations show qualitatively consistent pattern.
- ✓ If assuming the same mixing ratio for the lowest 100 hPa (~1000 m) of the atmosphere and no SO₂ above, 4 ppb translates into ~0.3 DU in column loading.



4+ Years of OMPS PBL SO₂ Research Product Now Available on NASA's SO₂ Website: <http://so2.gsfc.nasa.gov>

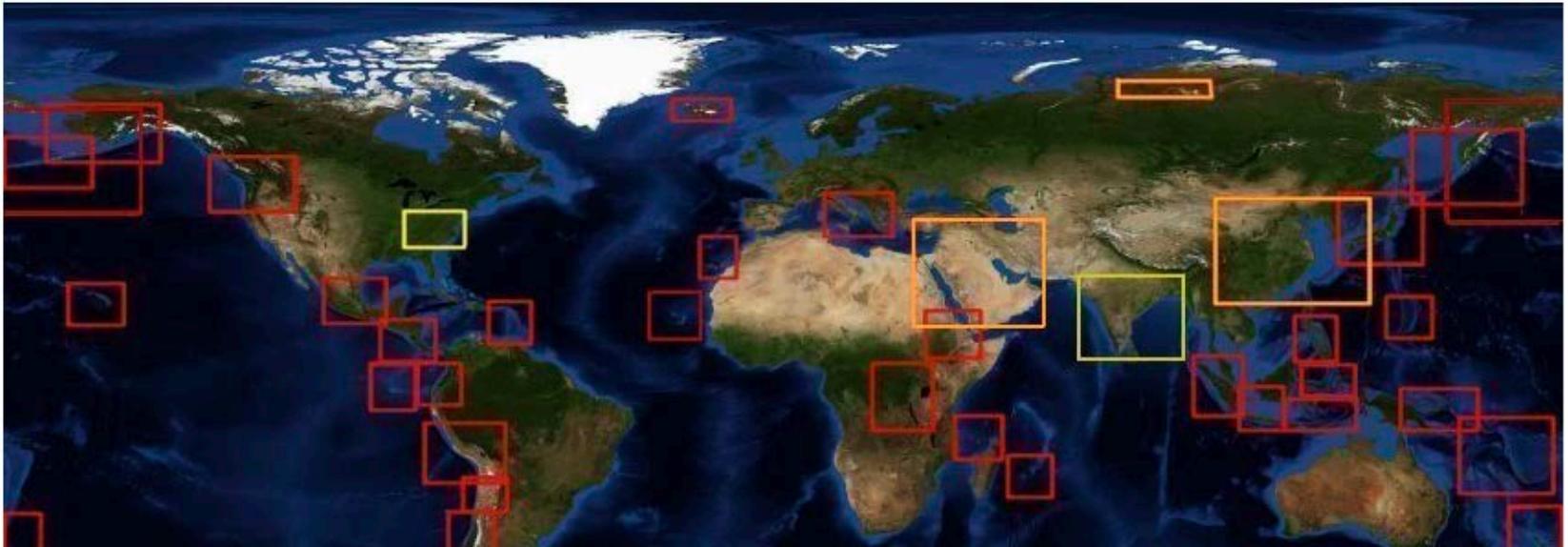
TOMS images (1979-2005) | AIRS images (2003-present) | OMI images (2004-present) | OMPS images (May 2012-present)

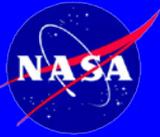
Global monthly OMI Boundary Layer SO₂ maps

Global monthly OMPS Boundary Layer SO₂ maps

Latest Daily (OMI/OMPS) Images of SO₂ (click on a highlighted rectangle)

Red = daily volcanic regions, **orange** = daily pollution regions, **yellow** = long-term pollution images





Conclusions

- The PCA SO₂ retrieval approach – data-driven, good quality, straightforward to implement.
- Operational OMI PCA PBL and volcanic SO₂ data show significant improvement over previous OMI data, also compare well with OMI DOAS SO₂ data using TROPOMI prototype algorithm [*Theys et al.*, 2015].
- Research OMPS PBL and volcanic SO₂ data based on PCA algorithms show good consistency with OMI data.



The capability of the OMPS Linear Fit SO₂ (LFSO2) algorithm for implementation at NDE

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C. Trevor Beck, Lawrence E. Flynn

NOAA/NESDIS/STAR

Kai Yang

University of Maryland

Goal for LFSO2 implementation at NOAA

1. Provide near real time ***alerts*** of volcanic SO₂ clouds.
2. Provide O₃ ***corrections*** when large amounts of SO₂ are present.
3. Provide ***accurate SO₂ total column amounts*** to address the shortfall of the existing products in the Version-8 ozone algorithm.

Residuals and Linearization

The algorithm starts from N-values: $N_m(\Omega, \Xi, R, \lambda_i) = N(\Omega, \Xi, R, \lambda_i) + \varepsilon_r$ (1)

We linearize the problem with differentials at $\Omega = \Omega_0$, $\Xi = \Xi_0$, $R = R_0$:

$$\begin{aligned}
 N_m(\lambda_2) - N_0(\lambda_2) &= \Delta\Omega \left. \frac{dN(\lambda_2)}{d\Omega} \right|_{\Omega=\Omega_0} + \Delta\Xi \left. \frac{dN(\lambda_2)}{d\Xi} \right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^2 c_j (\lambda_2 - \lambda_0)^j \right) \left. \frac{dN(\lambda_2)}{dR} \right|_{R=R_0} + \varepsilon_r \\
 N_m(\lambda_3) - N_0(\lambda_3) &= \Delta\Omega \left. \frac{dN(\lambda_3)}{d\Omega} \right|_{\Omega=\Omega_0} + \Delta\Xi \left. \frac{dN(\lambda_3)}{d\Xi} \right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^2 c_j (\lambda_3 - \lambda_0)^j \right) \left. \frac{dN(\lambda_3)}{dR} \right|_{R=R_0} + \varepsilon_r \\
 N_m(\lambda_4) - N_0(\lambda_4) &= \Delta\Omega \left. \frac{dN(\lambda_4)}{d\Omega} \right|_{\Omega=\Omega_0} + \Delta\Xi \left. \frac{dN(\lambda_4)}{d\Xi} \right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^2 c_j (\lambda_4 - \lambda_0)^j \right) \left. \frac{dN(\lambda_4)}{dR} \right|_{R=R_0} + \varepsilon_r \quad (2) \\
 &\dots \\
 &\dots \\
 N_m(\lambda_i) - N_0(\lambda_i) &= \Delta\Omega \left. \frac{dN(\lambda_i)}{d\Omega} \right|_{\Omega=\Omega_0} + \Delta\Xi \left. \frac{dN(\lambda_i)}{d\Xi} \right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^2 c_j (\lambda_i - \lambda_0)^j \right) \left. \frac{dN(\lambda_i)}{dR} \right|_{R=R_0} + \varepsilon_r
 \end{aligned}$$

$N_0(\lambda)$: radiative transfer model computed at $N_0(\Omega_0, \Xi_0, R_0, \lambda)$.

$N_m(\lambda)$: measured N-value.

$N_m(\lambda) - N_0(\lambda)$: V8TOZ Algorithm output residuals.

15-Granule Bias Estimates

The ozone retrieval provided residual includes biases along-orbit. To eliminate these residual biases, A 15-granule implementation technique is designed. Residual averages $\langle \psi(\lambda) \rangle$ over three five-granule intervals (corresponding to $\sim 10^\circ$ latitude) are calculated at the 12 wavelength bands and 35 cross tracks. Each individual average residual within these three averaged intervals are calculated by interpolation. The corrected residual, $\psi(\lambda) = N_m(\lambda) - N_0(\lambda) - \langle \psi(\lambda) \rangle$ is called the “adjust residual”, then:

$$\begin{aligned}
 \psi(\lambda_2) &= \Delta\Omega \left. \frac{dN(\lambda_2)}{d\Omega} \right|_{\Omega=\Omega_0} + \Delta\Xi \left. \frac{dN(\lambda_2)}{d\Xi} \right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^2 c_j (\lambda_2 - \lambda_0)^j \right) \left. \frac{dN(\lambda_2)}{dR} \right|_{R=R_0} + \varepsilon_r \\
 \psi(\lambda_3) &= \Delta\Omega \left. \frac{dN(\lambda_3)}{d\Omega} \right|_{\Omega=\Omega_0} + \Delta\Xi \left. \frac{dN(\lambda_3)}{d\Xi} \right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^2 c_j (\lambda_3 - \lambda_0)^j \right) \left. \frac{dN(\lambda_3)}{dR} \right|_{R=R_0} + \varepsilon_r \\
 \psi(\lambda_4) &= \Delta\Omega \left. \frac{dN(\lambda_4)}{d\Omega} \right|_{\Omega=\Omega_0} + \Delta\Xi \left. \frac{dN(\lambda_4)}{d\Xi} \right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^2 c_j (\lambda_4 - \lambda_0)^j \right) \left. \frac{dN(\lambda_4)}{dR} \right|_{R=R_0} + \varepsilon_r \\
 &\dots \\
 &\dots \\
 \psi(\lambda_i) &= \Delta\Omega \left. \frac{dN(\lambda_i)}{d\Omega} \right|_{\Omega=\Omega_0} + \Delta\Xi \left. \frac{dN(\lambda_i)}{d\Xi} \right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^2 c_j (\lambda_i - \lambda_0)^j \right) \left. \frac{dN(\lambda_i)}{dR} \right|_{R=R_0} + \varepsilon_r
 \end{aligned} \tag{3}$$

These linear equations can be converted into a matrix expression.

Matrix Formulation

$$\begin{pmatrix} \psi(\lambda_2) \\ \psi(\lambda_3) \\ \cdot \\ \psi(\lambda_i) \\ \cdot \\ \psi(\lambda_{11}) \end{pmatrix} = \begin{pmatrix} \frac{dN(\lambda_2)}{d\Omega} & \frac{dN(\lambda_2)}{d\Xi} & \frac{dN(\lambda_2)}{dR} & (\lambda_2 - \lambda_0) \frac{dN(\lambda_2)}{dR} & (\lambda_2 - \lambda_0)^2 \frac{dN(\lambda_2)}{dR} \\ \frac{dN(\lambda_3)}{d\Omega} & \frac{dN(\lambda_3)}{d\Xi} & \frac{dN(\lambda_3)}{dR} & (\lambda_3 - \lambda_0) \frac{dN(\lambda_3)}{dR} & (\lambda_3 - \lambda_0)^2 \frac{dN(\lambda_3)}{dR} \\ \dots & & & & \\ \frac{dN(\lambda_i)}{d\Omega} & \frac{dN(\lambda_i)}{d\Xi} & \frac{dN(\lambda_i)}{dR} & (\lambda_i - \lambda_0) \frac{dN(\lambda_i)}{dR} & (\lambda_i - \lambda_0)^2 \frac{dN(\lambda_i)}{dR} \\ \cdot & & & & \\ \dots & & & & \\ \frac{dN(\lambda_{11})}{d\Omega} & \frac{dN(\lambda_{11})}{d\Xi} & \frac{dN(\lambda_{11})}{dR} & (\lambda_{11} - \lambda_0) \frac{dN(\lambda_{11})}{dR} & (\lambda_{11} - \lambda_0)^2 \frac{dN(\lambda_{11})}{dR} \end{pmatrix} \begin{pmatrix} \Delta\Omega \\ \Delta\Xi \\ \Delta R \\ c_1 \\ c_2 \end{pmatrix} + \begin{pmatrix} \varepsilon(\lambda_2) \\ \varepsilon(\lambda_3) \\ \cdot \\ \varepsilon(\lambda_i) \\ \cdot \\ \varepsilon(\lambda_{11}) \end{pmatrix}$$

The sensitivities differ depending upon the assumed height of the SO₂ layer. Estimates of the total column SO₂ using this Matrix formula is obtained for three different heights: Lower Troposphere (TRL), Middle Troposphere (TRM) and Lower Stratosphere (STL). Other technique is used to estimate Planetary Boundary Layer (PBL) SO₂.

Retrieval Parameters

Name	Type	Description	Dimension	Units	Range
s_AlgorithmFlag_PBL	32 bit integer	PBL algorithm flag	105 x 15	Unitless	0, 1, 11
s_AlgorithmFlag_STL	32 bit integer	STL algorithm flag	105 x 15	Unitless	0, 1, 2, 11, 12
s_AlgorithmFlag_TRL	32 bit integer	TRL algorithm flag	105 x 15	Unitless	0, 1, 2, 11, 12
s_AlgorithmFlag_TRM	32 bit integer	TRM algorithm flag	105 x 15	Unitless	0, 1, 2, 11, 12
s_QualityFlags_PBL	32 bit integer	PBL quality flag	105 x 15	Unitless	0 ~ 65535
s_QualityFlags_STL	32 bit integer	STL quality flag	105 x 15	Unitless	0 ~ 65535
s_QualityFlags_TRL	32 bit integer	TRL quality flag	105 x 15	Unitless	0 ~ 65535
s_QualityFlags_TRM	32 bit integer	TRM quality flag	105 x 15	Unitless	0 ~ 65535
s_STLO3	32 bit float	STL corrected total column of O3	105 x 15	Dobson	0 ~ 1000
s_TRLO3	32 bit float	TRL corrected total column of O3	105 x 15	Dobson	0 ~ 1000
s_TRMO3	32 bit float	TRM corrected total column of O3	105 x 15	Dobson	0 ~ 1000
s_ColumnamountSO2_STL	32 bit float	STL total column of SO2	105 x 15	Dobson	-10 ~ 2000
s_ColumnamountSO2_TRL	32 bit float	TRL total column of SO2	105 x 15	Dobson	-10 ~ 2000
s_ColumnamountSO2_TRM	32 bit float	TRM total column of SO2	105 x 15	Dobson	-10 ~ 2000
s_deltaRefl331	32 bit float	Delta Reflectivity at 331 nm	105 x 15	Percent	-100 ~ 100

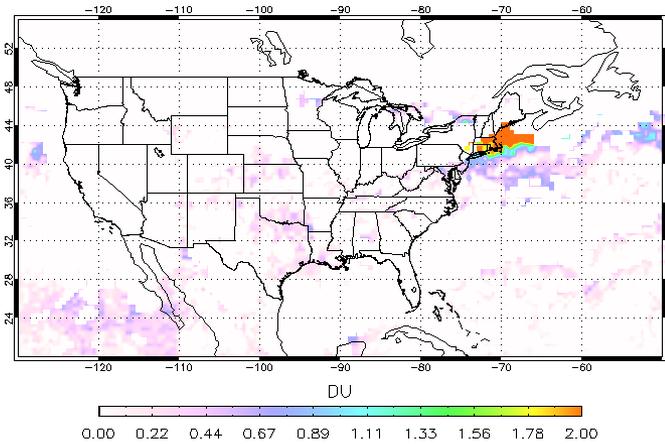
Retrieval Parameters

Name	Type	Description	Dimension	Units	Range
s_ChiSquareLfit	32 bit float	Chi-square of linear fit	105 x 15	Unitless	> 0
s_dN_dSO2_STL	32 bit float	dN/dSO2(STL)	12 x 105 x 15	Per Dobson	-1 ~ 100
s_dN_dSO2_TRL	32 bit float	dN/dSO2(TRL)	12 x 105 x 15	Per Dobson	-1 ~ 1000
s_dN_dSO2_TRM	32 bit float	dN/dSO2(TRM)	12 x 105 x 15	Per Dobson	-1 ~ 100
s_Slope	32 bit float	C_1 in linear equ.	105 x 15	Unitless	-1 ~ 1
s_Qterm	32 bit float	C_2 in linear equ.	105 x 15	Unitless	-1 ~ 1
s_ResidualAdjustment	32 bit float	Averaged residual of nvalue	12 x 105 x 15	Unitless	-10 ~ 10
s_ColumnamountSO2_PBL	32 bit float	Planetary Boundary Layer (PBL) SO2	105 x 15	Dobson	-300 ~ 1000
s_ColumnamountSO2_PBLbrd	32 bit float	PBL SO2 by BRD method	105 x 15	Dobson	-10 ~ 2000
s_ColumnamountSO2_STLbrd	32 bit float	STL SO2 by BRD method	105 x 15	Dobson	-10 ~ 2000
s_ColumnamountSO2_TRMbrd	32 bit float	TRM SO2 by BRD method	105 x 15	Dobson	-10 ~ 2000
s_SO2indexP1	32 bit float	Partial adjust residual for 310 and 311	105 x 15	Unitless	-100 ~ 100
s_SO2indexP2	32 bit float	Partial adjust residual for 311 and 313	105 x 15	Unitless	-100 ~ 100
s_SO2indexP3	32 bit float	Partial adjust residual for 313 and 314	105 x 15	Unitless	-100 ~ 100

Products from the LFSO2 algorithm

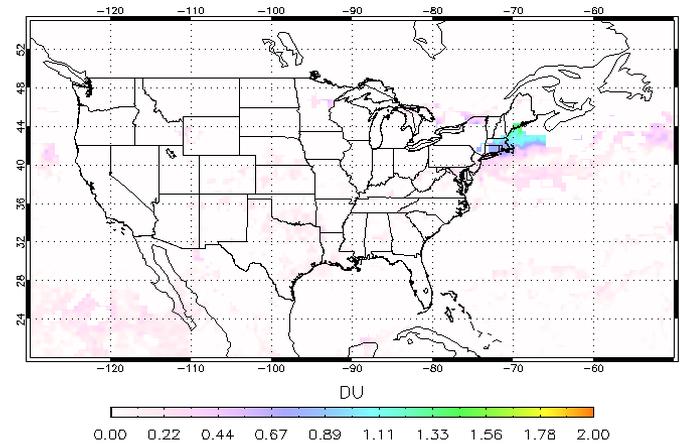
Umkhr-0: 0~5.5km

OMPS V8TOS trl SO₂ 2016/01/03



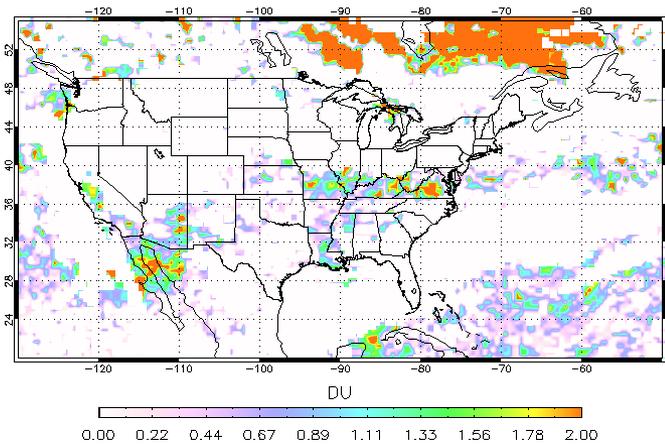
Umkhr-1: 5.5~10.3 km

OMPS V8TOS trm SO₂ 2016/01/03



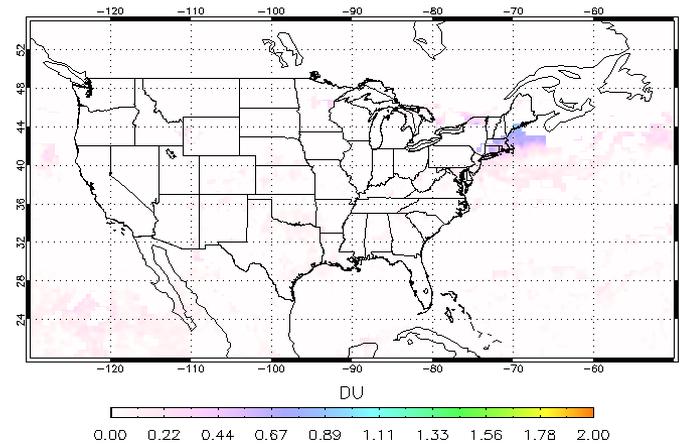
PBL: 0~2km

OMPS V8TOS pbl SO₂ 2016/01/03



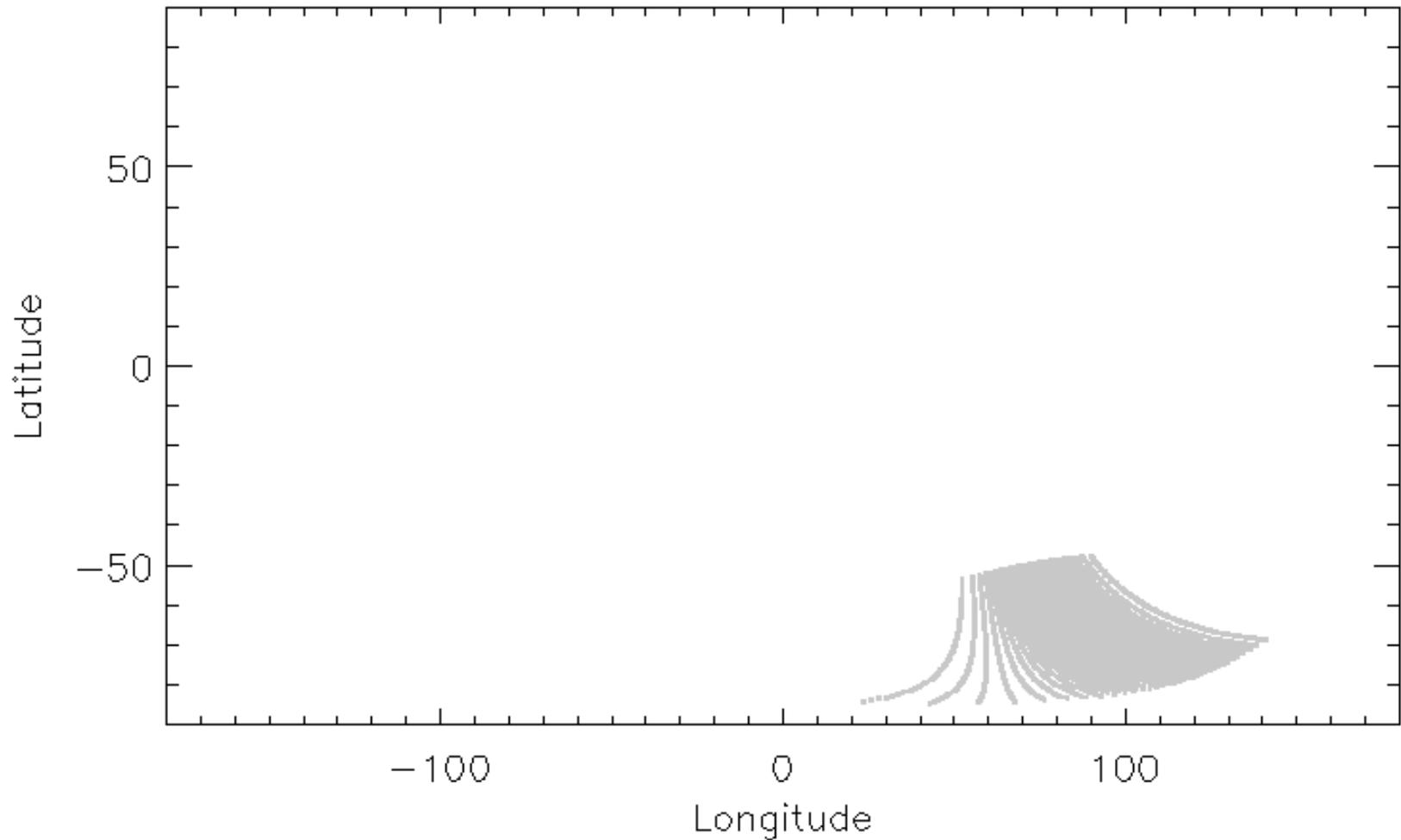
Umkhr-3: 14.7~19.1km

OMPS V8TOS stl SO₂ 2016/01/03



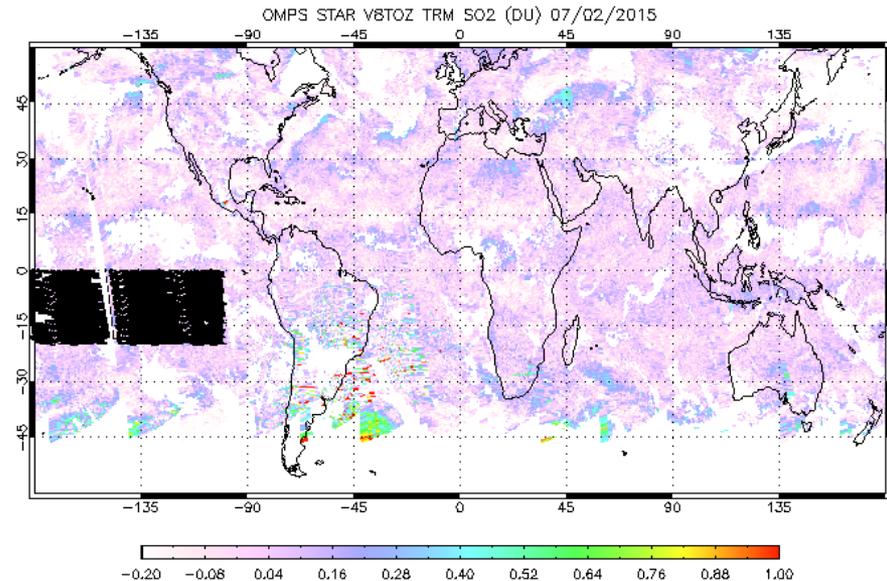
Strategy for running LFSO2

Strategy for near real time LFSO2 processing



Estimates minimum detectable SO_2 for single IFOV

	# IFOV	Average (DU)	STD (DU)
STL	5480	0.0037	0.069
TRM	5480	0.0057	0.09
TRL	5480	0.0125	0.18
PBL	5480	0.0624	0.6



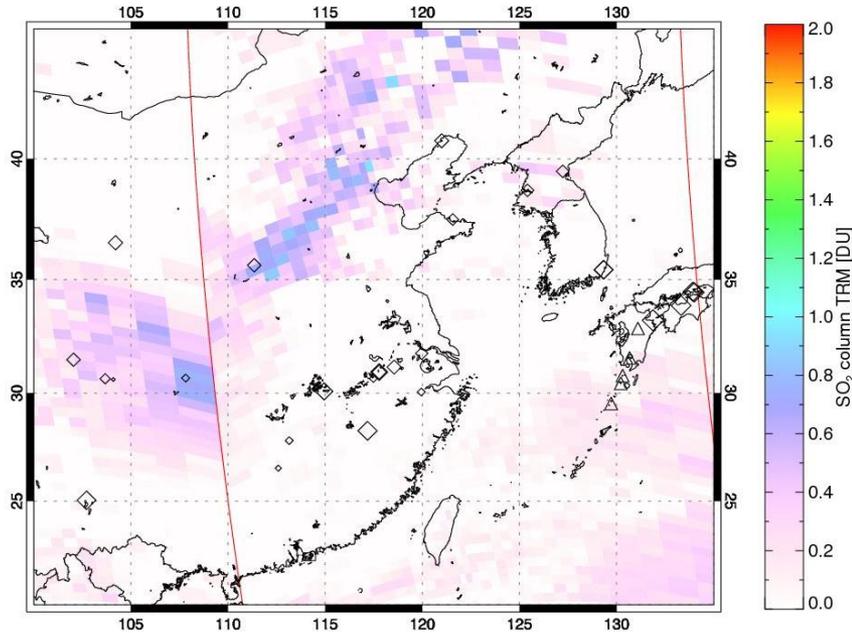
by Jianguo Niu System Research Group Inc.

SO₂ in 5~10km (TRM) over East China

From PEATE SO₂ website

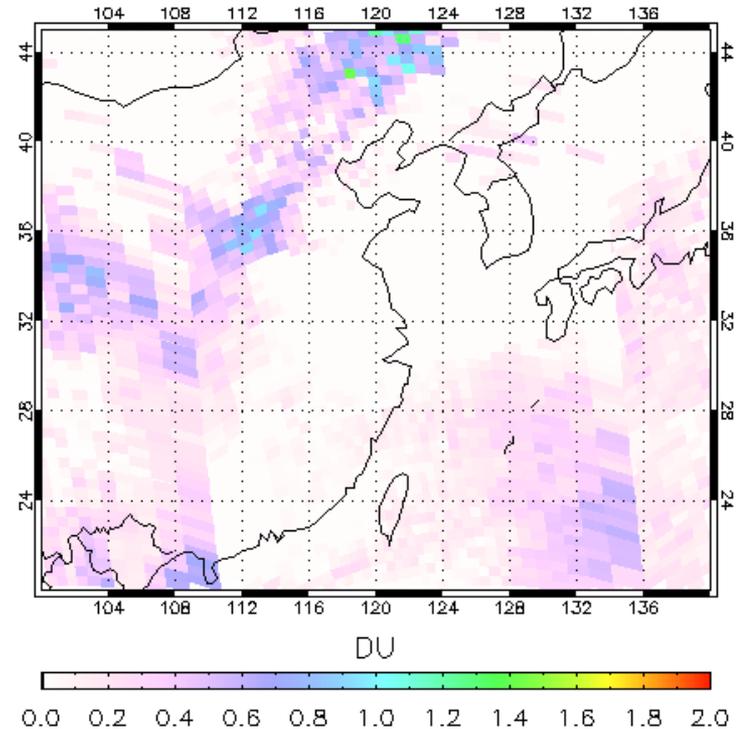
Suomi NPP/OMPS - 01/12/2016 03:24-06:52 UT

SO₂ mass: 0.006 kt; Area: 412 km²; SO₂ max: 0.94 DU at lon: 117.23 lat: 39.69 ; 05:09UTC



From Star LFSO2

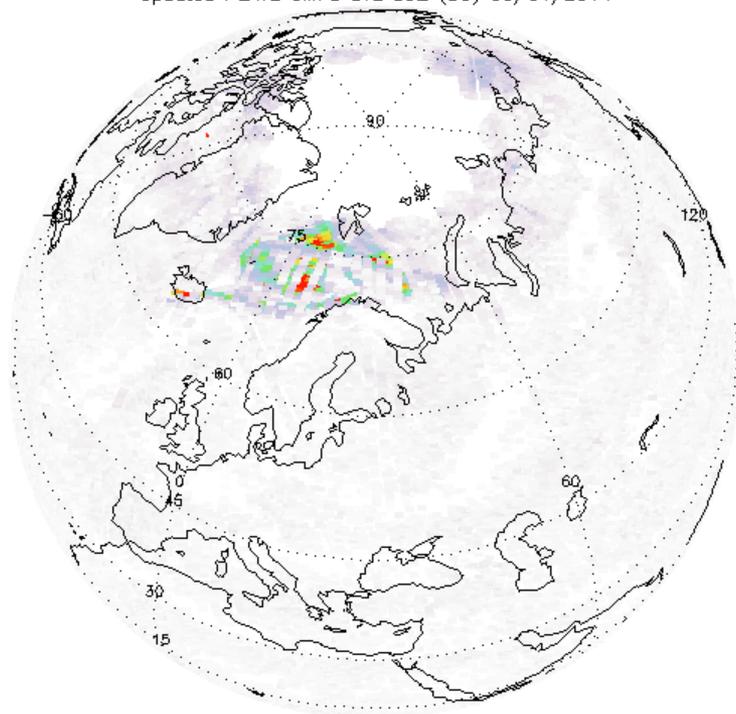
SNPP/OMPS V8TOS TRM SO₂ 01/12/2016



Example-1: Iceland Bardarbunga volcano eruption

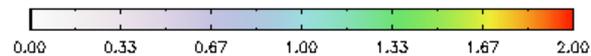
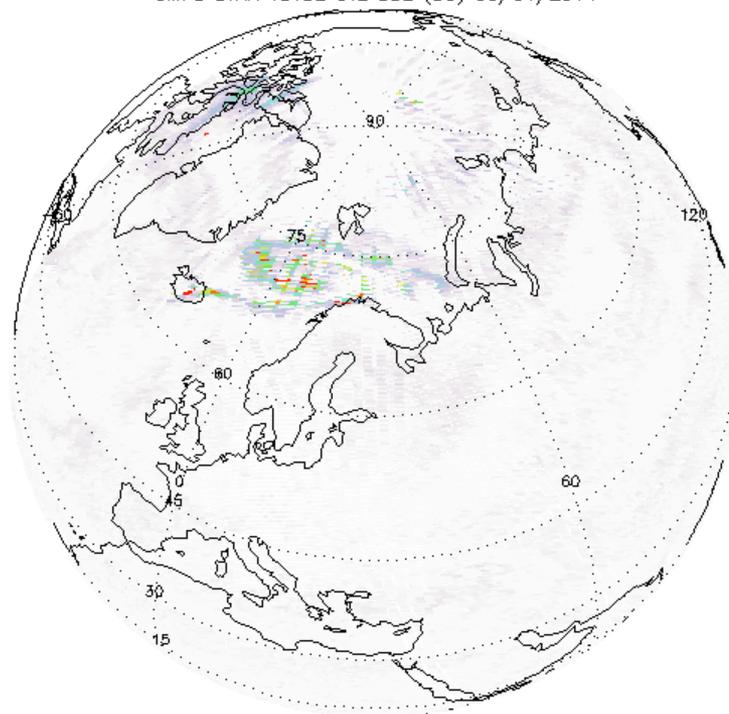
PEATE algorithm's product

Updated PEATE OMPS STL SO2 (DU) 09/04/2014

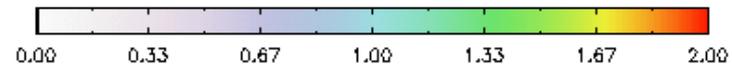
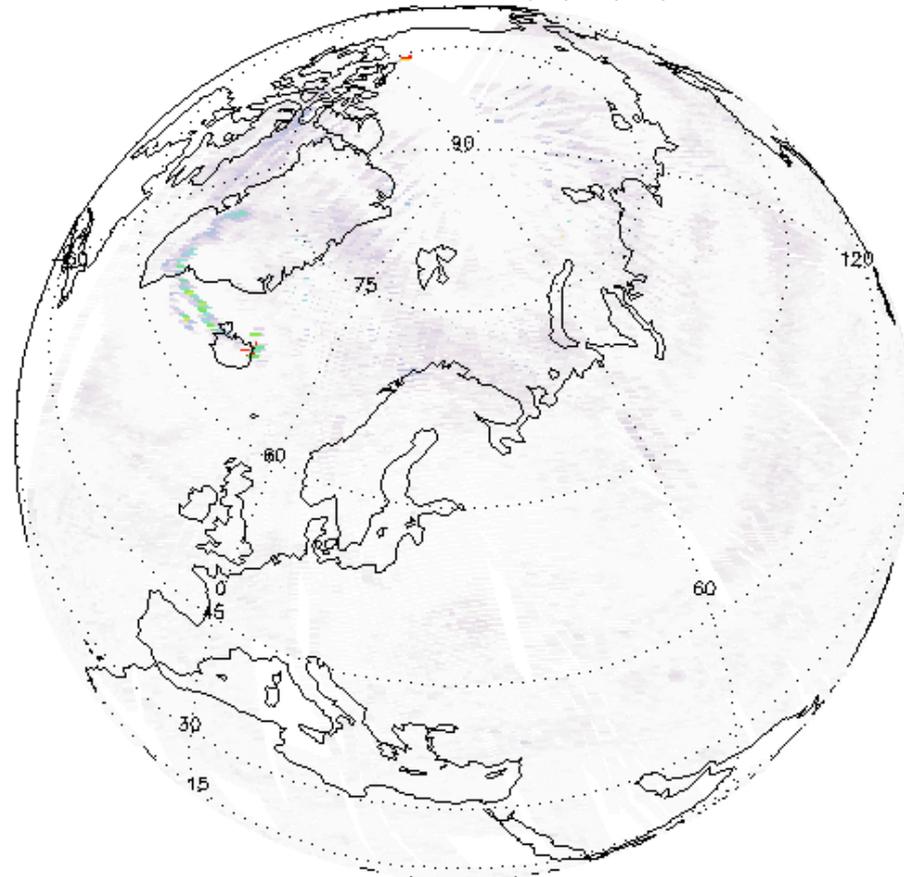


STAR products

OMPS STAR V8TOZ STL SO2 (DU) 09/04/2014



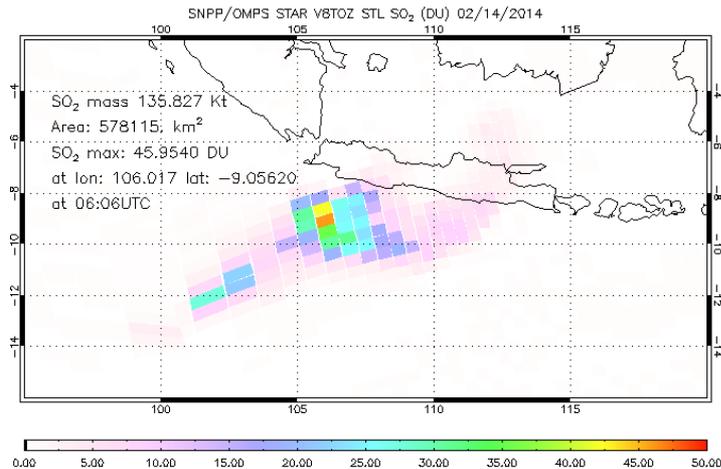
OMPS STAR V8TOZ STL SO2 (DU) 09/01/2014



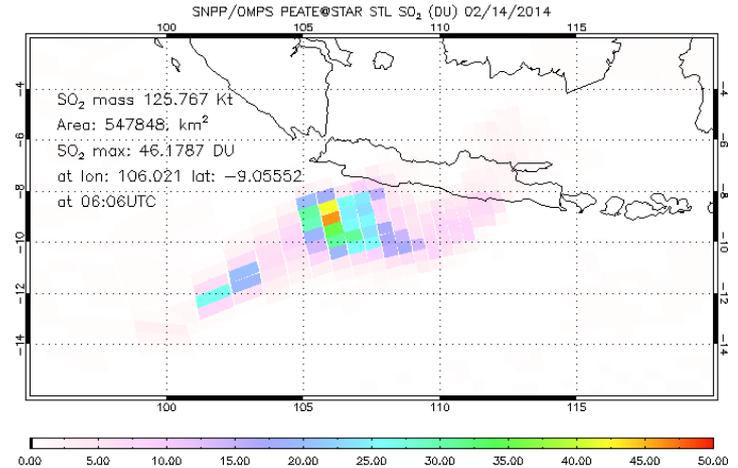
by Jianguo Niu System Research Group Inc.

Example-2: Indonesia Kelud volcano eruption February 14, 2014

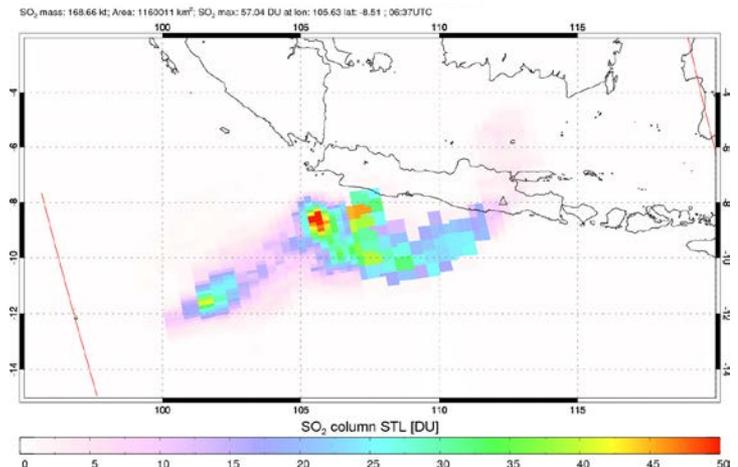
STAR V8+NMSO2



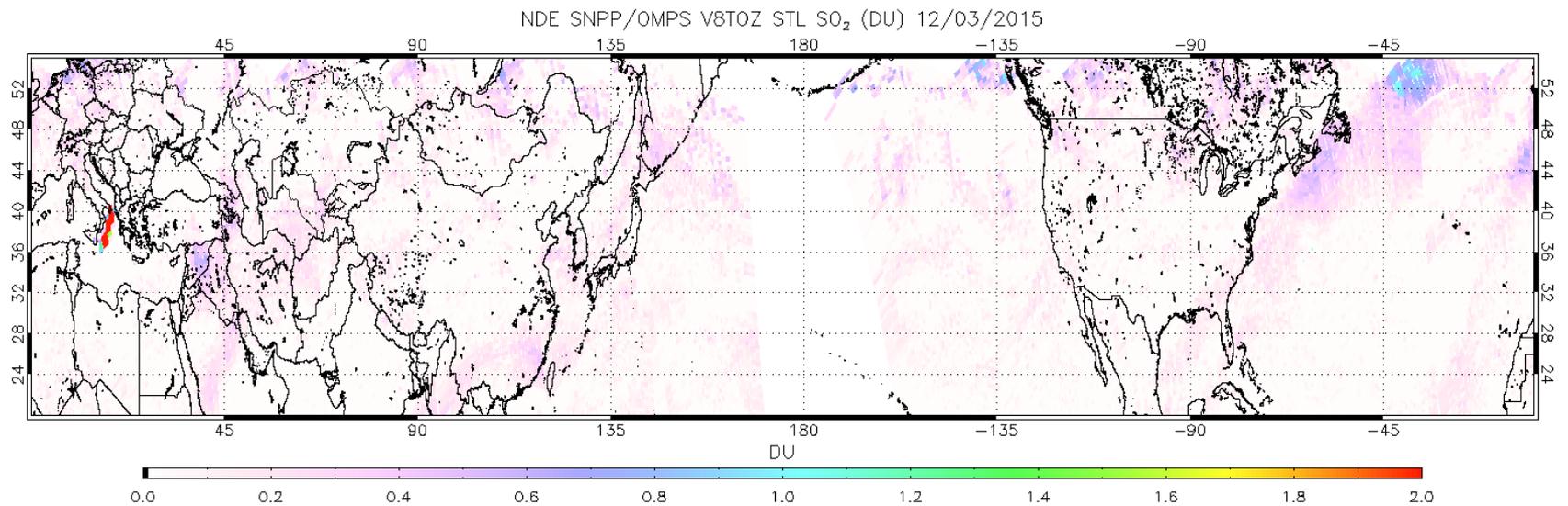
STAR/PEATE updated original



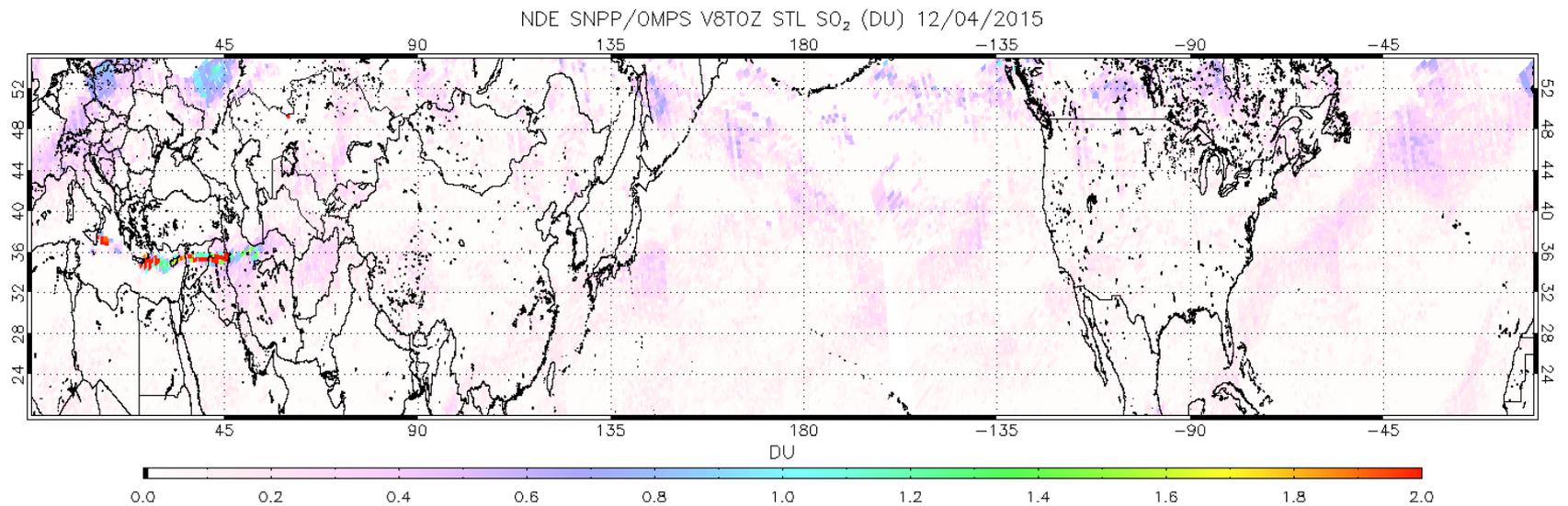
Provided by
NASA PEATE



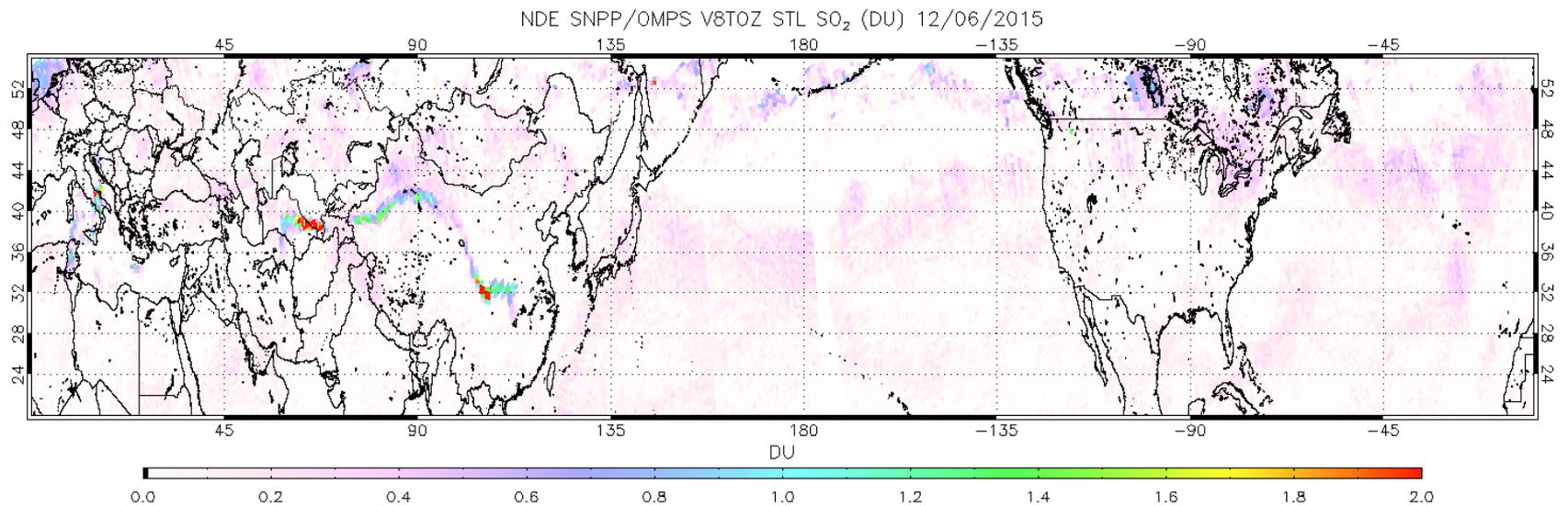
Example 3-1: Sicily Volcano eruption and transportation



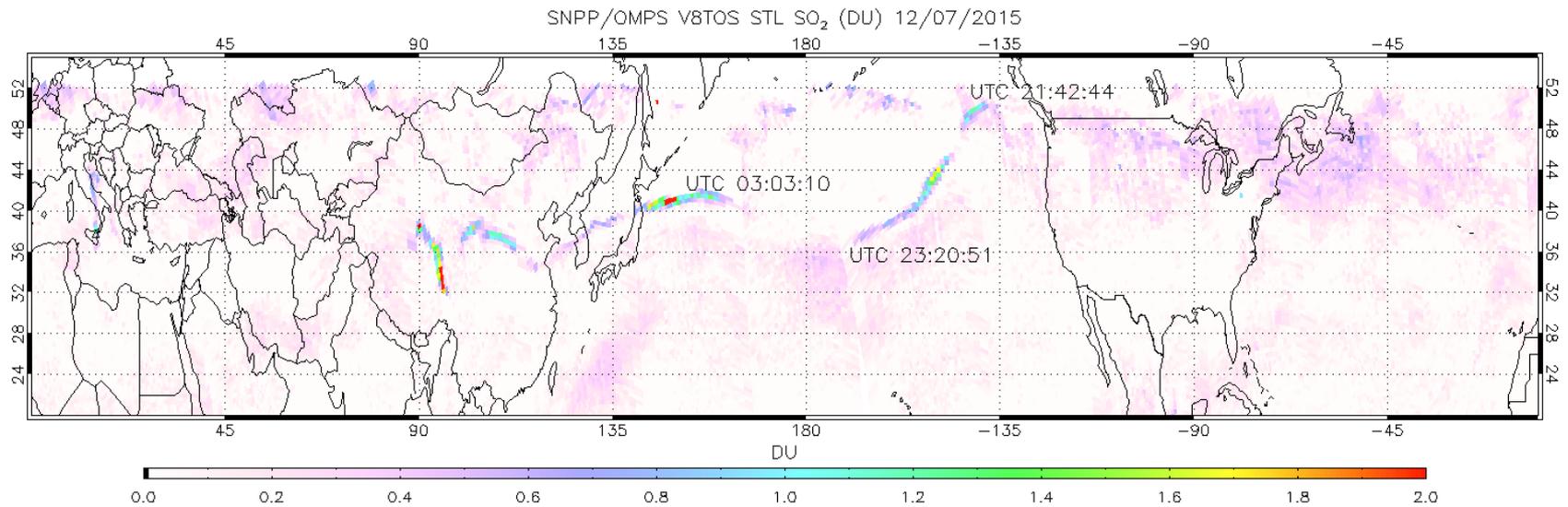
Example 3-2: Sicily Volcano eruption and transportation



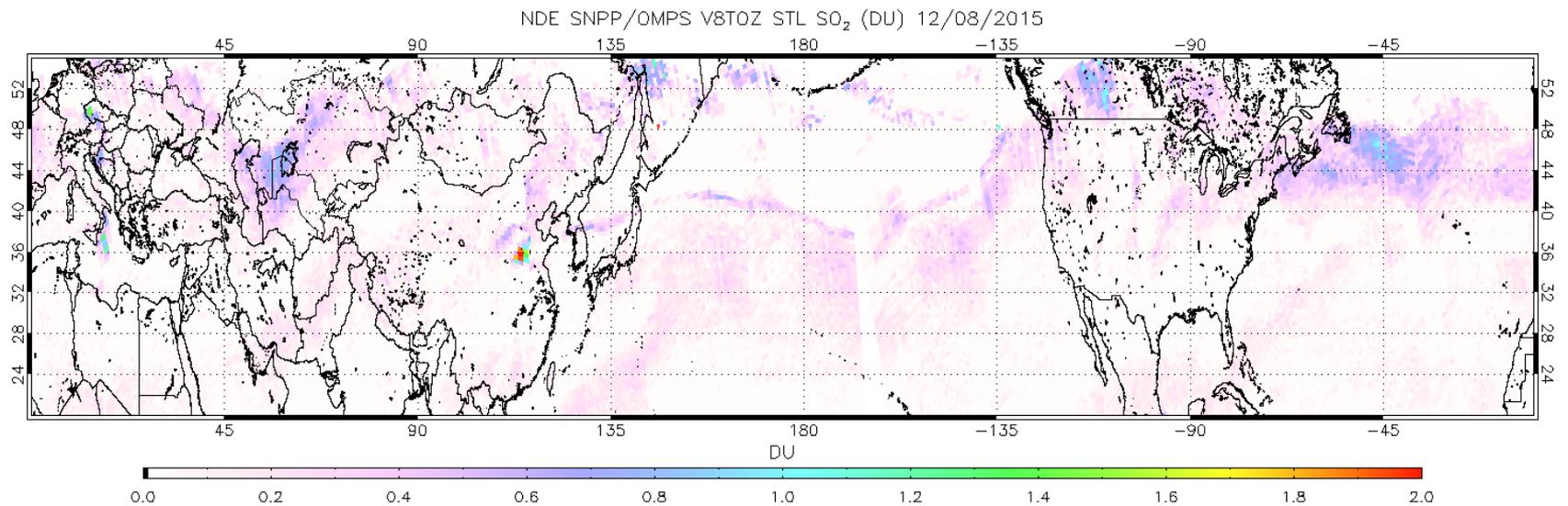
Example 3-3: Sicily Volcano eruption and transportation



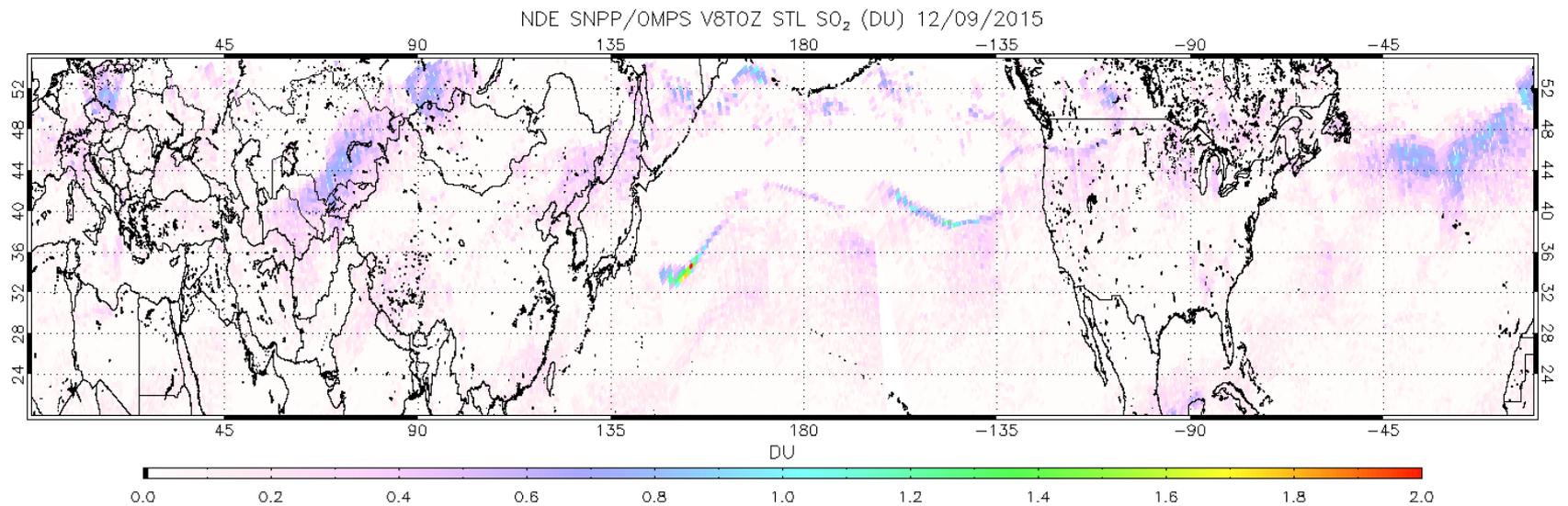
Example 3-4: Sicily Volcano eruption and transportation



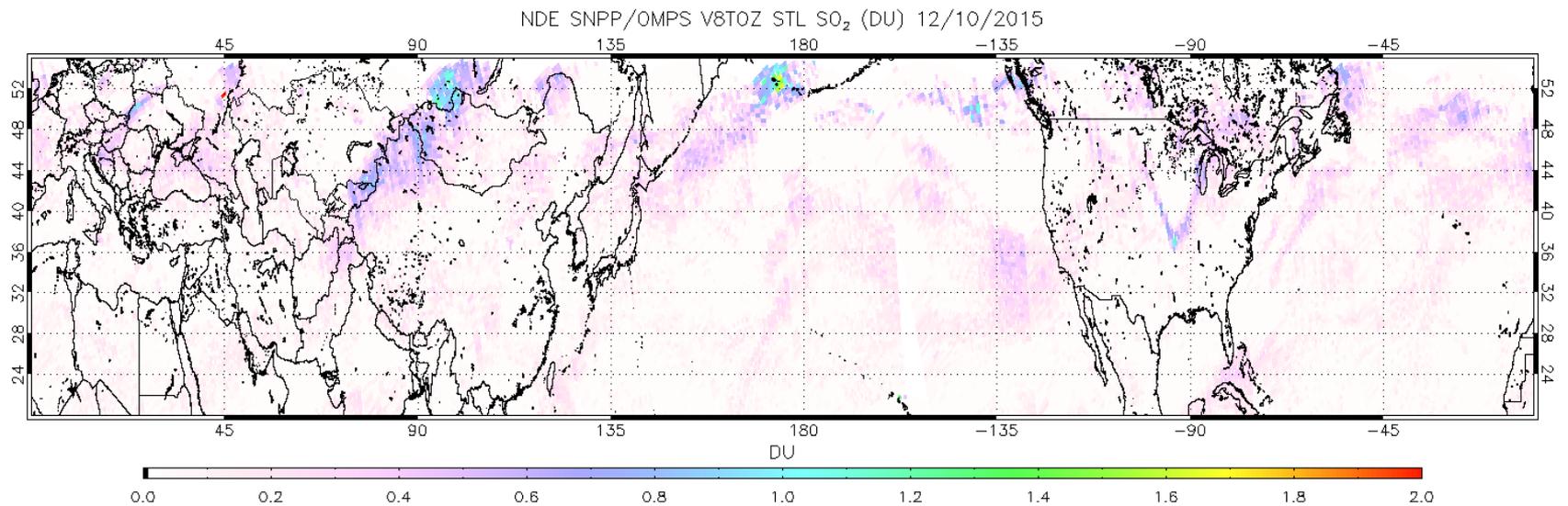
Example 3-5: Sicily Volcano eruption and transportation



Example 3-6: Sicily Volcano eruption and transportation

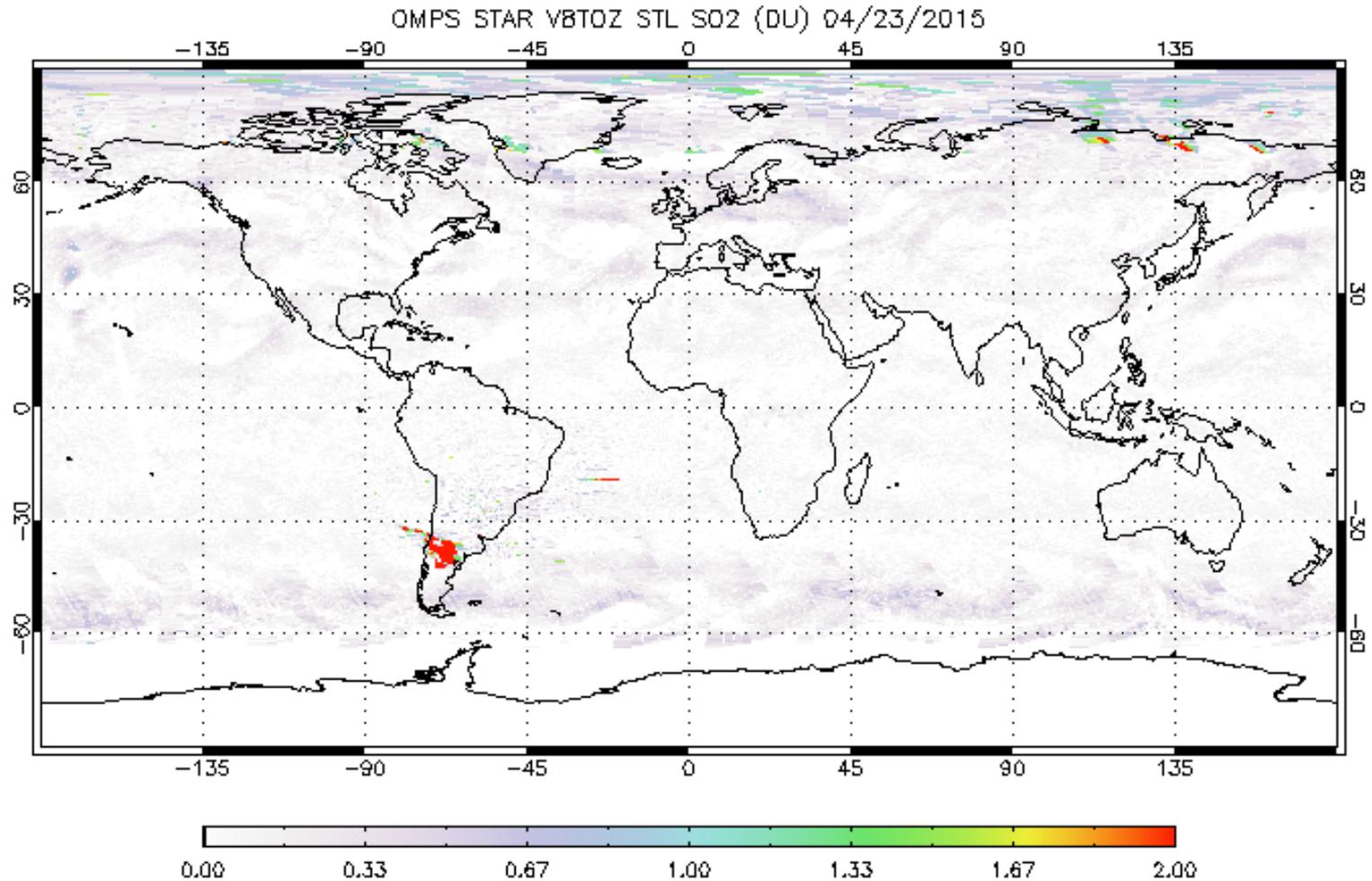


Example 3-7: Sicily Volcano eruption and transportation



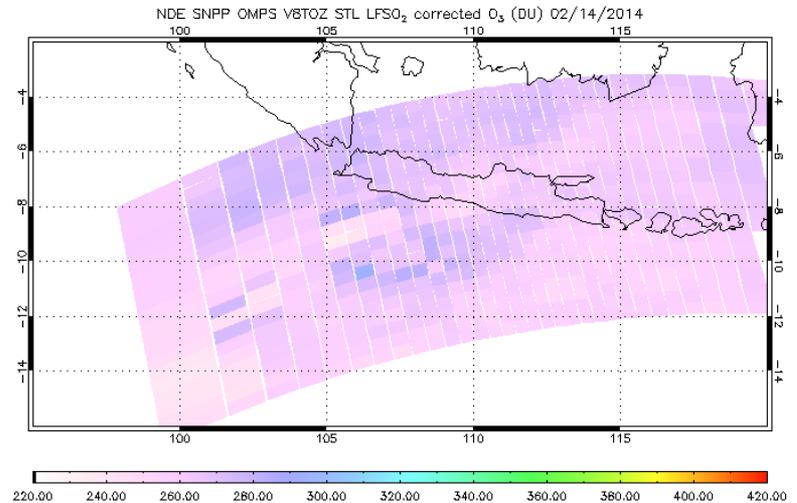
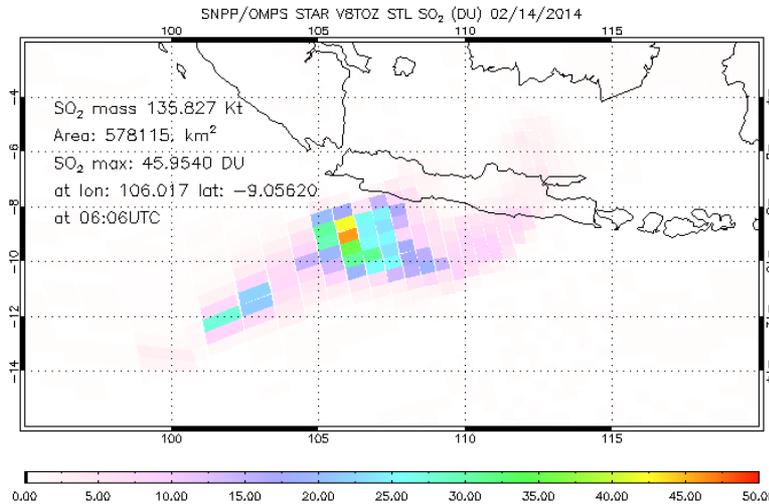
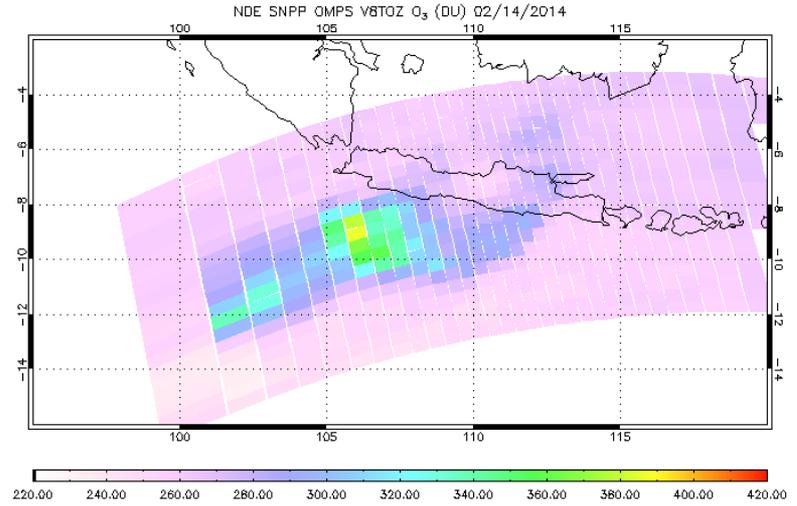
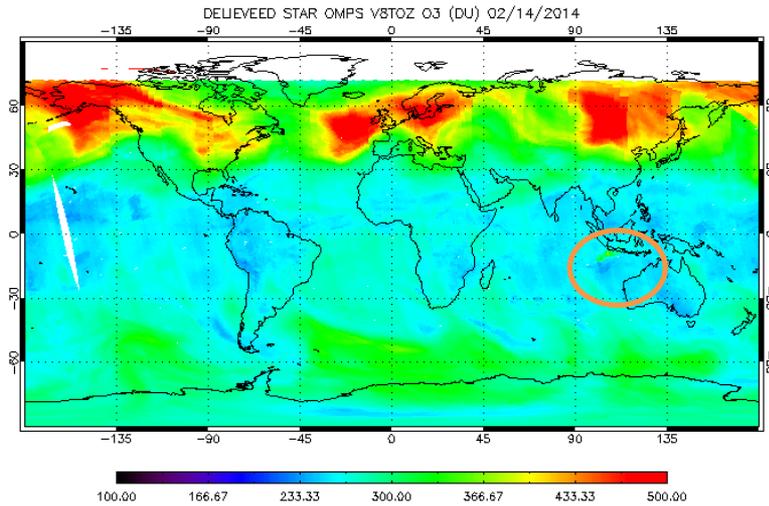
Example 4: Chile Calbuco volcano

4/23/2015 to 5/04/2015



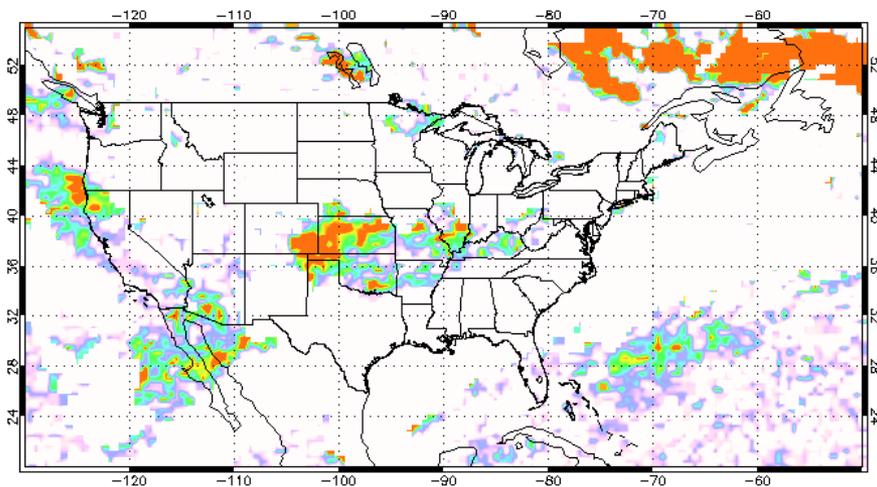
Example-5: Ozone correction by assuming SO₂ in STL for Indonesia Kelud volcano eruption case

February 14, 2014



Daily PBL and TRL SO₂ maps over the US January to June 2016

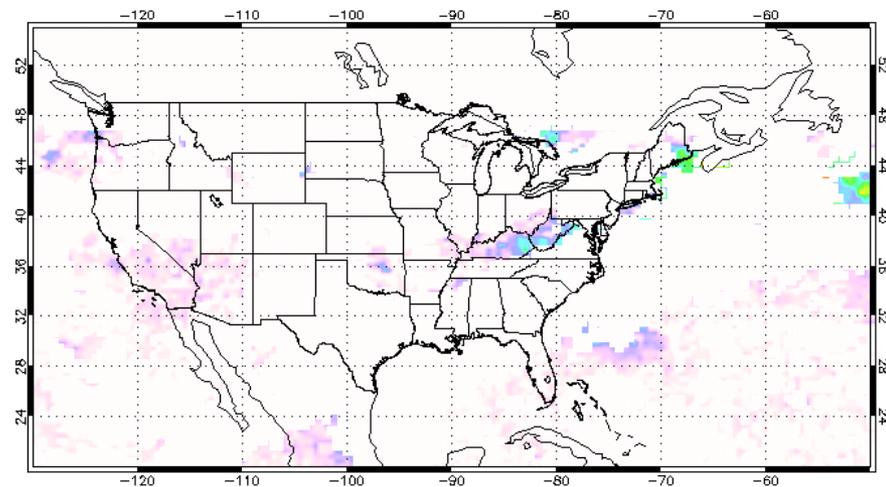
OMPS V8TOS pbl SO₂ 2016/01/01



DU

0.00 0.22 0.44 0.67 0.89 1.11 1.33 1.56 1.78 2.00

OMPS V8TOS trl SO₂ 2016/01/01



DU

0.00 0.22 0.44 0.67 0.89 1.11 1.33 1.56 1.78 2.00

Summary

1. A 15-granule implementation provide a reliable alert to volcanic SO₂ cloud.
2. LFSO2 retrieval provides a total column O₃ correction when thick SO₂ appears in the atmosphere.
3. Provide accurate SO₂ total column amount for V8TOZ product.
4. Shown that OMPS Nadir Mapper possesses high sensitivity to monitor SO₂ as a pollutant in the atmosphere.



Marco Fulle - www.stromboli.net

DEVELOPMENT OF MULTI-SENSOR SO₂ PRODUCTS FOR JPSS



Michael J. Pavolonis

Physical Scientist

National Environmental Satellite, Data, and Information Service

Center for Satellite Applications and Research

JPSS Science Team Meeting

11 August 2016

Outline

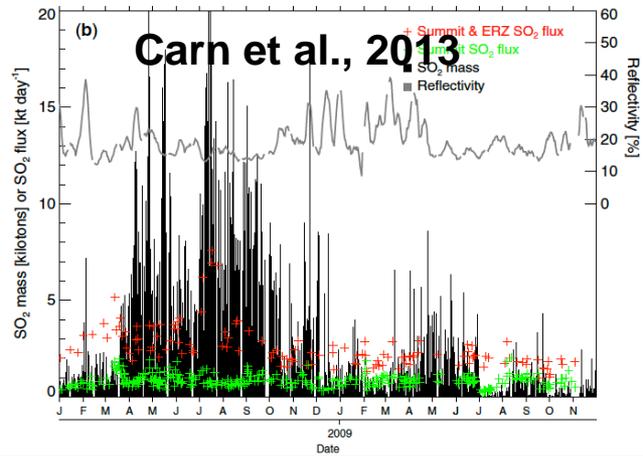
- Importance of SO₂ monitoring
- Strengths and weaknesses of different satellite measurements
- Measurement integration plan
- Collaboration

Outline

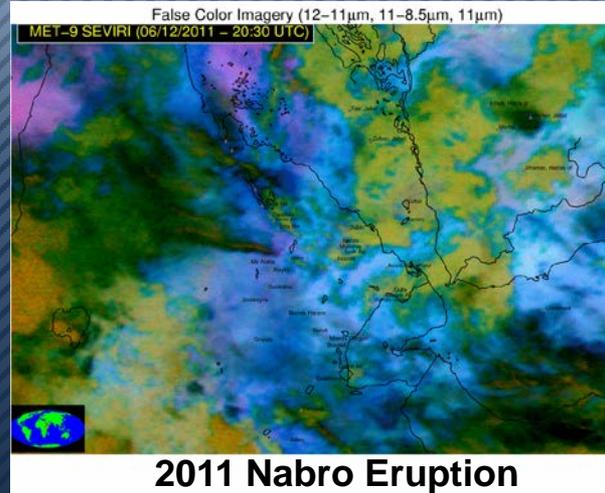
- Importance of SO₂ monitoring
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Motivation

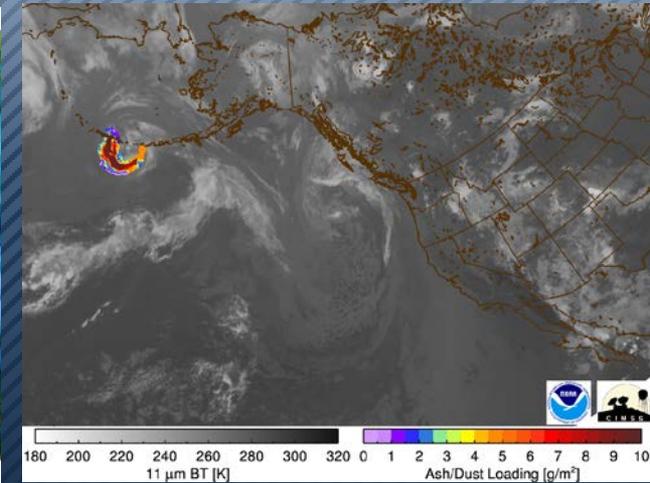
Volcano Monitoring



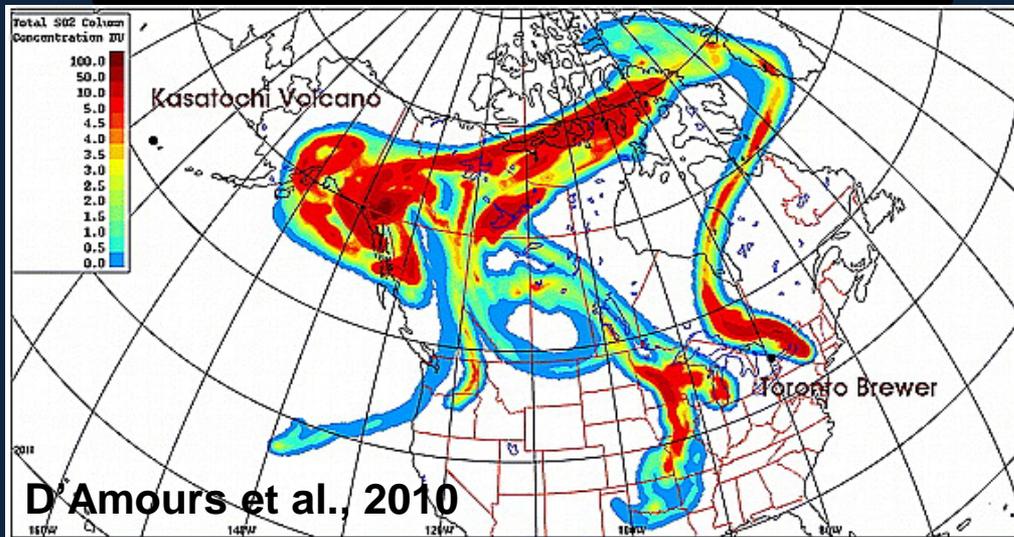
Hazard Avoidance



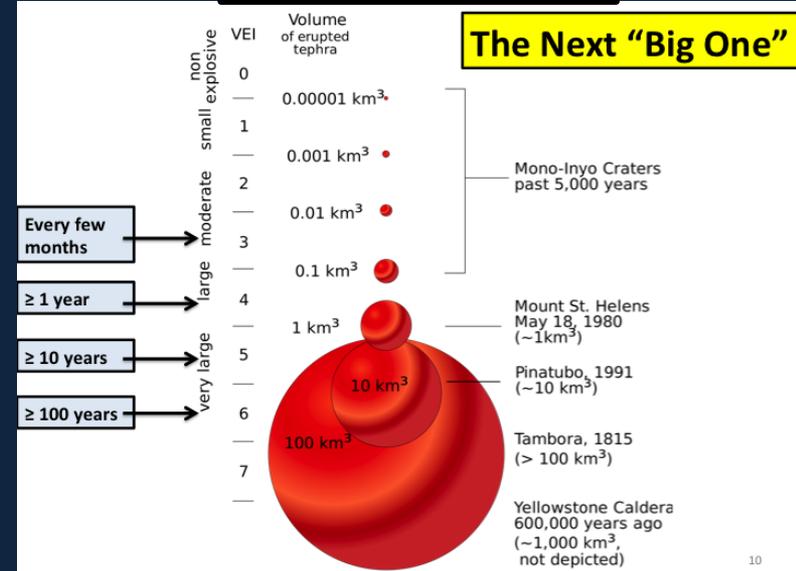
Volcanic Ash Tracking



Dispersion and Transport Modeling



Climate



End Users

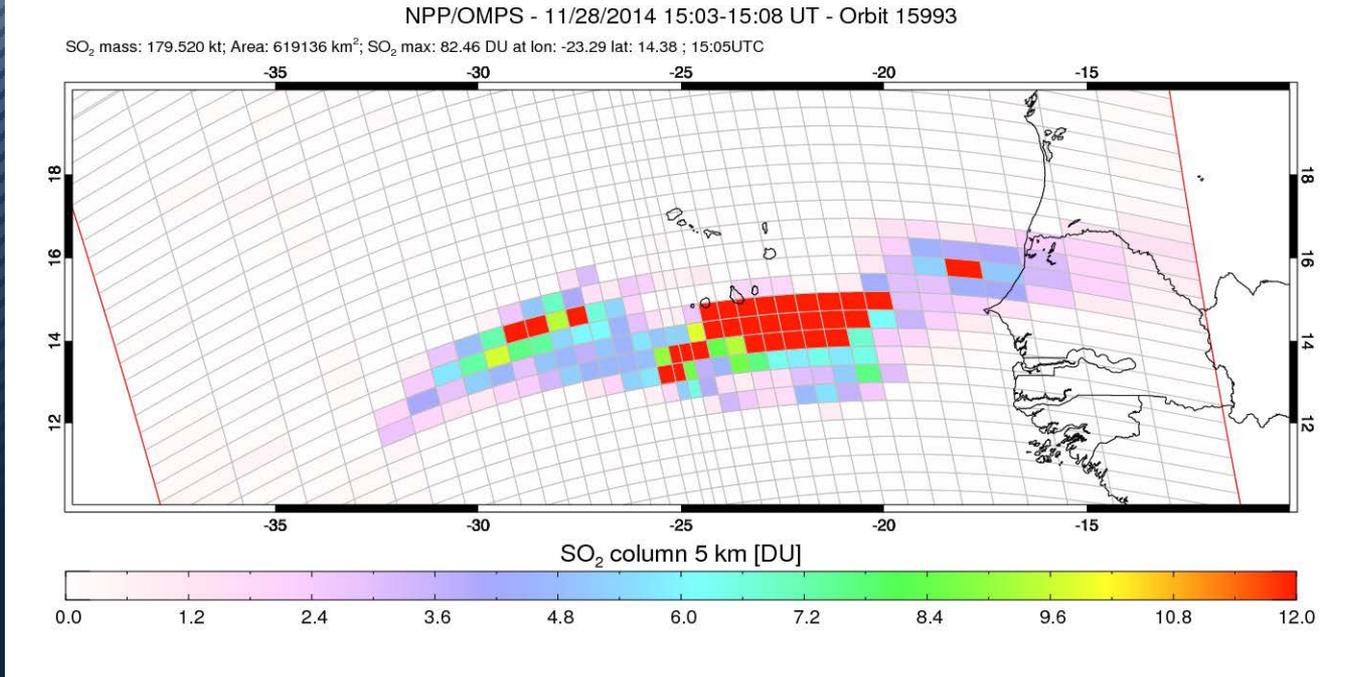
- Volcanic Ash Advisory Centers
- Meteorological Watch Offices
- Weather Forecast Offices
- Volcano Observatories (including the USGS)
- Military
- Operational modeling community (dispersion, weather, and climate)
- Research Community

Outline

- Importance of SO₂ monitoring
- Strengths and weaknesses of different satellite measurements
- Measurement integration plan
- Collaboration

Ultra-Violet (OMPS)

Source: NASA GSFC

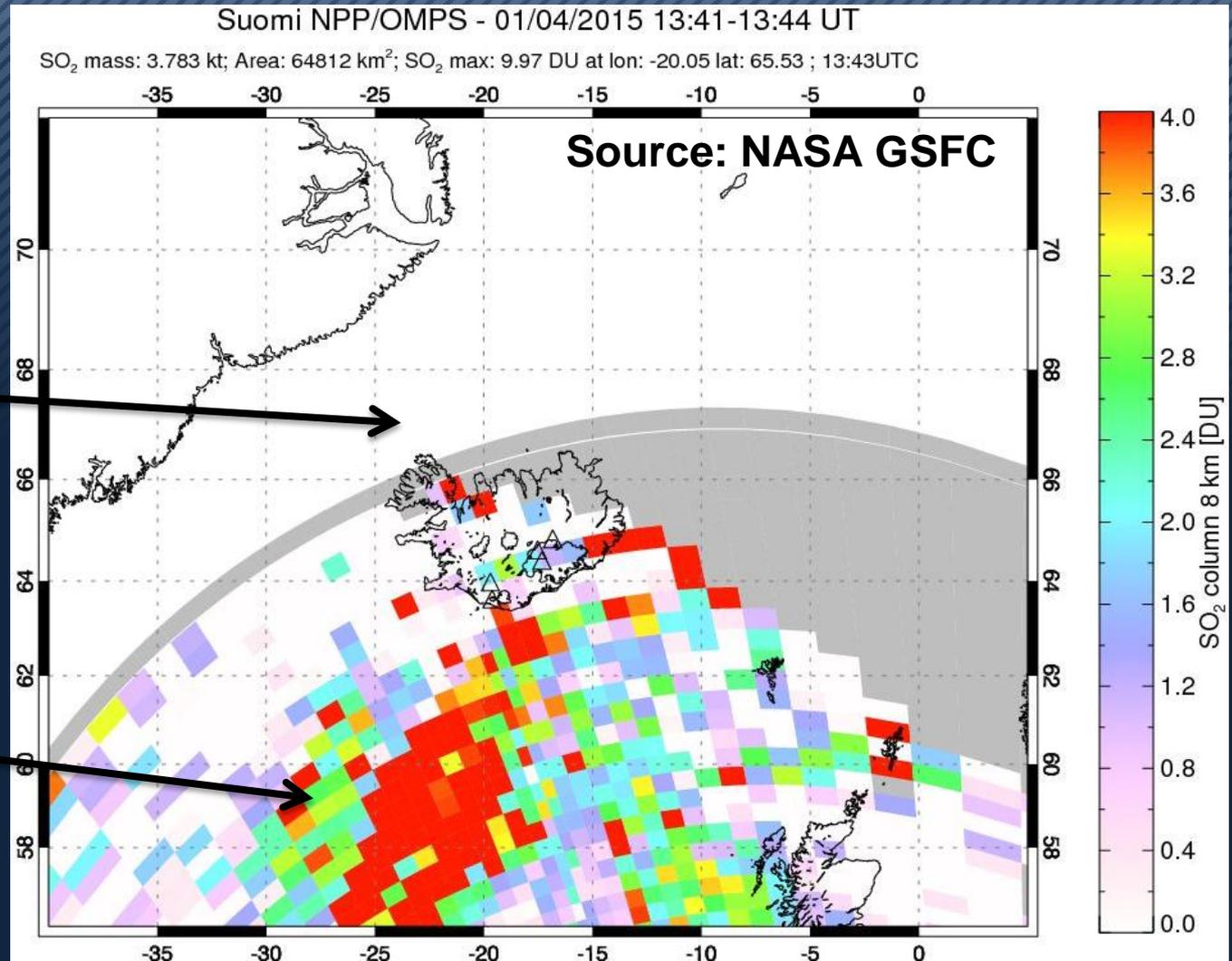


Major Strengths:

- Very sensitive to the presence of SO₂ under many conditions including in the presence of clouds (liquid, ice, and aerosol) and over bright surfaces
- Sensitive to SO₂ loading, some sensitivity to SO₂ height

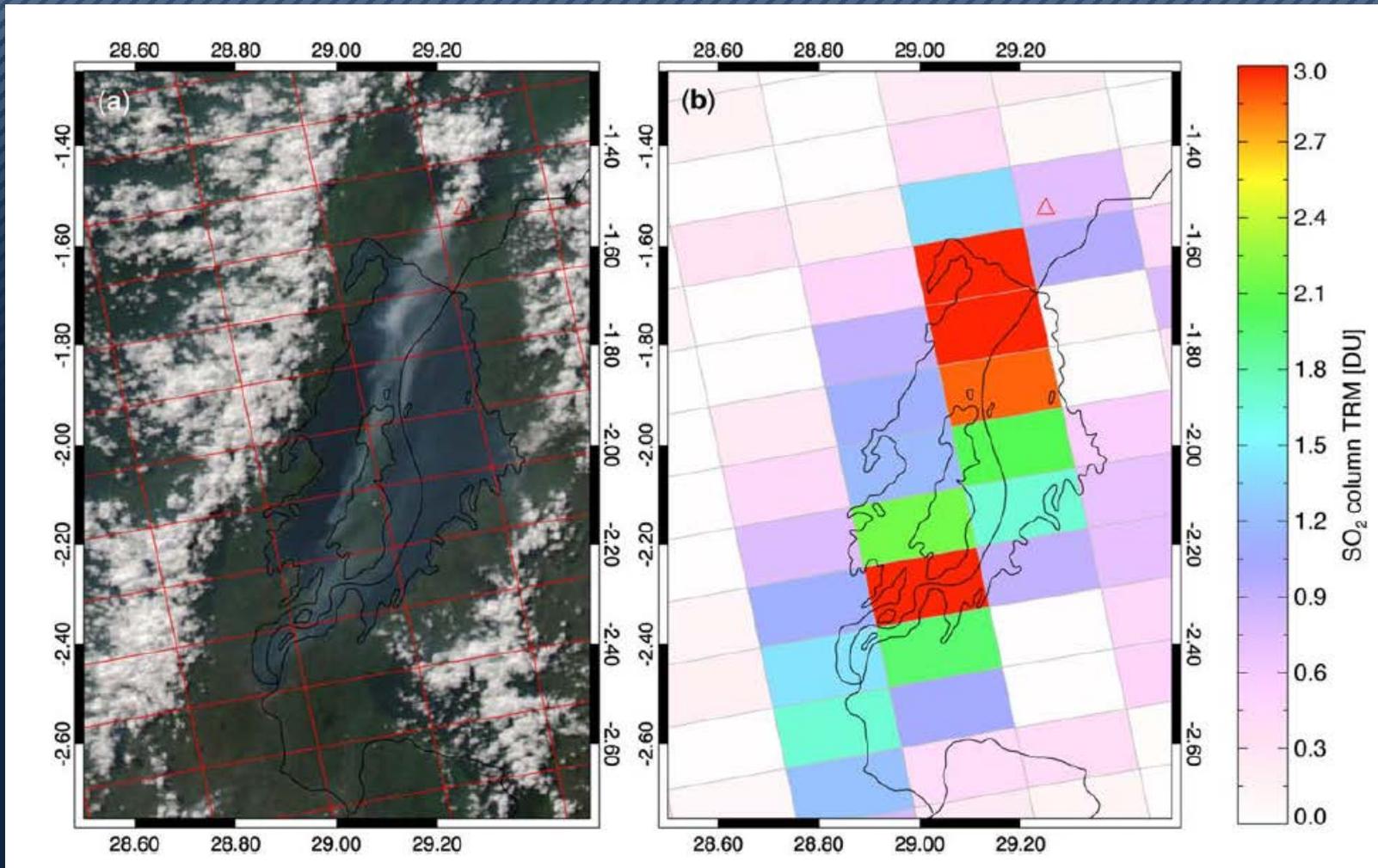
Ultra-Violet (OMPS)

Weakness: Sensitive to solar zenith angle



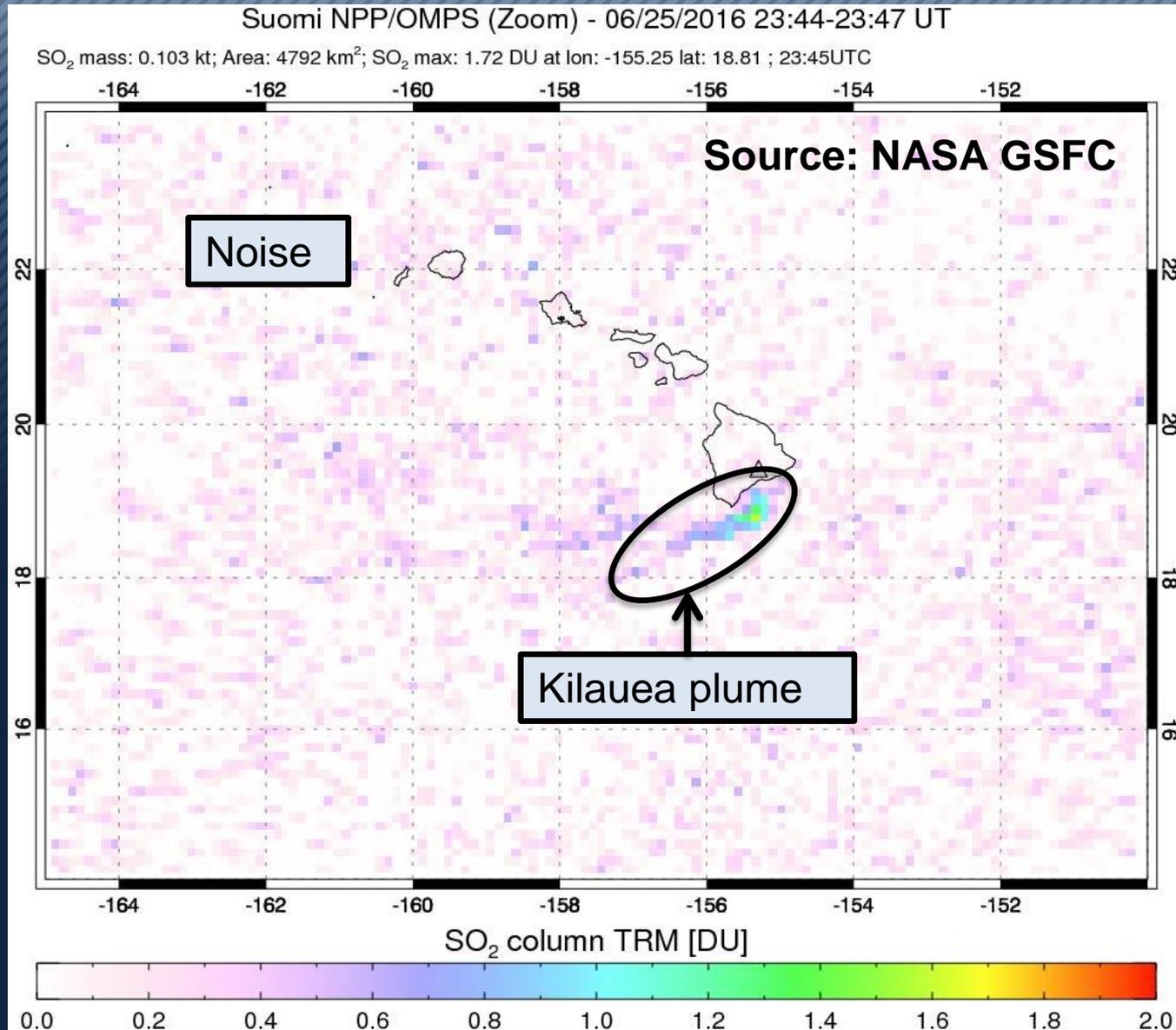
Ultra-Violet (OMPS)

Weakness: Large footprint size relative to spatial scale of many SO₂ plumes

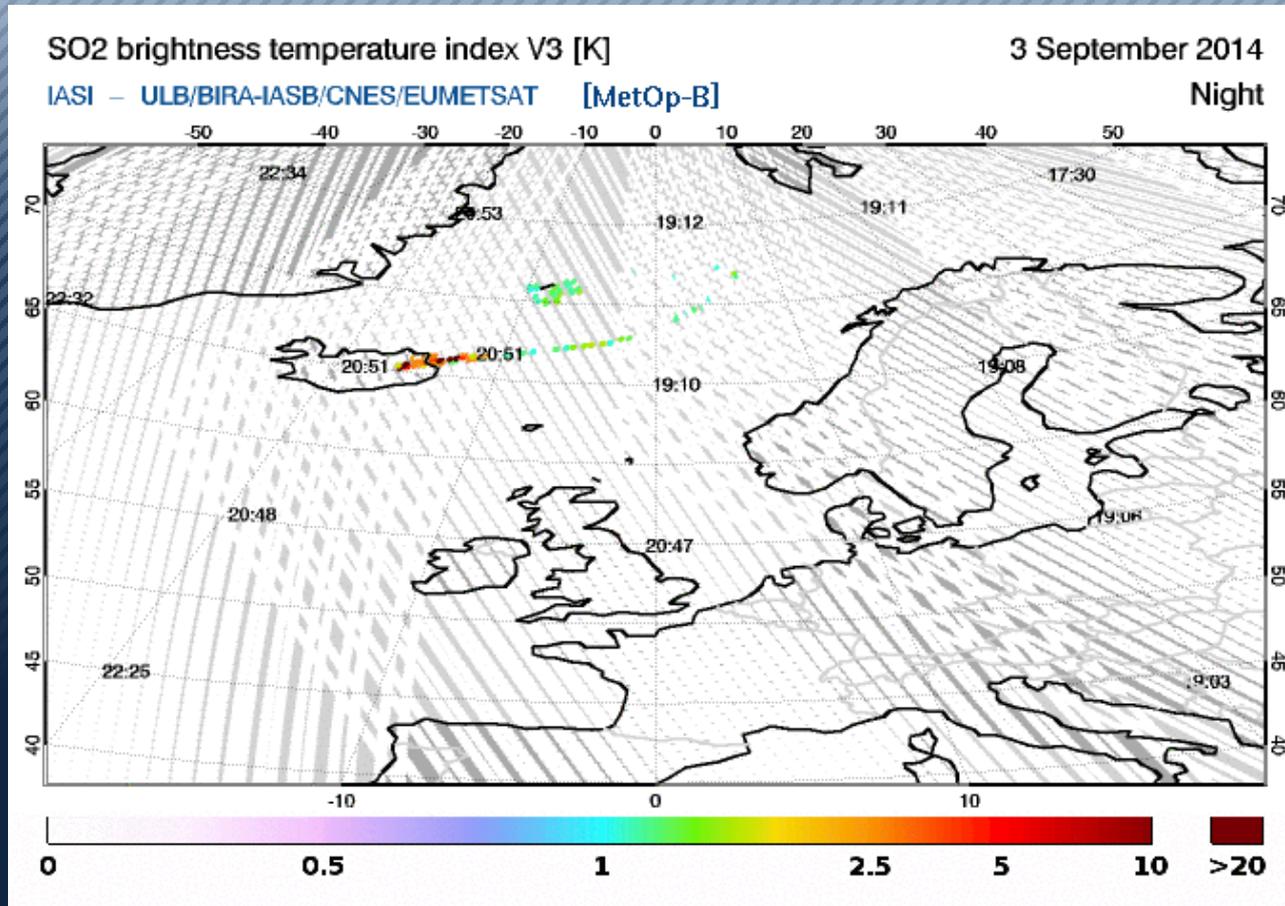


Ultra-Violet (OMPS)

Weakness: Noise



Hyperspectral Infrared (CrIS)

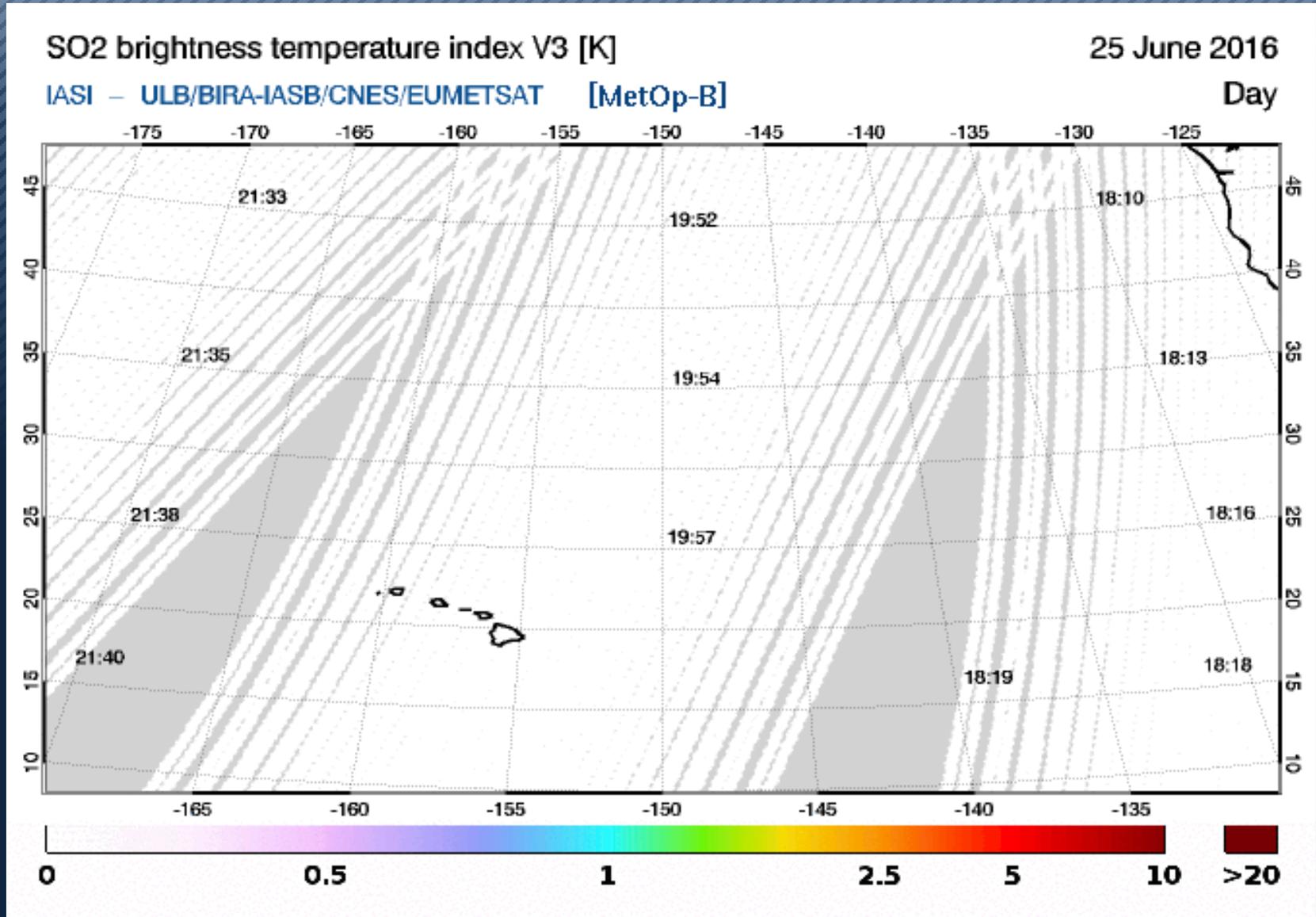


Major Strengths:

- Provides information on SO₂ day and night
- Provides sensitivity to SO₂ loading and height

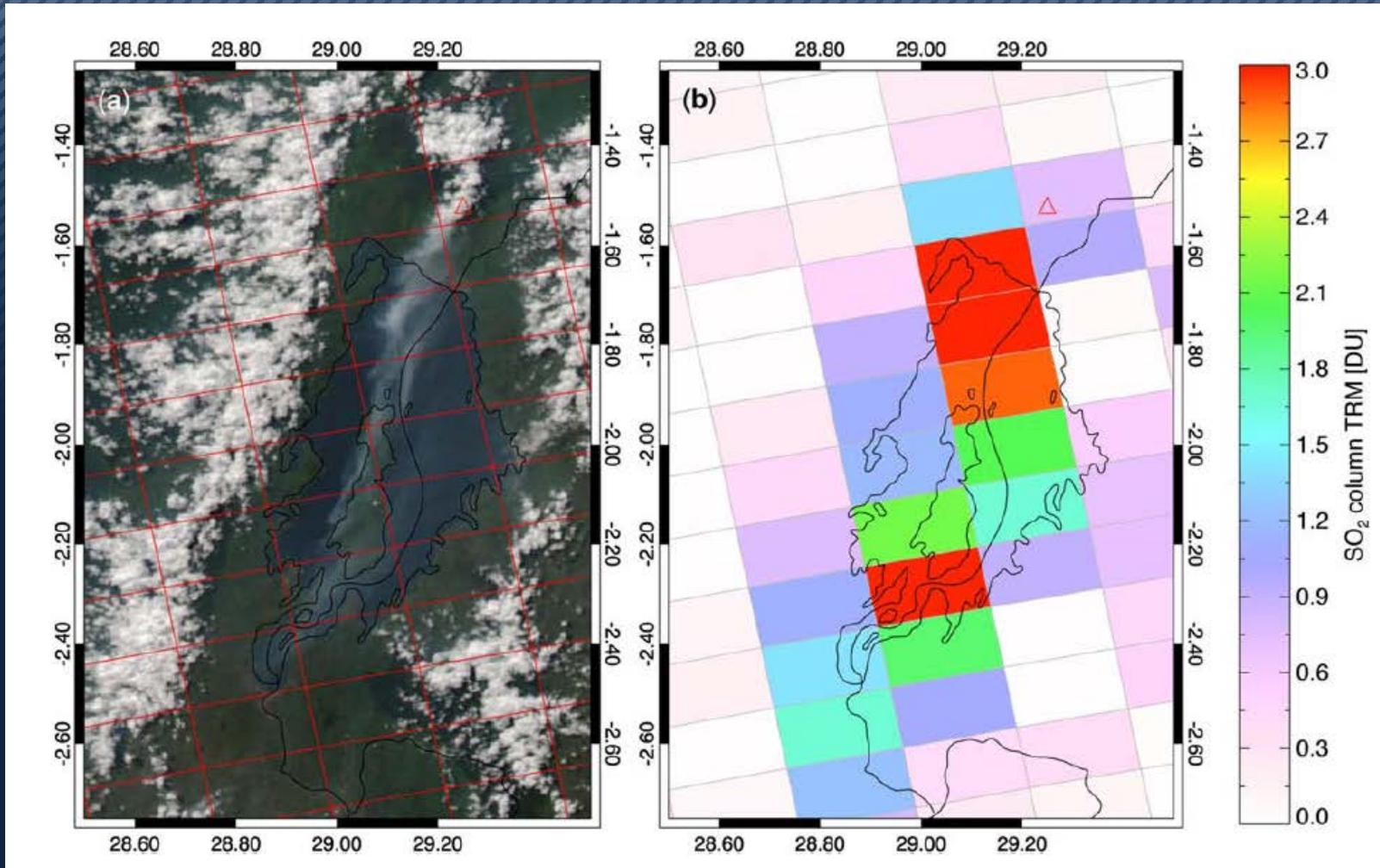
Hyperspectral Infrared (CrIS)

Weakness: Less sensitive to lower tropospheric SO₂

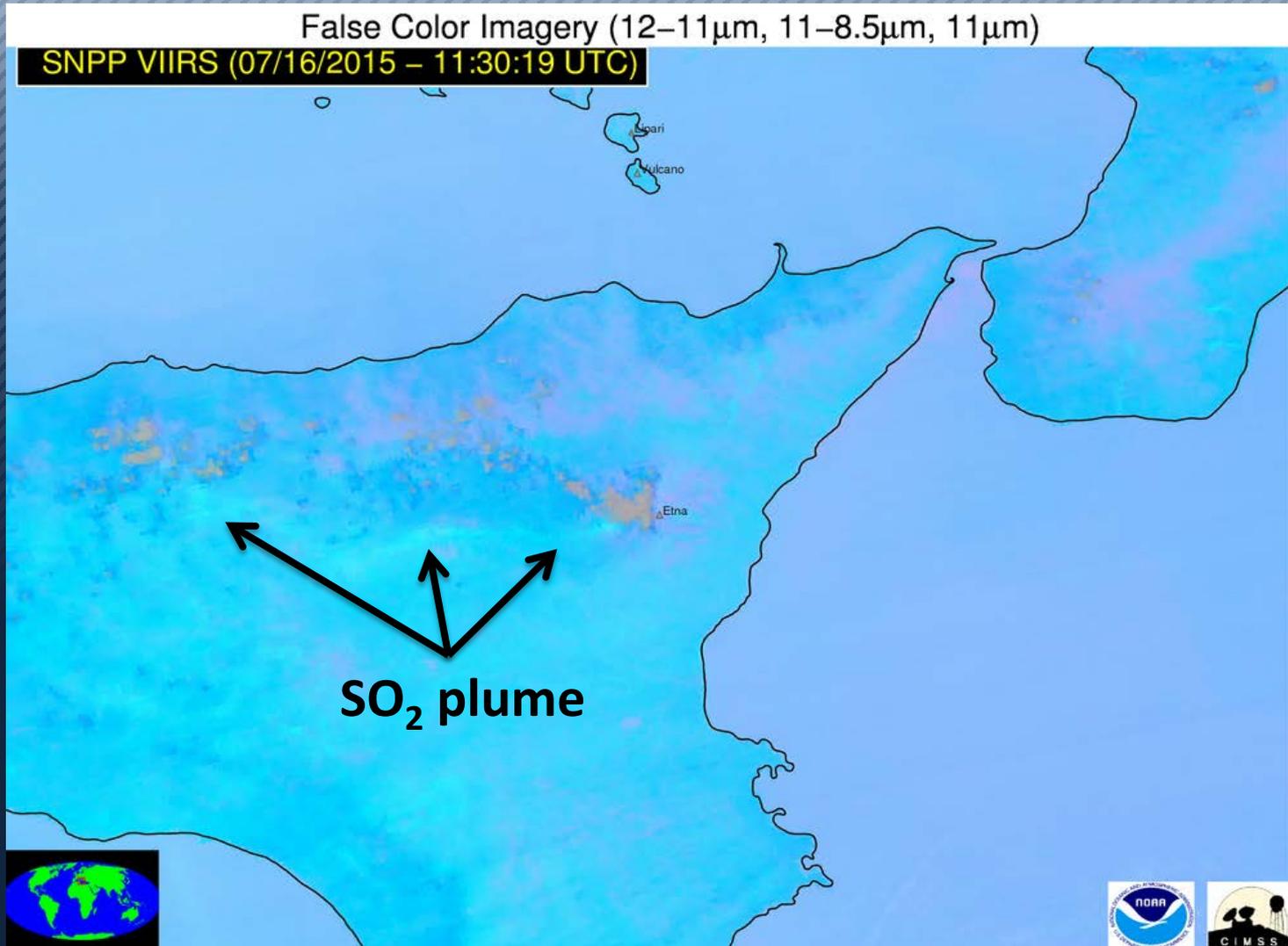


Hyperspectral Infrared (CrIS)

Weakness: Large footprint size relative to spatial scale of many SO₂ plumes



Narrow-band Imager (VIIRS)

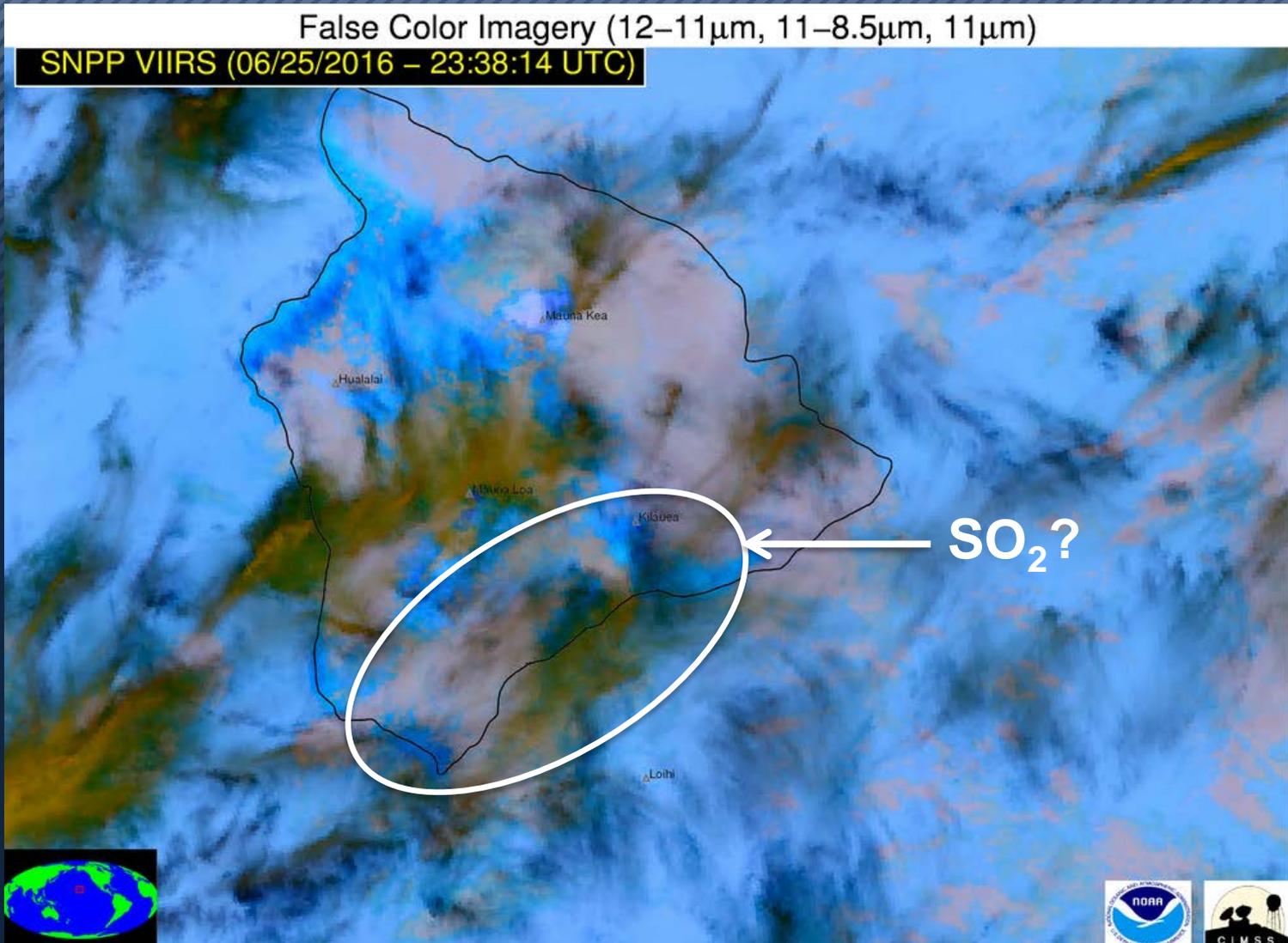


Major Strengths:

- Provides high spatial resolution imagery of SO₂ clouds and plumes under many conditions day and night.

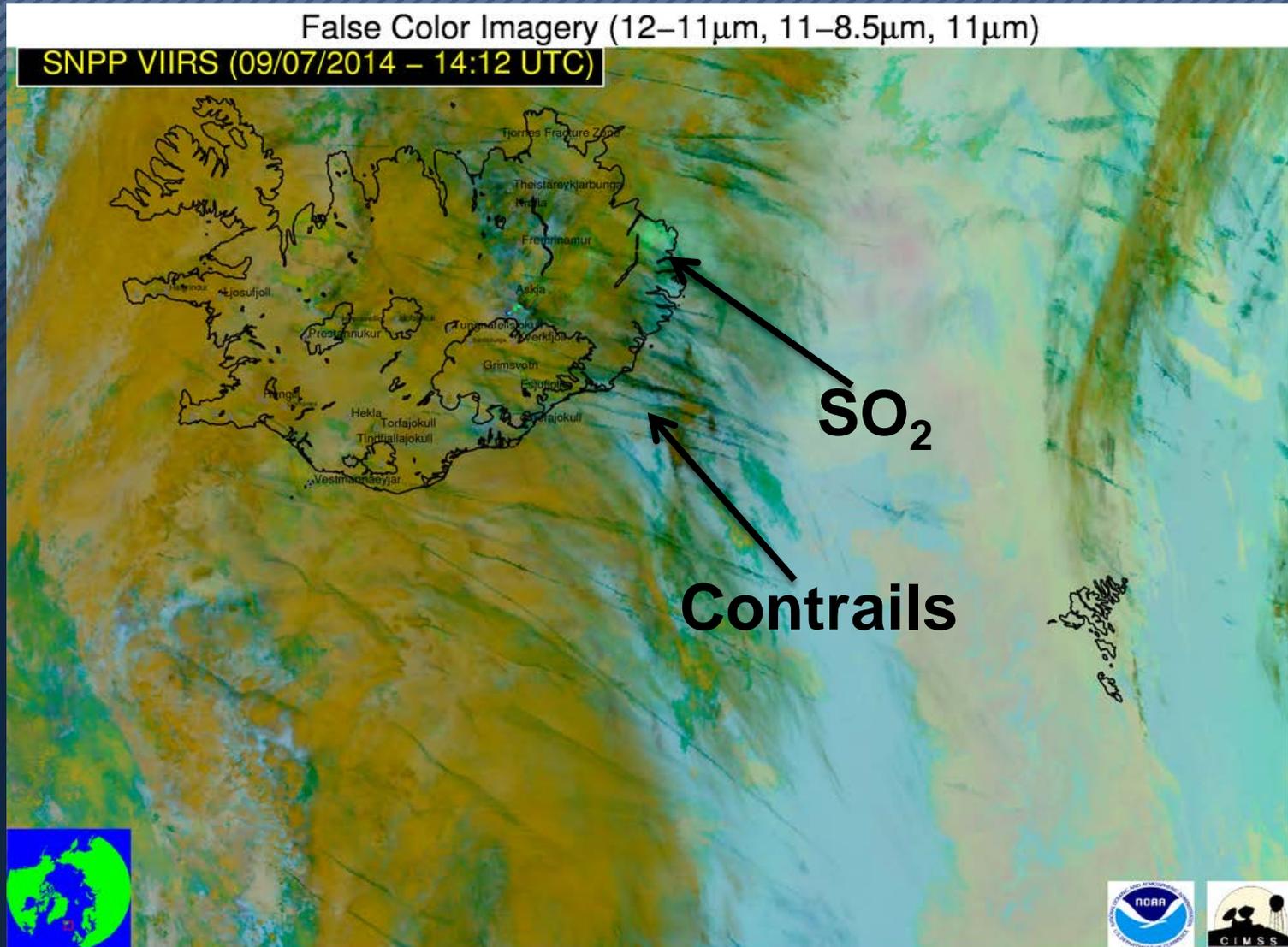
Narrow-band Imager (VIIRS)

Weakness: Larger lower limit of detection, especially in the presence of clouds



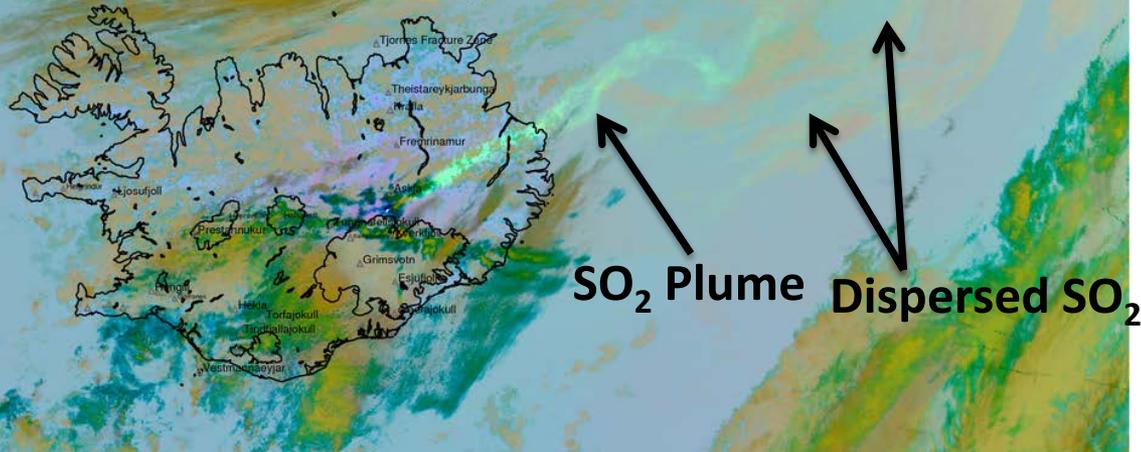
Narrow-band Imager (VIIRS)

Weakness: Challenging to extract quantitative information without additional constraints



False Color Imagery (12–11 μ m, 11–8.5 μ m, 11 μ m)

SNPP VIIRS (09/03/2014 – 13:46 UTC)

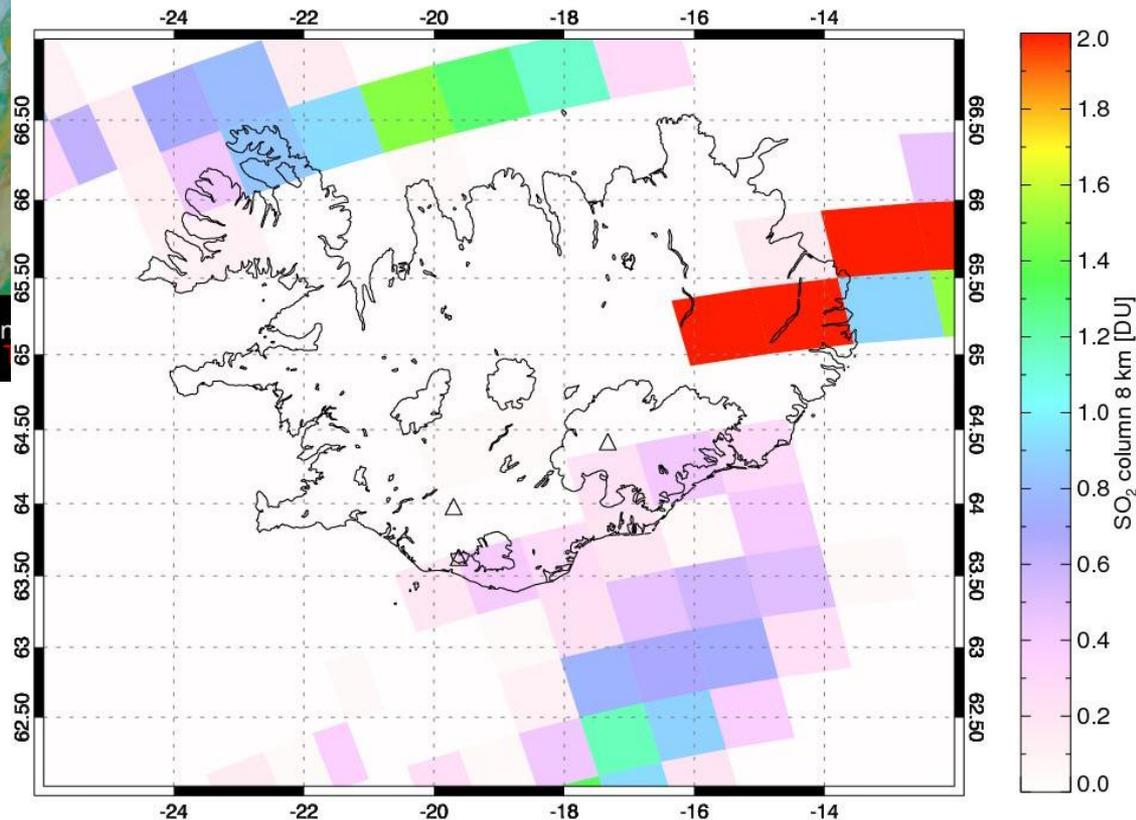


A multi-sensor SO₂ analysis is needed

Suomi NPP/OMPS - 09/03/2014 13:49-13:51 UT

SO₂ mass: 0.983 kt; Area: 75083 km²; SO₂ max: 3.19 DU at lon: -13.24 lat: 65.75 ; 13:50UTC

NASA GSFC



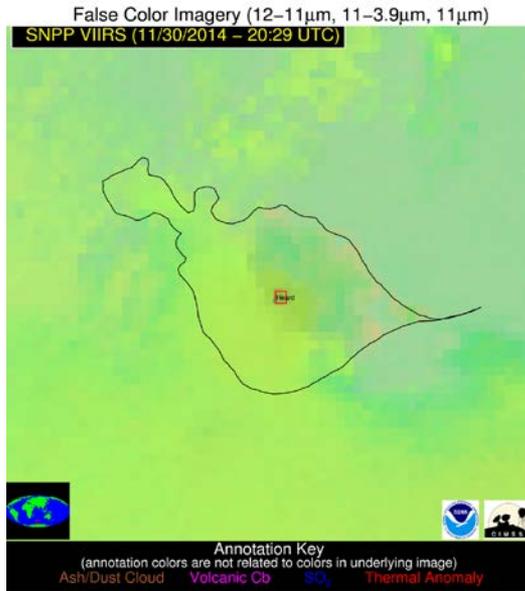
Annotation Key
(annotation colors are not related to colors in ur
Ash/Dust Cloud Volcanic Cb SO₂

Outline

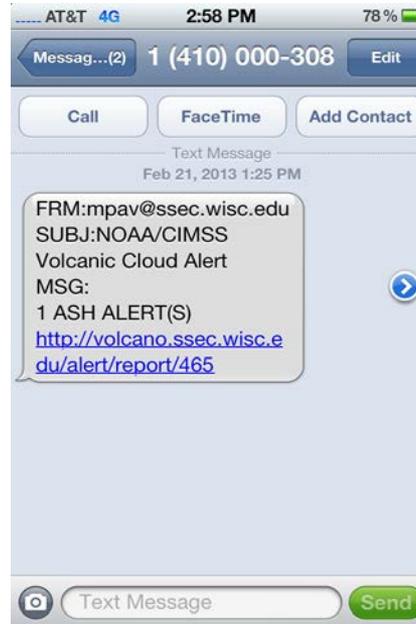
- Importance of SO₂ monitoring
- Strengths and weaknesses of different satellite measurements
- **Measurement integration plan**
- Collaboration

VOLcanic Cloud Analysis Toolkit (VOLCAT)

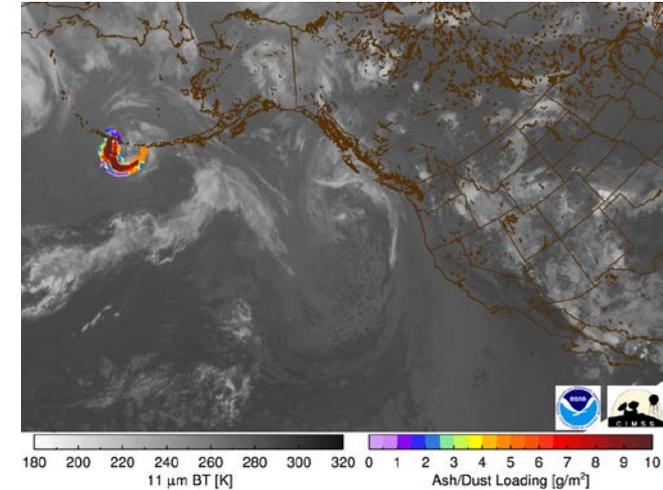
1). Unrest Alerts



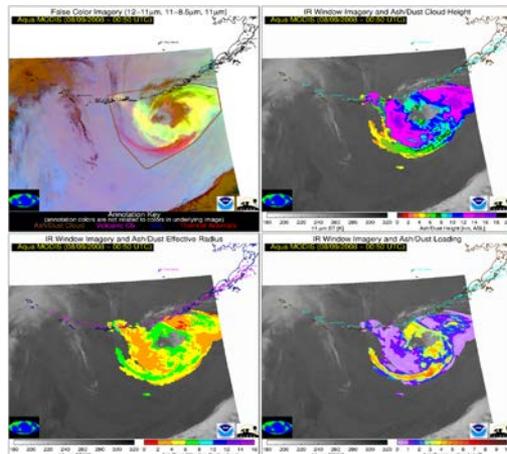
2). Eruption Alerts



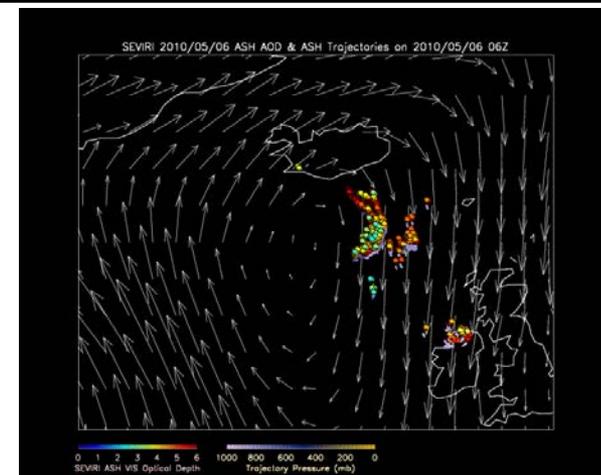
3). Volcanic Cloud Tracking



4). Volcanic Cloud Characterization



5). Dispersion Forecasting



Spectrally Enhanced Cloud Objects (SECO) Method for SO₂ Detection

- Automatically extract coherent SO₂ features from OMPS and CrIS using cloud object analysis
- Construct an *a priori* probability from OMPS and CrIS and utilize it in VIIRS implementation of SECO method
- Final SO₂ detection results are at the VIIRS resolution and are overlaid on VIIRS imagery
- The fused JPSS SO₂ detection results can then be used to aid in SO₂ detection and tracking from GEO satellites

SO₂ Retrieval Options

- Utilize existing OMPS SO₂ loading products
- A variation on published methods (e.g. NUCAPS, Carboni et al. 2012; Clarisse et al., 2014) will be used to retrieve SO₂ loading and effective height from CrIS
- Optimal estimation readily allows the results from one sensor to influence another through the *a priori*. Thus, the result from OMPS or CrIS, which ever is deemed to be of higher quality, can be used to constrain the VIIRS retrieval, while allowing for small-scale spatial variability to be captured
- Many details TBD – this is R&D, not manufacturing!

References

- Pavolonis, M. J., W. F. Feltz, A. K. Heidinger, and G. M. Gallina, 2006: A daytime complement to the reverse absorption technique for improved automated detection of volcanic ash. *J.Atmos.Ocean.Technol.*, **23**, 1422-1444.
- Pavolonis, M. J., 2010: Advances in Extracting Cloud Composition Information from Spaceborne Infrared Radiances-A Robust Alternative to Brightness Temperatures. Part I: Theory. *Journal of Applied Meteorology and Climatology*, **49**, 1992-2012, doi:10.1175/2010JAMC2433.1 ER.
- Pavolonis, M., A. Heidinger, and J. Sieglaff, 2013: Automated retrievals of volcanic ash and dust cloud properties from upwelling infrared measurements, *J. Geophysical Research*, **118(3)**, 1436-1458.
- Pavolonis, M., J. Sieglaff, and J. Cintineo (2015a), Spectrally Enhanced Cloud Objects (SECO): A Generalized Framework for Automated Detection of Volcanic Ash and Dust Clouds using Passive Satellite Measurements, Part I: Multispectral Analysis, *Journal Geophysical Research*, **120**, 7813-7841.
- Pavolonis, M., J. Sieglaff, and J. Cintineo (2015b) Spectrally Enhanced Cloud Objects (SECO): A Generalized Framework for Automated Detection of Volcanic Ash and Dust Clouds using Passive Satellite Measurements, Part II: Cloud Object Analysis and Global Application, *Journal Geophysical Research*, **120**, 7842-7870.

Outline

- Importance of SO₂ monitoring
- Strengths and weaknesses of different satellite measurements
- Measurement integration plan
- Collaboration

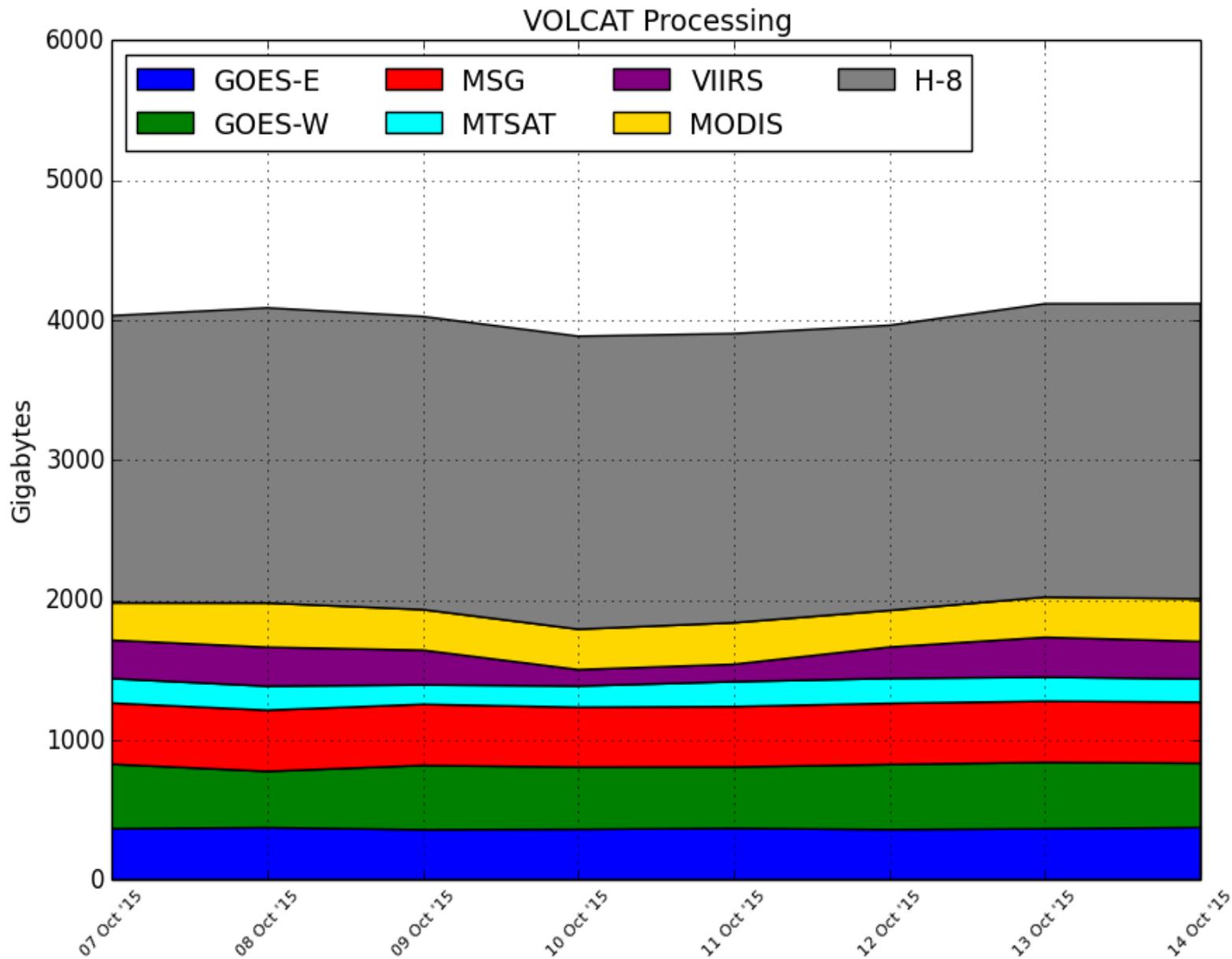
Collaborations

- Fusing information from many sensors is challenging. Collaborations with hyperspectral UV and IR SO₂ remote sensing groups at NASA and in academia are needed.
- In addition, a collaborative effort with the USGS, academia, and international partners (e.g. IMO) is needed to validate the fused JPSS SO₂ analysis.
- International collaboration is needed to work towards best practices for combining measurements from multiple satellite sensors – connection to WMO SCOPE-Nowcasting.
- Collaboration with the dispersion, weather, and climate modeling communities are critical to ensure that the impact of the information is maximized

Summary

- In support of NOAA's mission, NOAA's role in generating environmental intelligence related to SO₂ needs to be expanded (and integrated with information on volcanic ash) in collaboration with NASA, USGS, and international partners.
- The JPSS satellite series is a critical component of the SO₂ observing system
- A collaborative JPSS initiative is needed to ensure that the JPSS sensors are being fully utilized for SO₂ monitoring

“Big Data”

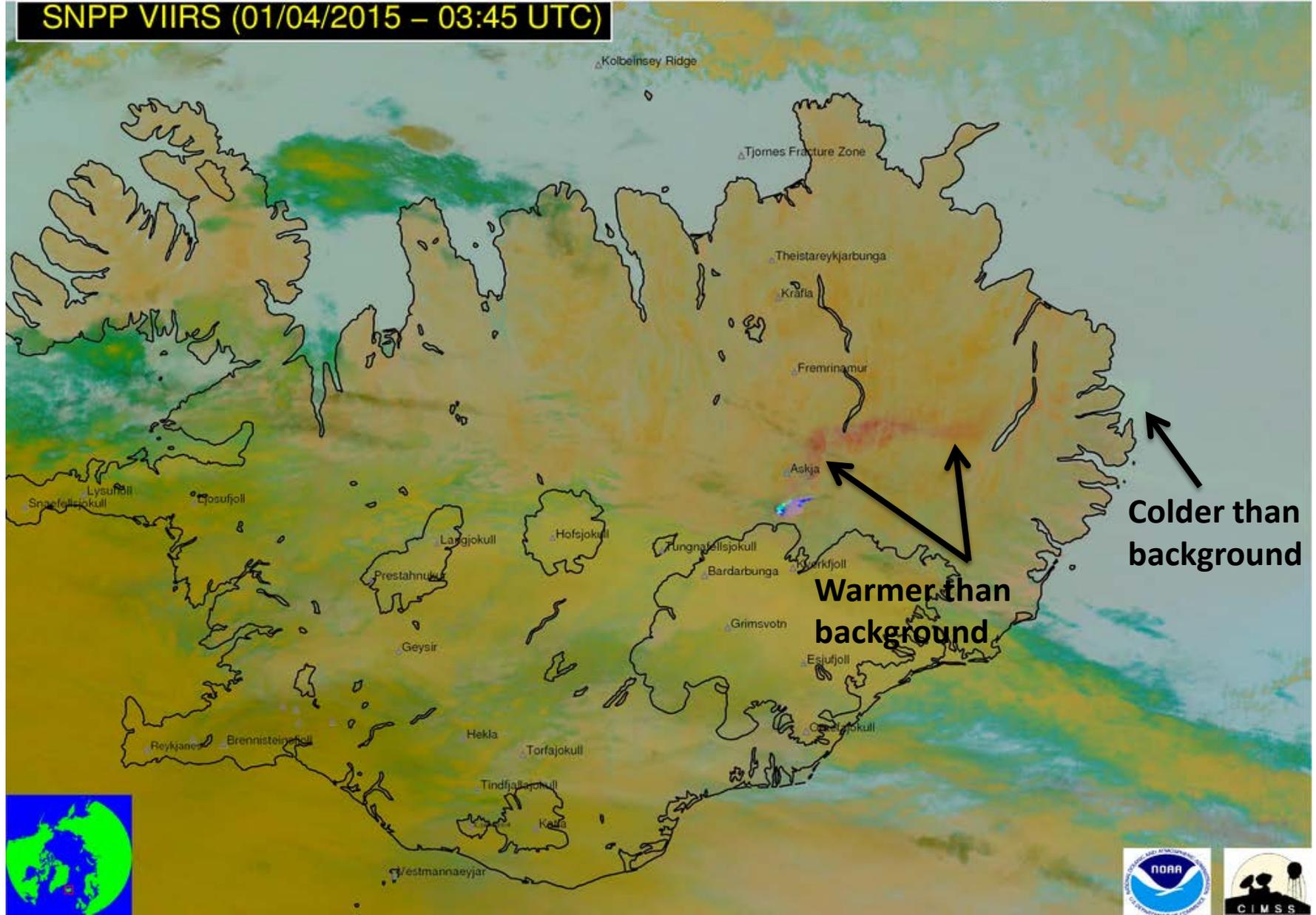


BACKUP SLIDES

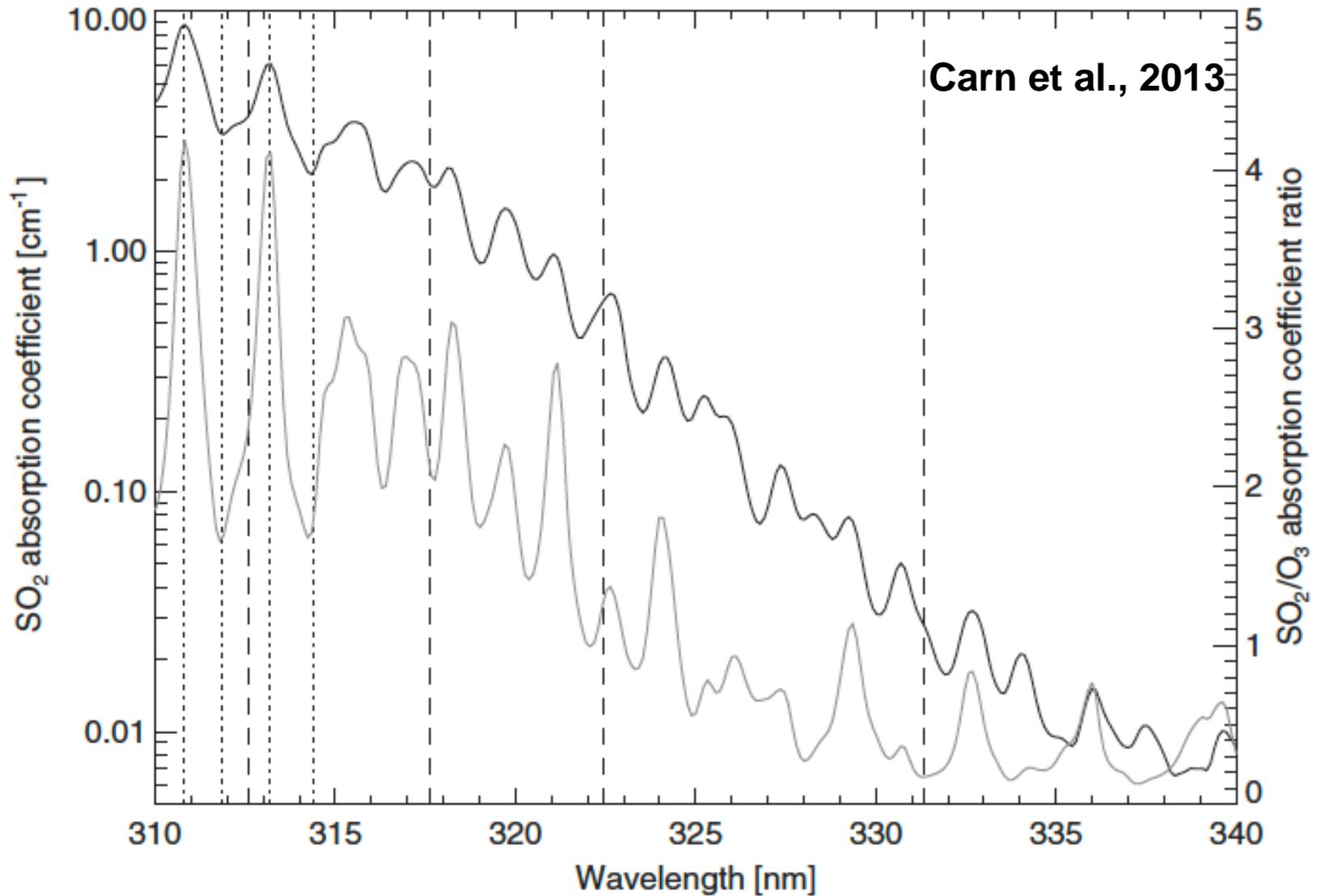
Nuances/Exceptions are Prevalent

False Color Imagery (12–11 μ m, 11–8.5 μ m, 11 μ m)

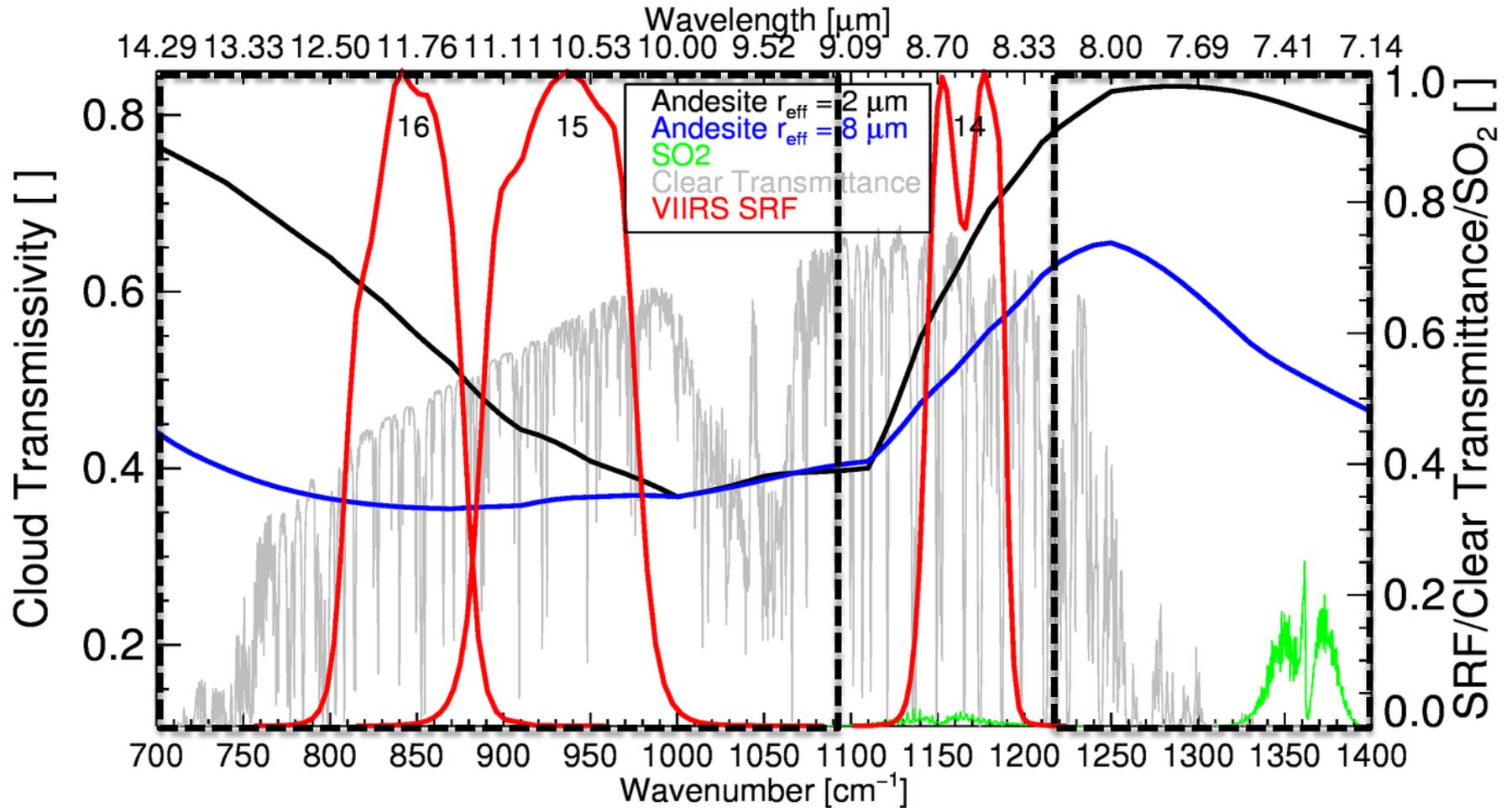
SNPP VIIRS (01/04/2015 – 03:45 UTC)



UV Sensitivity



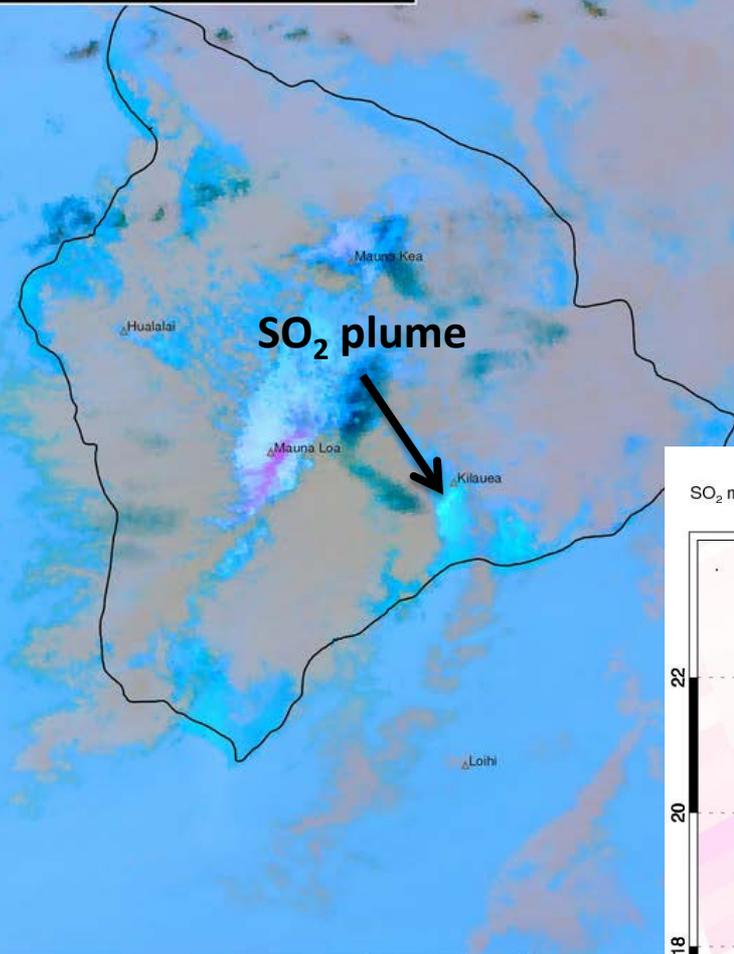
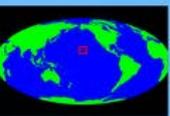
Infrared Sensitivity



False Color Imagery (12–11 μ m, 11–8.5 μ m, 11 μ m)

SNPP VIIRS (04/10/2015 – 23:30 UTC)

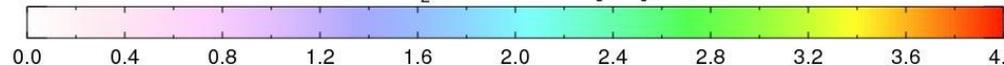
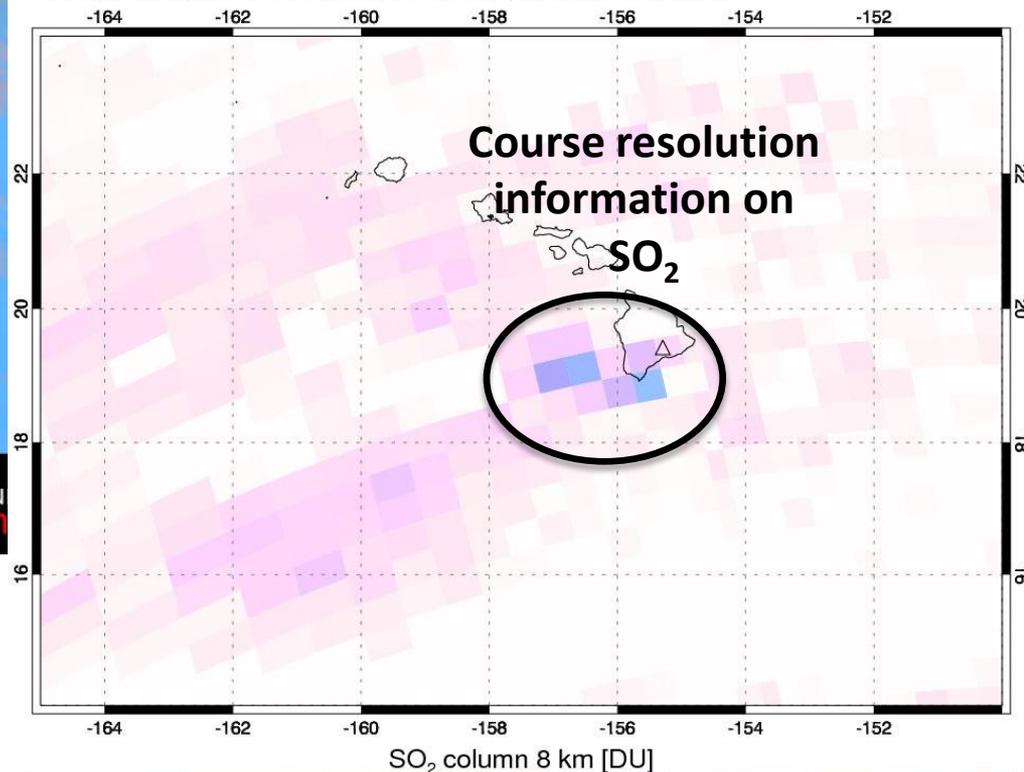
A multi-sensor SO₂ analysis is needed



Annotation Key
(annotation colors are not related to colors in u
Ash/Dust Cloud Volcanic Cb Th

Suomi NPP/OMPS - 04/10/2015 23:35-23:39 UT

SO₂ mass: 0.000 kt; Area: 0 km²; SO₂ max: 1.64 DU at lon: -155.50 lat: 18.86 ; 23:37UTC



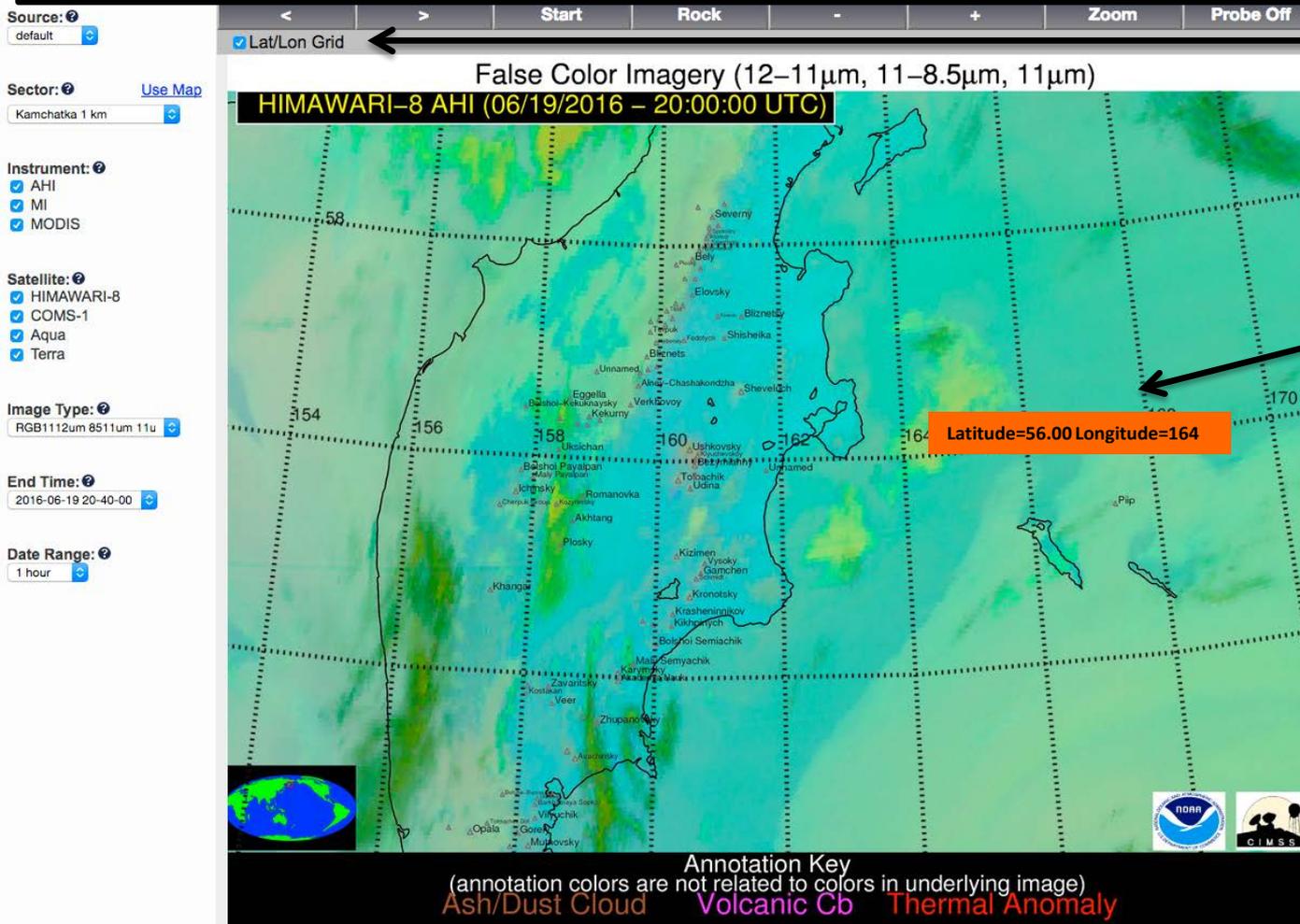
Optional Overlay Options: lat/lon grid, volcanoes, coast lines, VAAC boundaries, automated feature annotations

Image Probe: cursor readout of lat/lon and data value

Image Markup Tools: users can generate and export polygons and annotated images

SO₂: alerting, tracking, and characterization

Incorporation of Non-Satellite Tools: volcano web cameras, dispersion/trajectory modeling, and infrasound



Overlay options

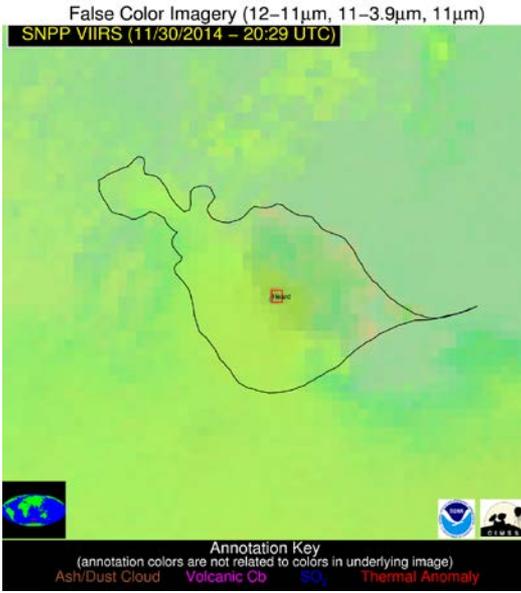
Image Probe

LEO and GEO satellite imagery are routinely generated for numerous geographic sectors that cover nearly every volcano in the world



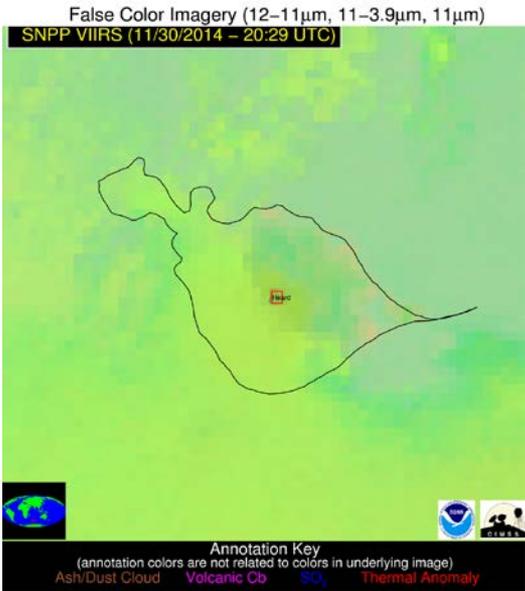
VOLCAT Goals

1). Unrest Alerts



VOLCAT Goals

1). Unrest Alerts

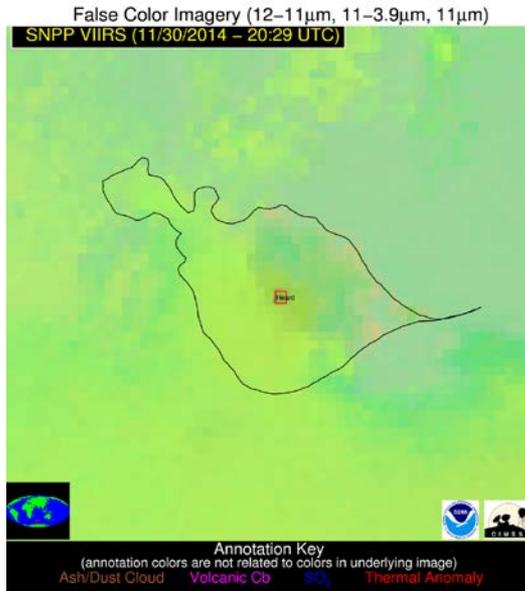


2). Eruption Alerts

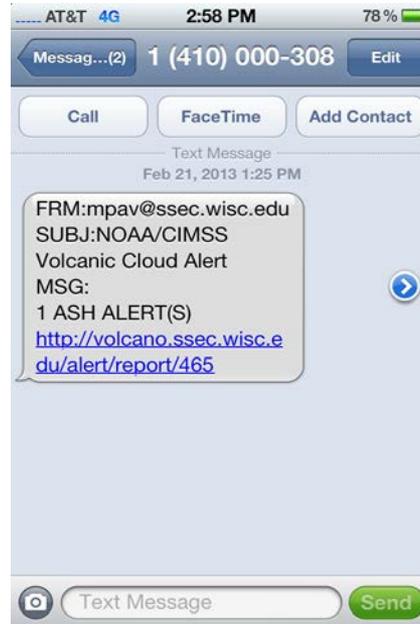


VOLCAT Goals

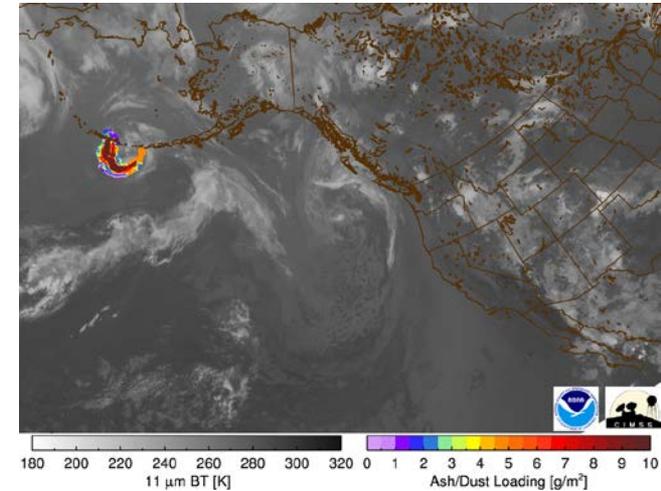
1). Unrest Alerts



2). Eruption Alerts

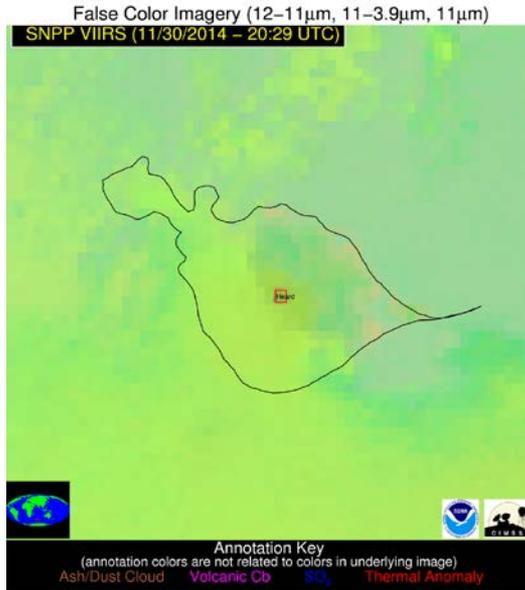


3). Volcanic Cloud Tracking

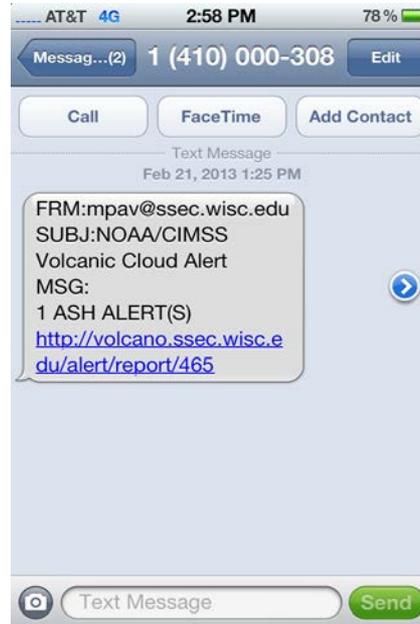


VOLCAT Goals

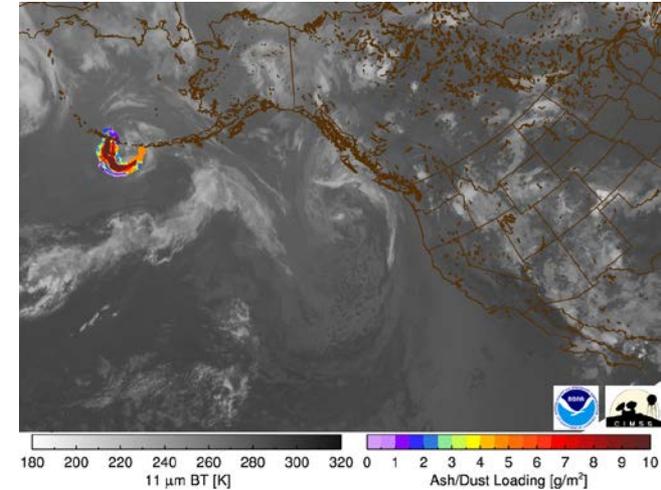
1). Unrest Alerts



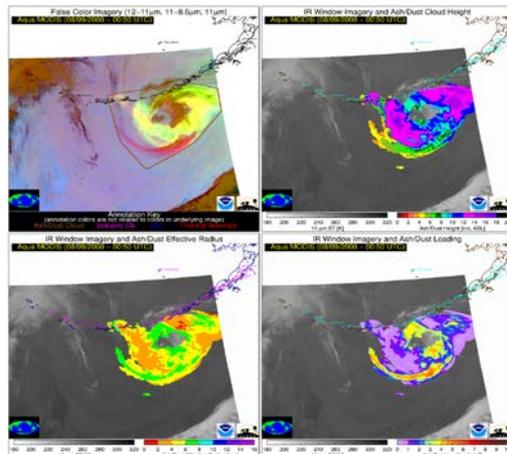
2). Eruption Alerts



3). Volcanic Cloud Tracking

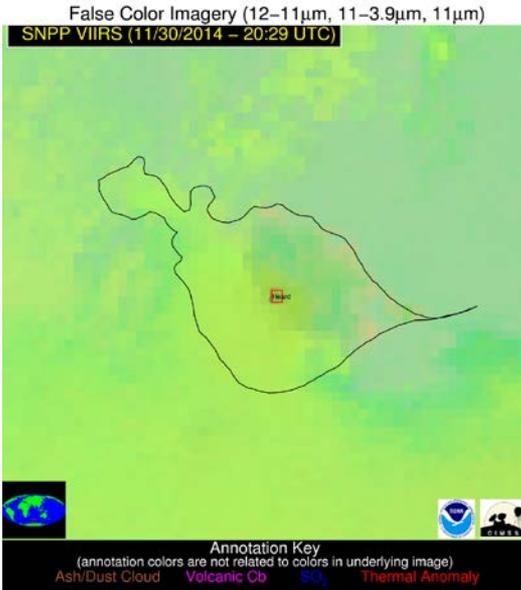


4). Volcanic Cloud Characterization

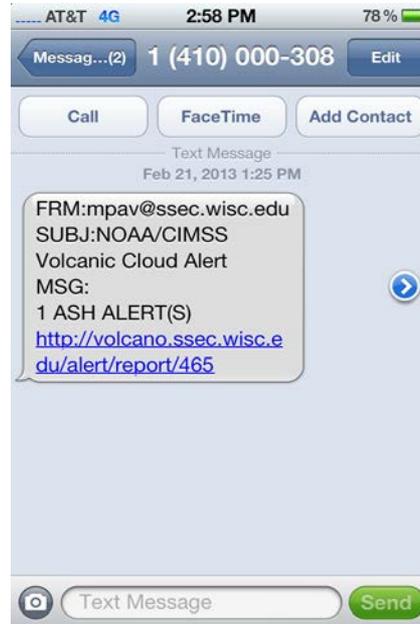


VOLCAT Goals

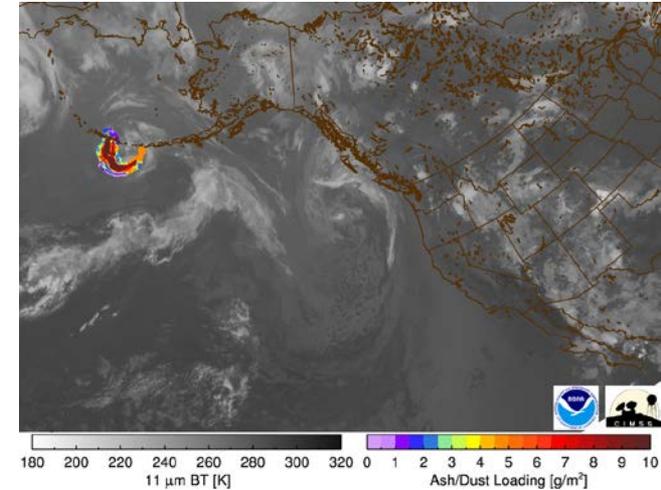
1). Unrest Alerts



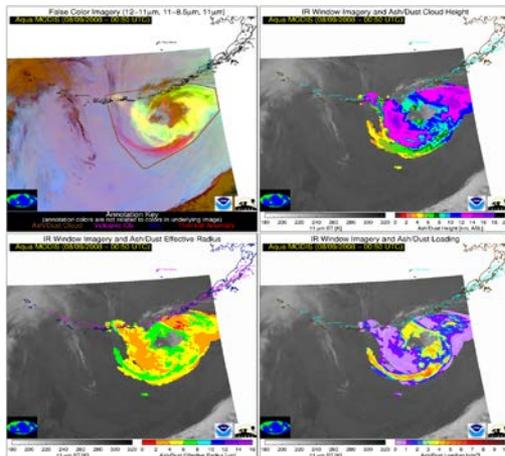
2). Eruption Alerts



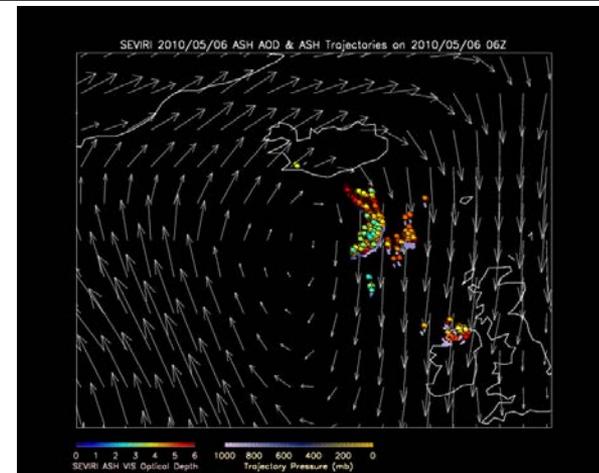
3). Volcanic Cloud Tracking



4). Volcanic Cloud Characterization

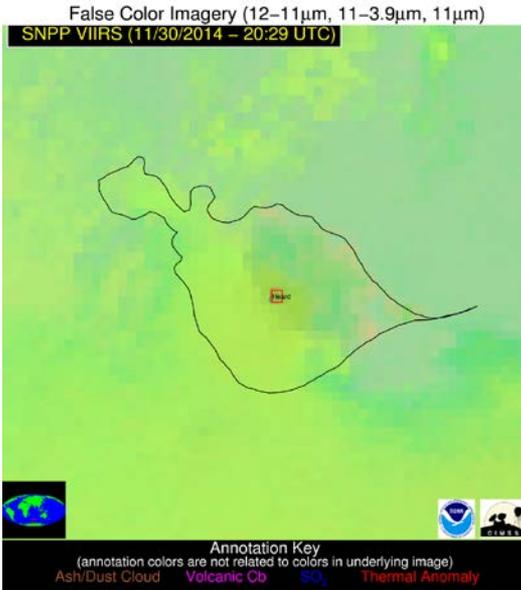


5). Dispersion Forecasting

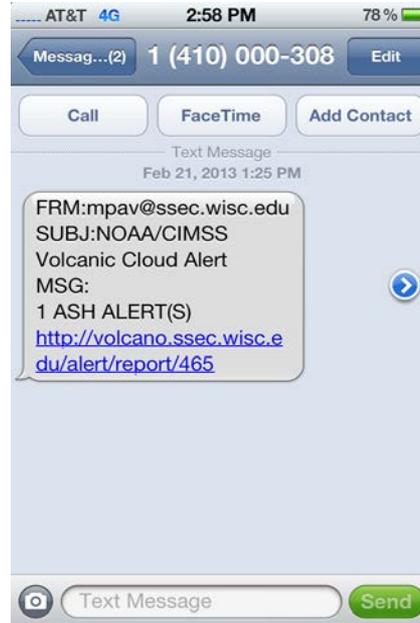


VOLCAT Goals

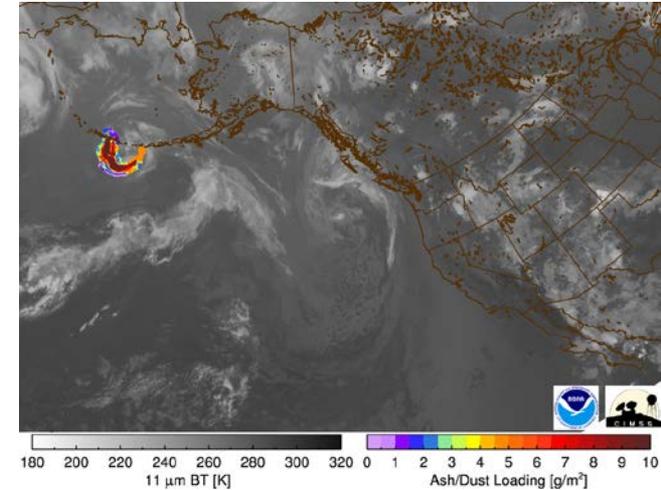
1). Unrest Alerts



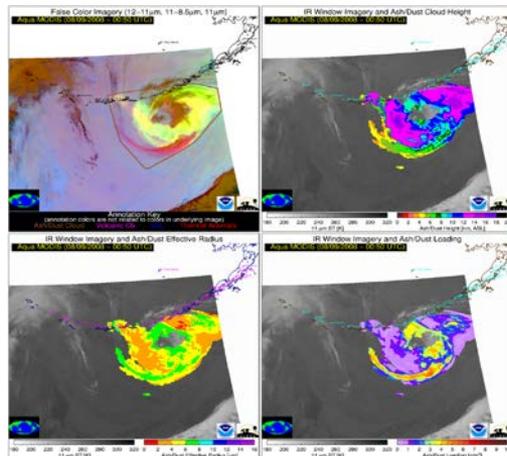
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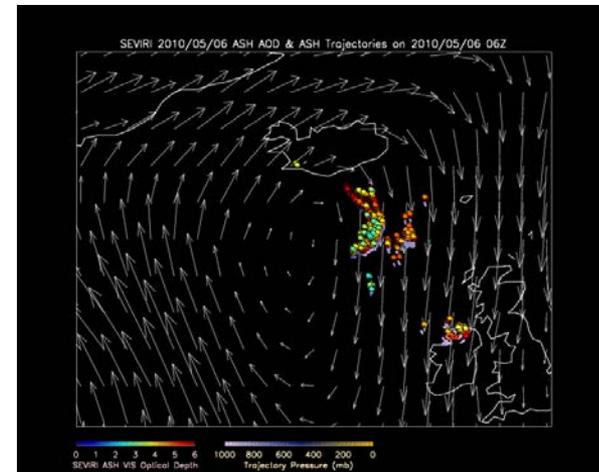
3). Volcanic Cloud Tracking

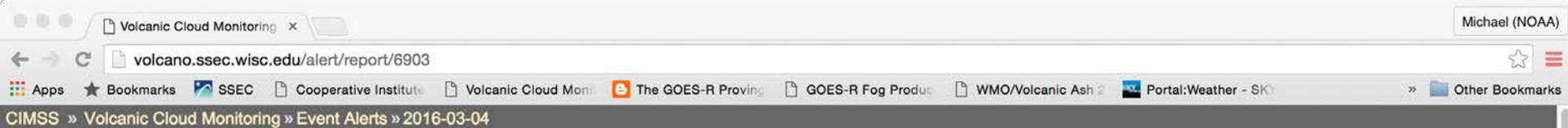


4). Volcanic Cloud Characterization



5). Dispersion Forecasting





Volcanic Cloud Monitoring — NOAA/CIMSS (BETA)



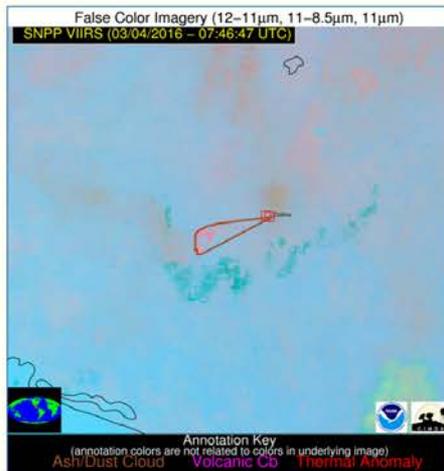
- Home
- Satellite Imagery
- Alerts
- Coverage Map
- Tutorials
- Admin
- Logout (mpav@ssec.wisc.edu)

Volcanic Cloud Alert Report

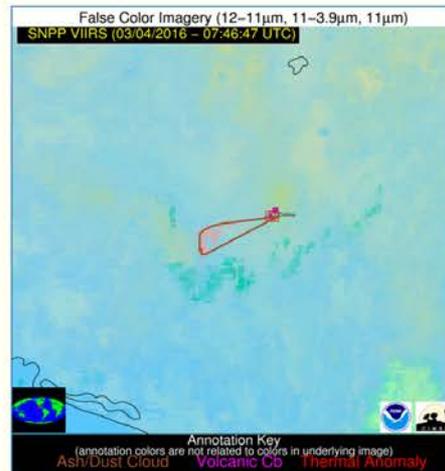
DATE:	2016-03-04
TIME:	07:46:47
Production Date and Time:	2016-03-04 10:44:46 UTC
PRIMARY INSTRUMENT:	NPP VIIRS

[More details ▼](#)

Possible Volcanic Ash Cloud



[False Color Image \(12-11, 11-8.5, 11\) \[zoomed-in\]](#)



[False Color Image \(12-11, 11-3.9, 11\) \[zoomed-in\]](#)

Basic Information

Volcanic Region(s)	Mexico and Central America
Country/Countries	Mexico
Volcanic Subregion(s)	Mexico
VAAC Region(s) of Nearby Volcanoes	Washington
Mean Object Date/Time	2016-03-04 07:46:47UTC
Radiative Center (Lat, Lon):	19.510 °, -103.620 °
	Colima (0.00 km) [Thermal Anomaly Present]
Nearby Volcanoes (meeting alert criteria):	Primavera, Sierra la (123.60 km)
	Mascota Volcanic Field (176.50 km)
	Michoacan-Guanajuato (199.50 km)
	Ceboruco (201.90 km)
Maximum Height [AMSL]	5.40 km; 17717 ft
90th Percentile Height [AMSL]	4.20 km; 13780 ft
Mean Tropopause Height [AMSL]	16.90 km; 55446 ft

[Show More ▲](#)

[View all event imagery ▶](#)

Volcanic Cloud Detection

The VOLCAT detection approach is multi-faceted and employs several different conceptual models to identify volcanic clouds across the spectrum of eruption cloud types.

- Spectral cloud objects [spectral signature]
- Plume [spectral signature + geometric properties]
- ~~– Puff [some spectral signature + cloud growth]~~
- ~~– Major Explosion [cloud growth]~~
- Tracking in time [spectral signature + feature tracking]





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Spectrally Enhanced Cloud Objects (SECO)

JGR - Pavolonis et al. (2015a)

JGR – Pavolonis et al. (2015b)

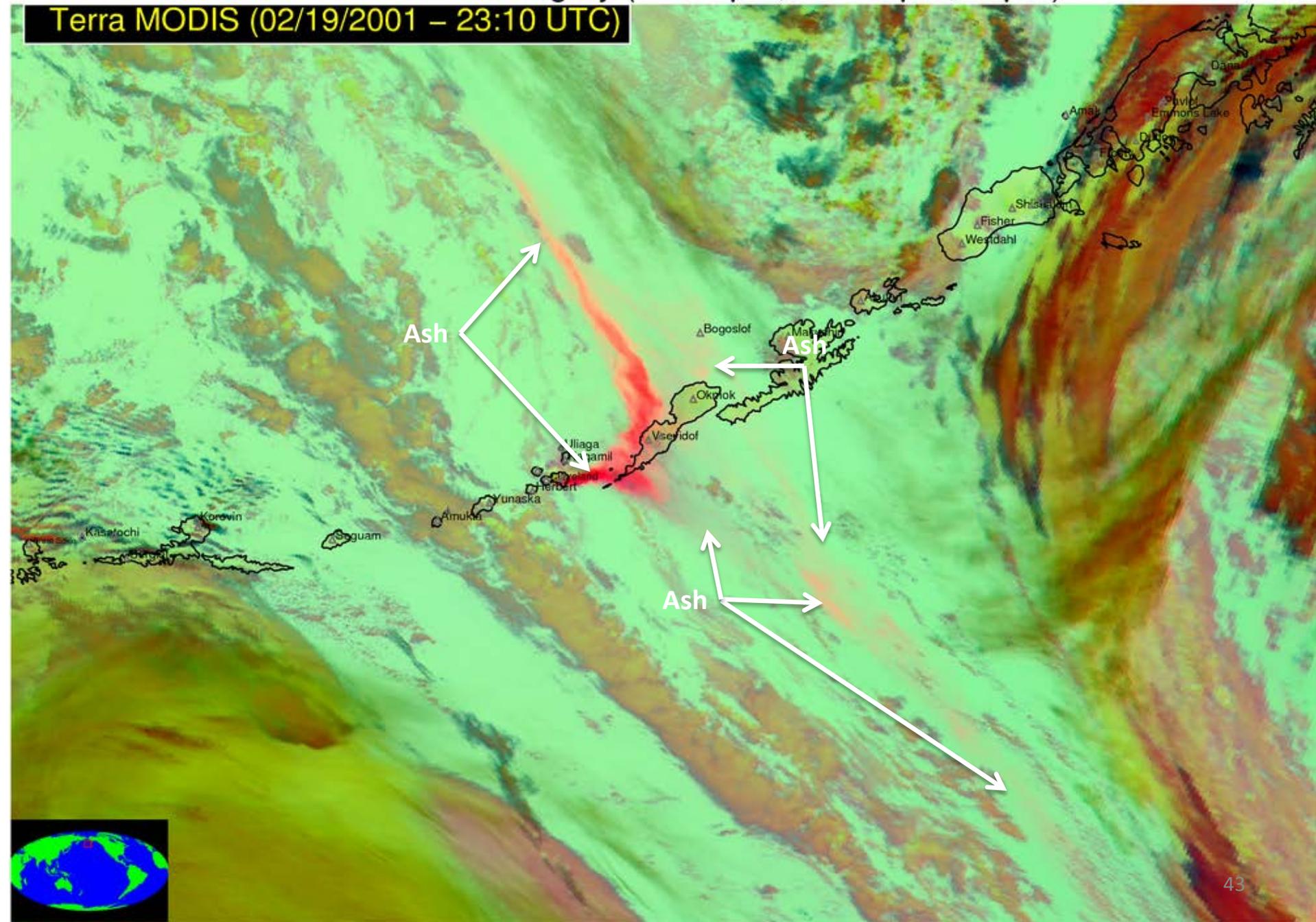


Rueters



False Color Imagery (12–11 μ m, 11–3.9 μ m, 11 μ m)

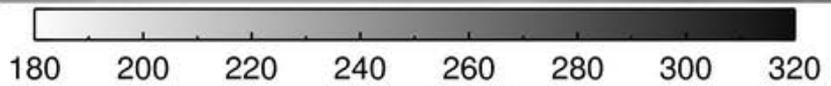
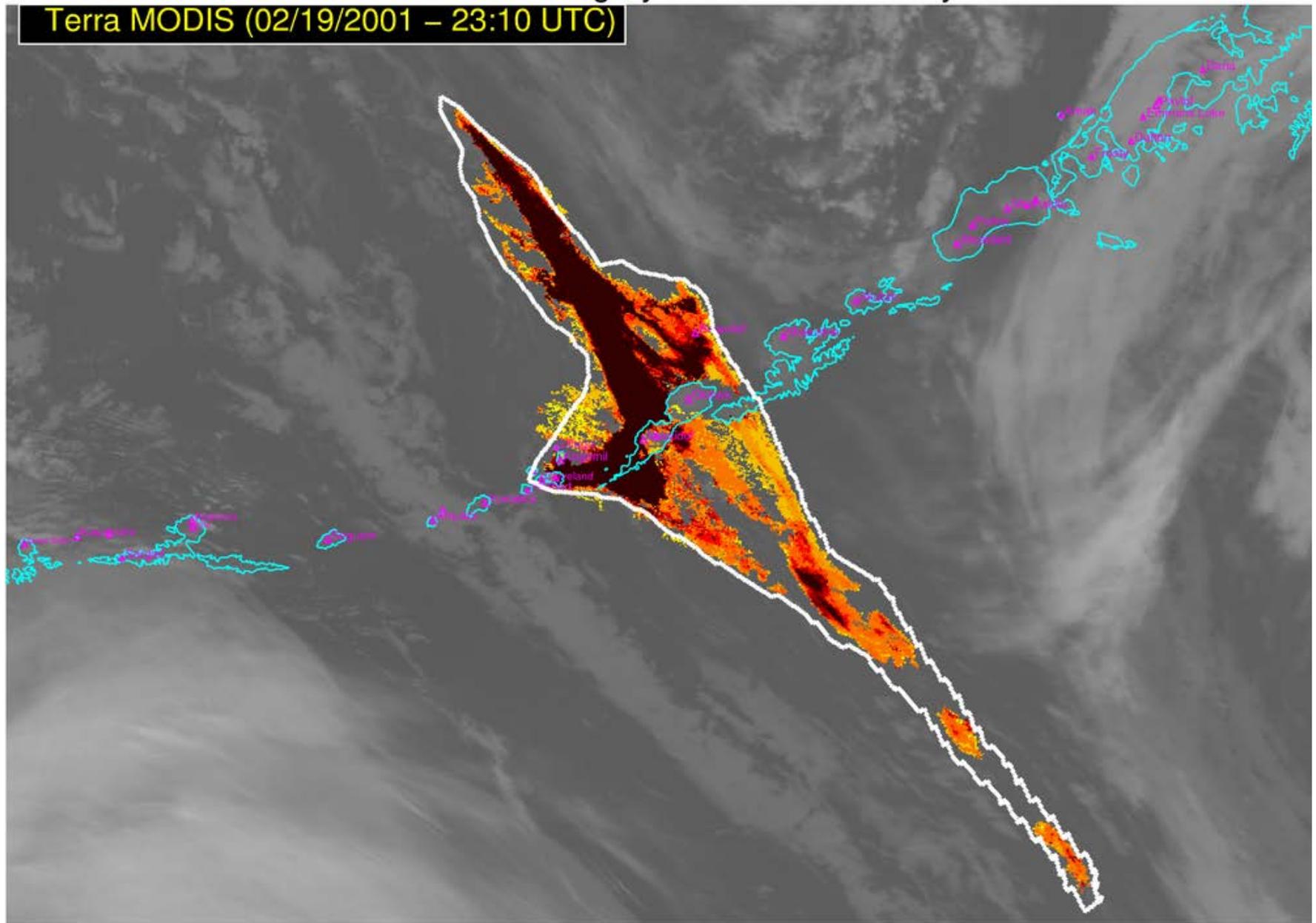
Terra MODIS (02/19/2001 – 23:10 UTC)



D

IR Window Imagery and Ash Probability

Terra MODIS (02/19/2001 – 23:10 UTC)



11 μm BT [K]

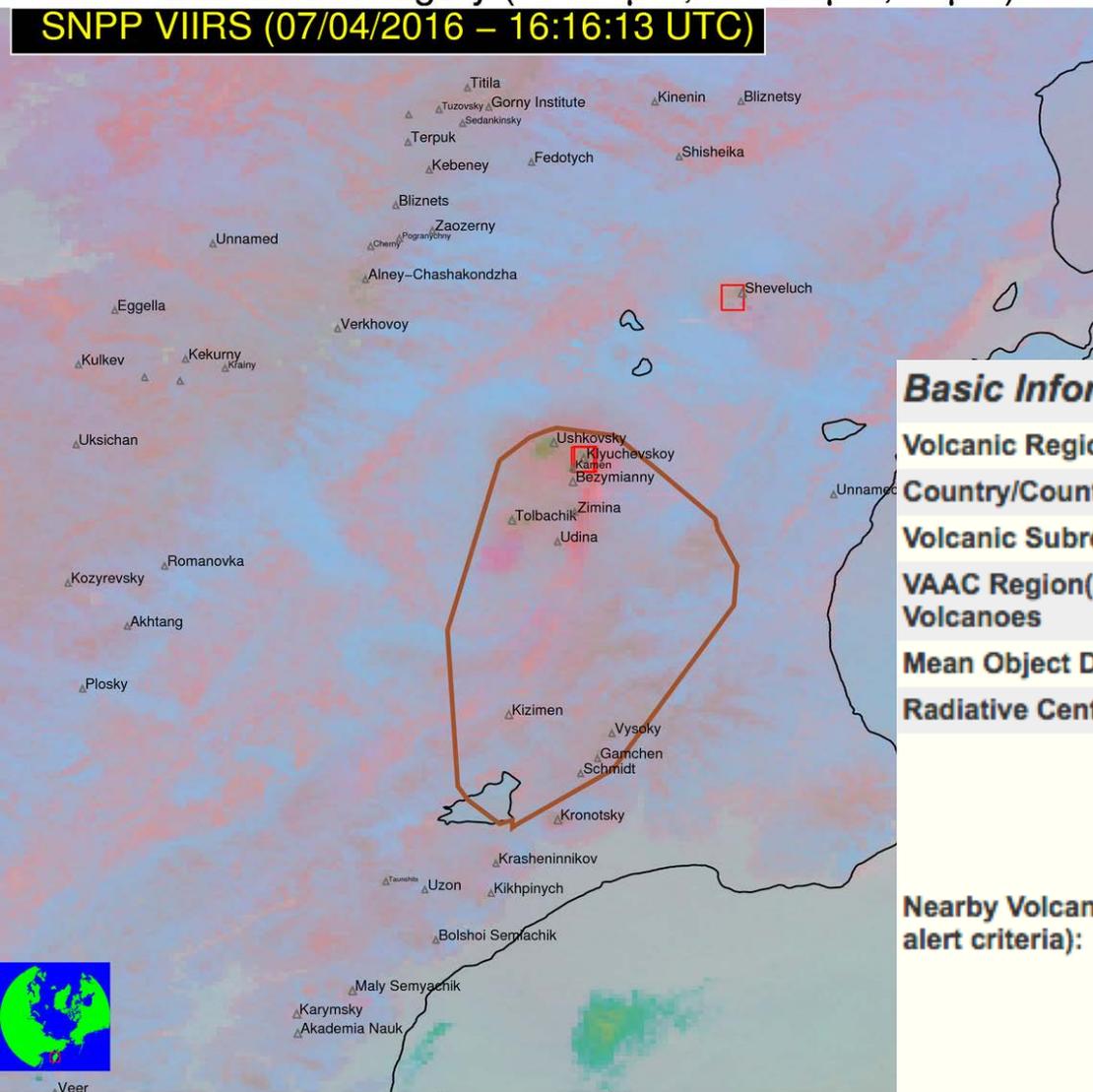


Ash/Dust Probability [%]

False Color Imagery (12–11µm, 11–8.5µm, 11µm)

SNPP VIIRS (07/04/2016 – 16:16:13 UTC)

Automated Determination of Source Volcano



Basic Information

Volcanic Region(s)	Kamchatka and Mainland Asia
Country/Countries	Russia
Volcanic Subregion(s)	Kamchatka Peninsula
VAAC Region(s) of Nearby Volcanoes	Tokyo
Mean Object Date/Time	2016-07-04 16:16:13UTC
Radiative Center (Lat, Lon):	56.060 °, 160.640 °

Nearby Volcanoes (meeting alert criteria):

- [Klyuchevskoy \(0.00 km\) \[Thermal Anomaly Present\]](#)
- [Kamen \(5.00 km\) \[Thermal Anomaly Present\]](#)
- [Bezymianny \(9.80 km\) \[Thermal Anomaly Present\]](#)
- [Ushkovskoy \(10.40 km\)](#)
- [Zimina \(21.70 km\)](#)

Maximum Height [AMSL]	6.70 km; 21982 ft
90th Percentile Height [AMSL]	4.40 km; 14436 ft
Mean Tropopause Height [AMSL]	12.00 km; 39370 ft

Annotation Key

(annotation colors are not related to colors in underlying image)

Ash/Dust Cloud Volcanic Cb Thermal A

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