Status of NUCAPS Full Spectral-Resolution Trace Gas EDR Validation

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  - **Ozone**
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    - **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.)
  - **Carbon Trace Gases**
    - **NASA Sounder Science Team:** *E. Olsen, T. Pagano, E. Fetzer* (NASA/JPL)
    - **Total Carbon Column Observing Network (TCCON)** (*D. Wunch* et al.) data were obtained from the TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center (CDIAC), tccon.onrl.gov

- 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.

- **STAR soundings team**: *A.K. Sharma, Q. Liu, T. King, W. W. Wolf* (STAR)

Outline

- **JPSS Sounder Trace Gas EDR Cal/Val Overview**
  - JPSS Level 1 Requirements
  - Validation Hierarchy recap
  - NUCAPS Algorithm
    - v1.5, nominal spectral-resolution (NSR) CrIS
    - v2.0 Phase 4, full spectral-resolution (FSR) CrIS
- **NUCAPS IR Ozone Profile EDR Product Evaluation**
  - v1.5 NSR Review
    - Global ozonesonde ensemble
  - v2.0 FSR (Phase 4) Status
    - Global Focus Day ECMWF
- **NUCAPS Carbon Trace Gas EDR Product Evaluation (Preliminary)**
  - Truth Datasets and Methodology
    - AIRS Version 6
    - TCCON
  - v2.0 FSR (Phase 4) Status
    - Carbon Monoxide (CO)
    - Methane (CH_4)
    - Carbon Dioxide (CO_2)

Status of NUCAPS FSR Trace Gas EDR Validation

JPSS SOUNDER TRACE GAS EDR CAL/VAL OVERVIEW

JPSS Specification Performance Requirements
CrIS Trace Gas EDR Uncertainty (O_3, CO, CO_2, CH_4)

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 Hierarchies

T/H_2O/O_3 Profiles

(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)
   - Limitation: Similar error characteristics
3. **Conventional PTU/O3 Sonde Matchup *Assessments***
   - WMO/GTS operational sondes or O3-sonde network (e.g., SHADOZ)
   - 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 distributions; mismatch errors; non-uniform radiosondes, assimilated into NWP
4. **Dedicated/Reference PTU/O3 Sonde Matchup *Assessments***
   - *Dedicated* for the purpose of satellite validation
   - Reference sondes: CFH, **GRUAN** corrected RS92/RS41
   - E.g., **ARM sites** (e.g., *Tobin et al.,* 2006), **AEROSE**, **CalWater/ACAPEX** , BCCSO, PMRF
   - Limitation: Small sample sizes, geographic coverage
5. **Intensive Field Campaign *Dissections***
   - Include dedicated sondes, some *not* assimilated into NWP models
   - Include ancillary datasets, ideally funded aircraft campaign(s)
   - E.g., **SNAP, SNPP, AEROSE, CalWater**, JAIVEX, AWEX-G, EAQUATE

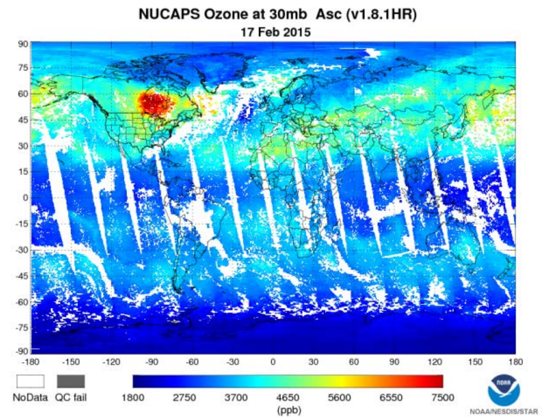
Carbon Trace Gases

1. **Numerical Model Global *Comparisons***
   - Examples: **ECMWF, NCEP/GFS**
   - Large, truly global samples acquired from Focus Days
   - Limitation: Not independent truth data
2. **Satellite Sounder EDR *Intercomparisons***
   - Examples: **AIRS, OCO-2, MLS**
   - Global samples acquired from Focus Days (e.g., AIRS)
   - Limitation: Similar error characteristics
3. **Surface-Based Spectrometer Network Matchup *Assessments***
   - **Total Carbon Column Observing Network (TCCON)**
   - Provide routine independent measurements representing global zones akin to RAOBs
   - Limitations: Small sample sizes, uncertainties in conversions to column abundances, different sensitivity to atmospheric layers
4. **Intensive Field Campaign *In Situ* Data *Assessments***
   - Include ancillary datasets, ideally funded aircraft campaign(s)
   - E.g., ATom, FIREX, HIPPO

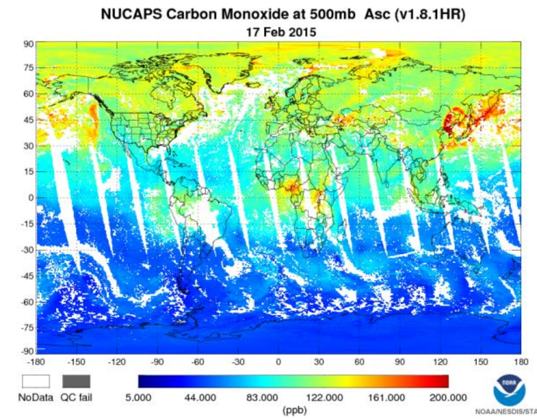
NOAA Unique Combined Atmospheric Processing System (NUCAPS) Algorithm (1/2)

- **Operational algorithm**
  - NOAA Enterprise Algorithm for CrIS/IASI/AIRS (*Susskind, Barnet and Blaisdell,* IEEE 2003; *Gambacorta et al.,* 2014)
  - Global non-precipitating conditions
  - Atmospheric Vertical Temperature, Moisture Profiles (AVTP, AVMP)
  - **Trace gas profiles** (**O_3, CO, CO_2, CH_4**)
- **Users**
  - Weather Forecast Offices (AWIPS)
    - Nowcasting / severe weather
    - Alaska (cold core)
  - NOAA/CPC (OLR)
  - **NOAA/ARL** (IR ozone, trace gases)
  - **NOAA TOAST** ozone product
  - Basic and applied science research (e.g., *Pagano et al.,* 2014)
    - Via NOAA Data Centers (e.g., CLASS)
    - Atmospheric chemistry research
    - Universities, peer-reviewed pubs

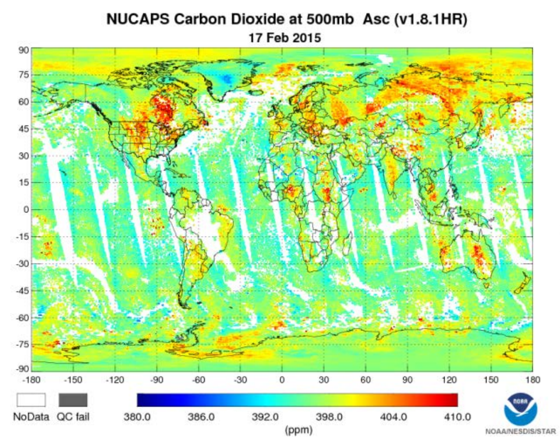
NUCAPS IR O_3



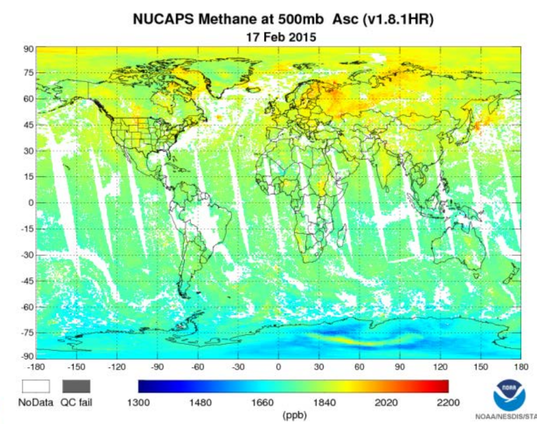
NUCAPS CO



NUCAPS CO_2



NUCAPS CH_4



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

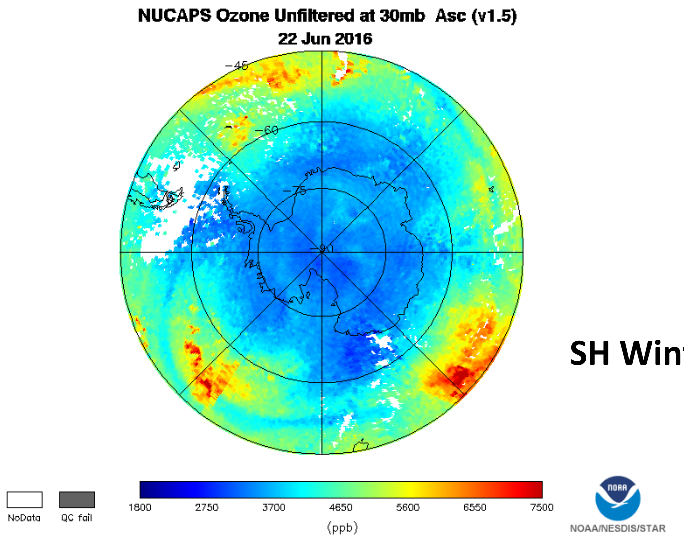
NUCAPS Offline Code Versioning

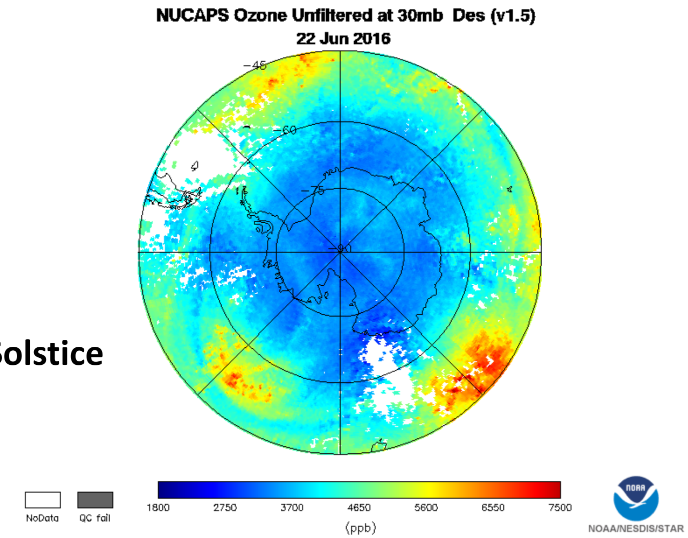
- **Version 1.5**
  - Operational system beginning in September 2013
  - Runs on CrIS nominal spectral-resolution (NSR) data
  - Validated Maturity for IR Ozone Profile EDR attained Oct 2016
  - Carbon trace gas EDR validation was not required
- **Versions 1.8.x to 1.9.x**
  - Preliminary offline experimental algorithms in preparation for CrIS full spectral-resolution (FSR) data
  - *Ad hoc* CrIS full-resolution radiative transfer algorithm (RTA) and bias correction coefficients
- **Version 2.0 (Phase 4)**
  - Uses **UMBC CrIS full-res (FSR) RTA** (L. Strow et al.)
  - Includes **IR-only version** (risk-mitigation for ATMS loss)
  - **Phase 4 Algorithm Readiness Review (ARR)** delivered on 6 July 2017
    - Draft ATBD delivered August 2017
    - Code currently being delivered and transitioned into operations

Status of NUCAPS FSR Trace Gas EDR Validation

IR OZONE PROFILE EDR

Science Application: Ozone Hole Over Antarctica

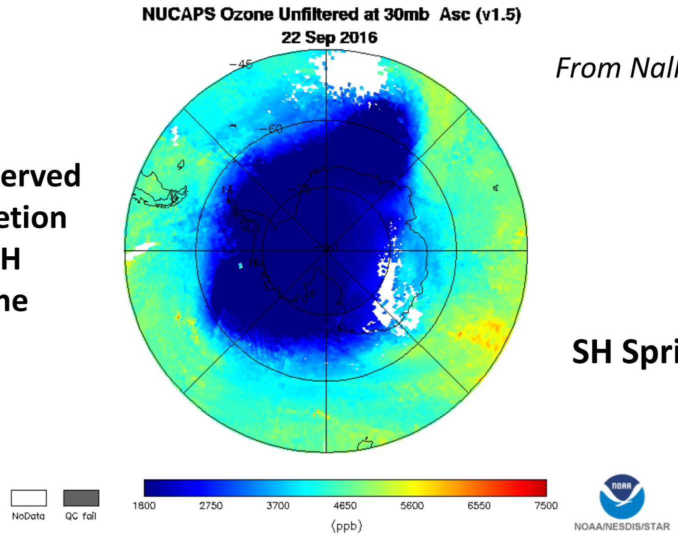


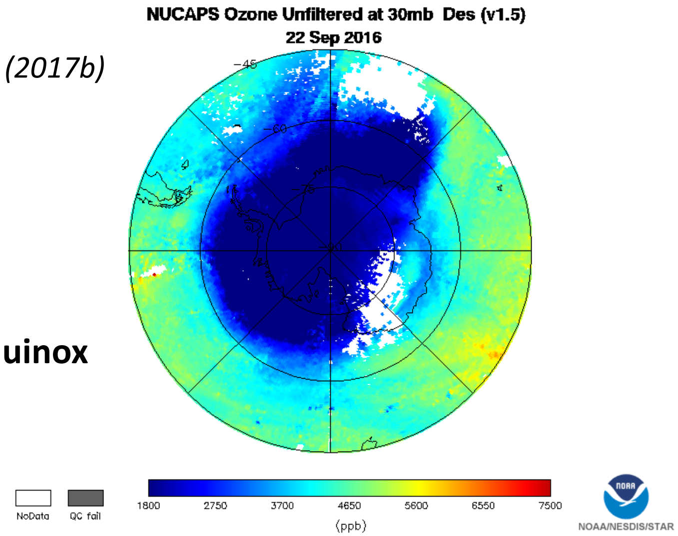


SH Winter Solstice

From Nalli et al. (2017b)

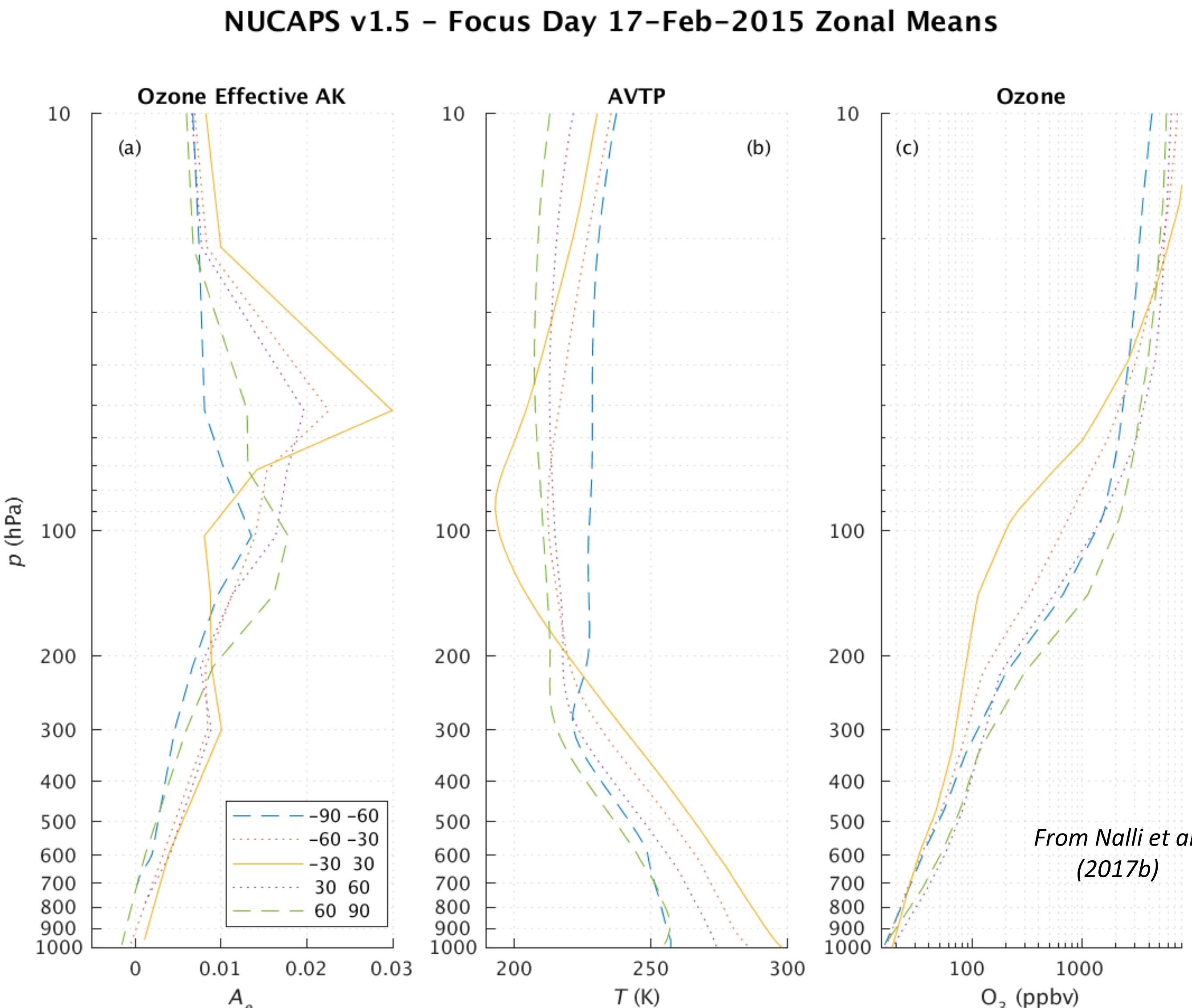
NUCAPS observed ozone depletion during SH springtime





SH Spring Equinox

NUCAPS IR Ozone and AVTP Zonal Means

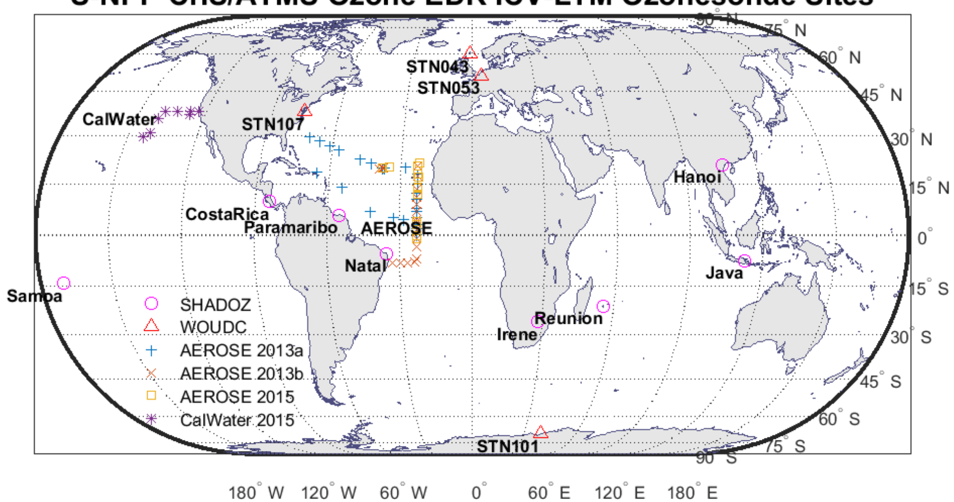


From Nalli et al. (2017b)

Collocated Ozonesondes for O_3 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

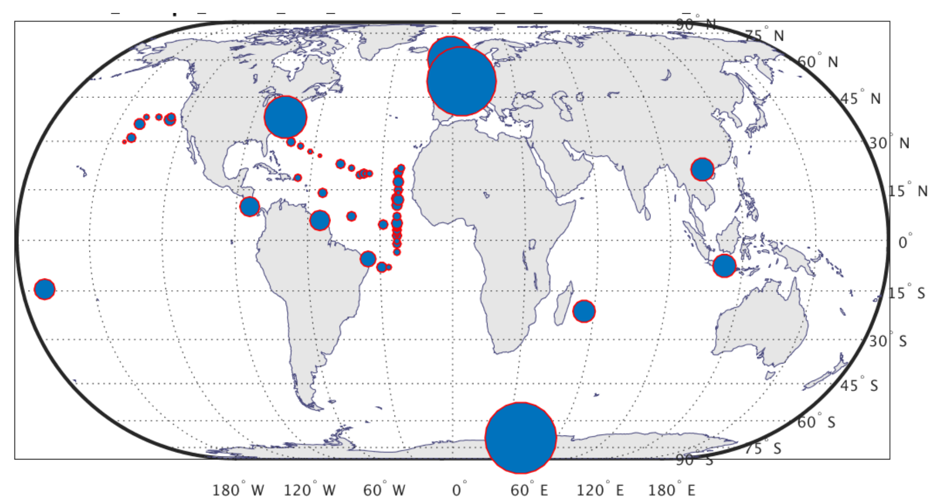
S-NPP CrIS/ATMS Ozone EDR ICV-LTM Ozonesonde Sites



From Nalli et al. (2017b)

Geographic Sample Histogram (Equal Area)

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

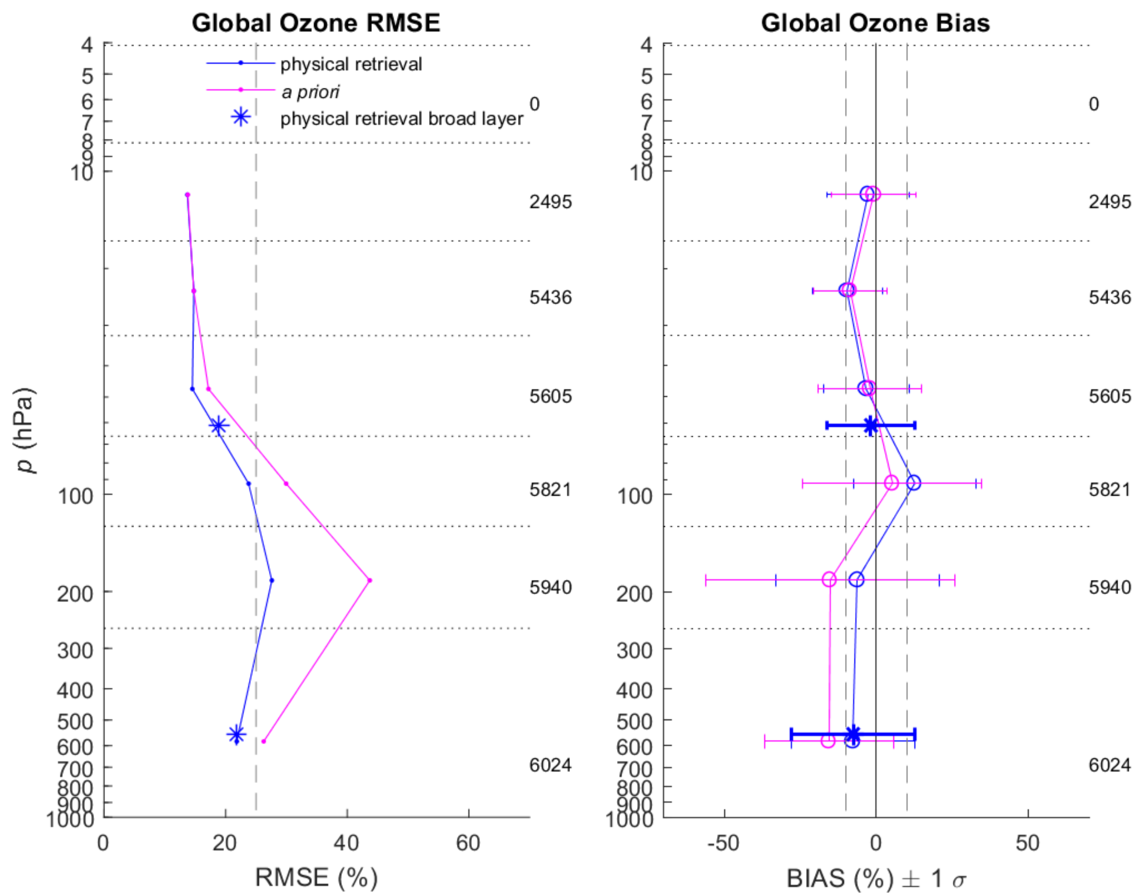


NUCAPS IR Ozone Profile Coarse-Layer Statistics

NSR (v1.5) versus Global Ozonesondes

Retrieval and ***A Priori***

IR+MW Yield = 62.2%

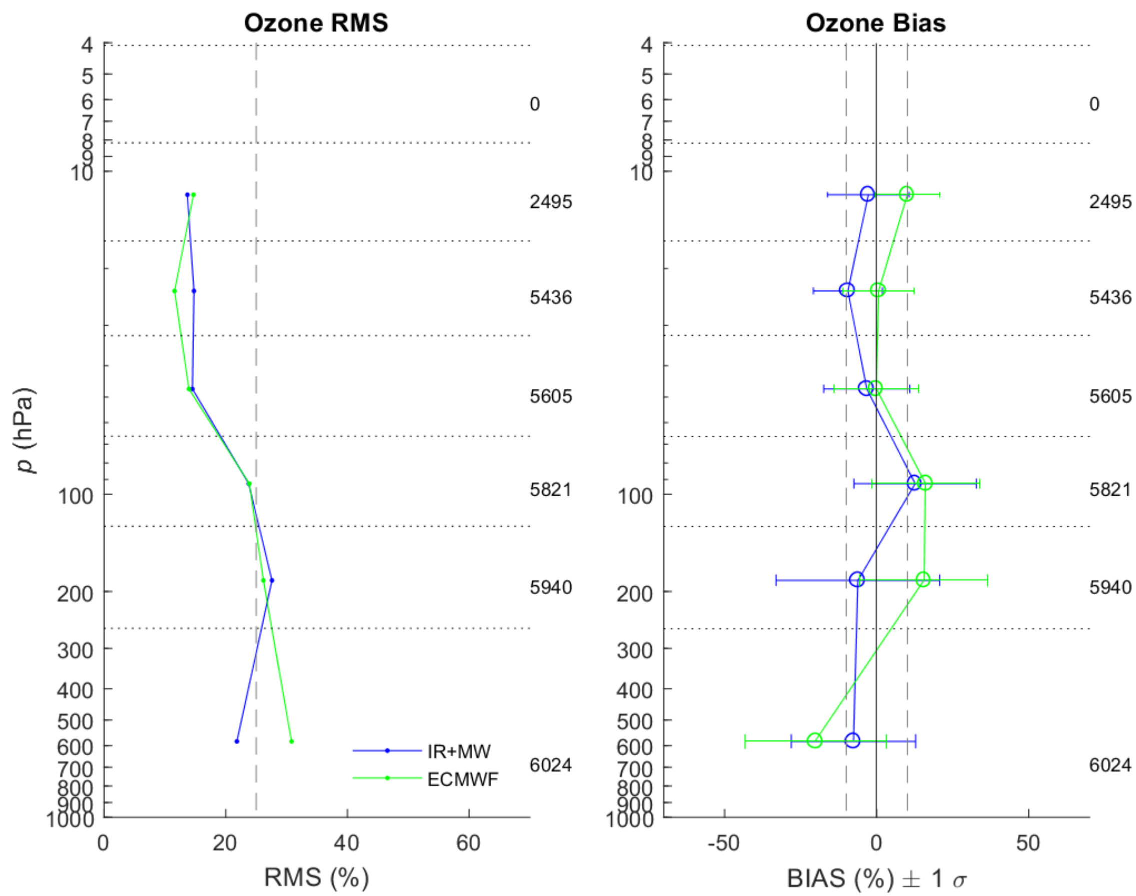


From Nalli et al. (2017)

NUCAPS IR Ozone Profile Coarse-Layer Statistics
NSR (v1.5) versus Global Ozonesondes

Retrieval and **ECMWF**

IR+MW Yield = 62.2%

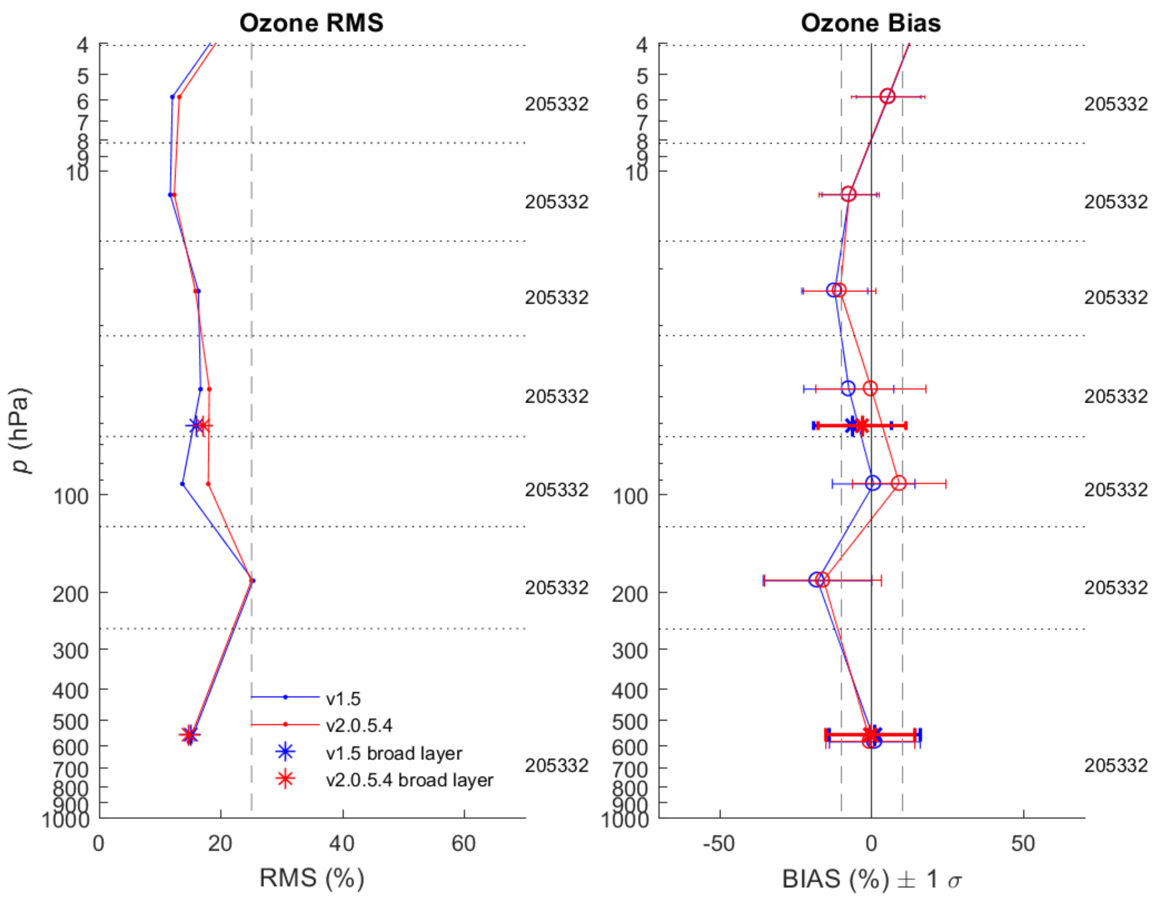


NUCAPS v2.0 FSR Ozone Profile Coarse-Layer Statistics
Global Focus Day 17-Feb-2015 ECMWF

NUCAPS FSR Ozone Versus ECMWF

V1.5 IR+MW
V2.0 IR+MW

v1.5 Yield = 63.4%
v2.0 Yield = 88.5%



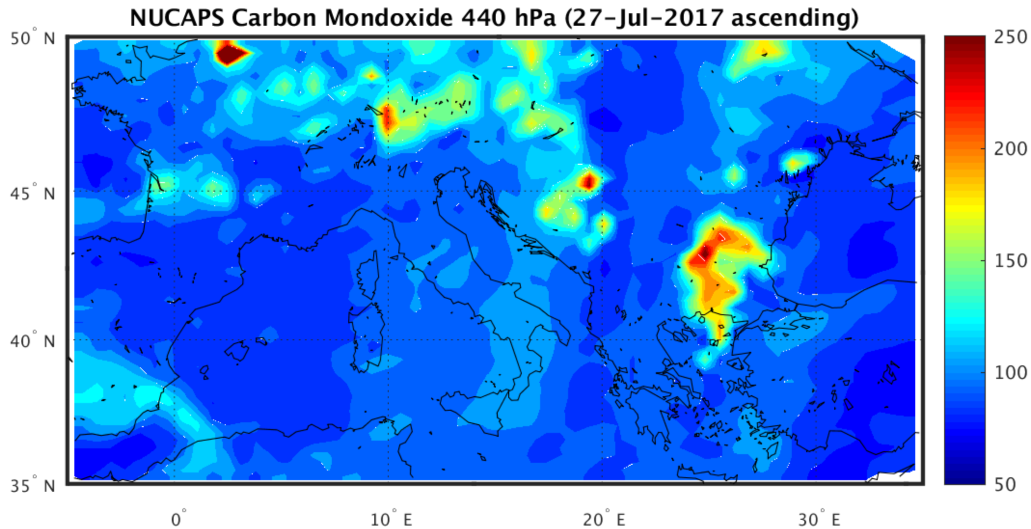
From Nalli et al. (2017)

Status of NUCAPS FSR Trace Gas EDR Validation

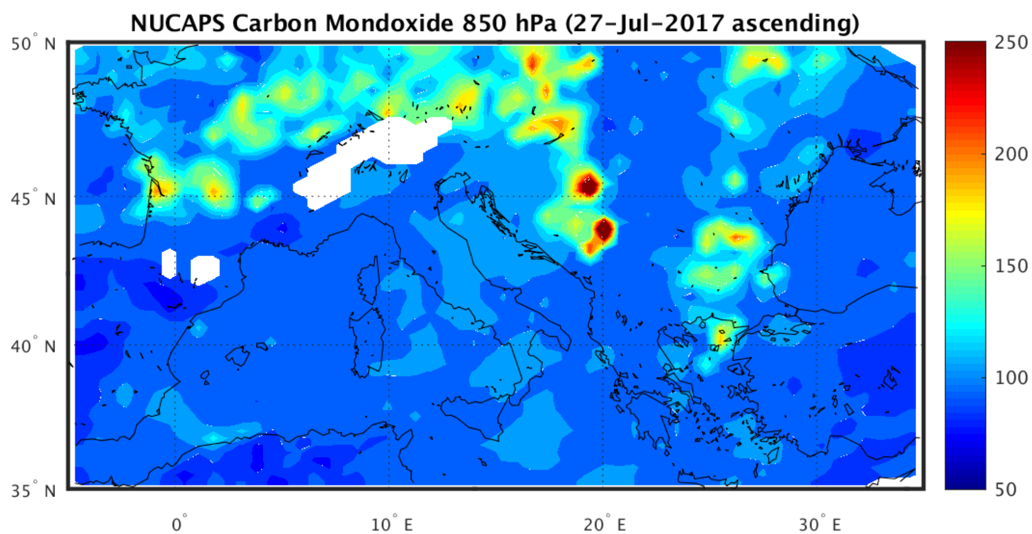
CARBON TRACE GAS EDR

Science Application:
Elevated CO From European Fires, 27 July 2017

440 hPa Layer



850 hPa Layer



Preliminary Methodology for Carbon Trace Gas Validation

- **Carbon trace gas EDR validation** versus JPSS program established uncertainty specifications is a **new sounder validation requirement** that began during the transition period to the FSR CrIS NUCAPS
- **In response to these new requirements, a validation strategy was devised** with preliminary validation of NUCAPS carbon trace gas EDRs conducted leveraging global truth datasets, including
  - **ECMWF from Global Focus Days** (Cal/Val Method #1)
  - **Satellite EDRs from Global Focus Days** (Cal/Val Method #2)
    - **Aqua AIRS v6**
      - **Ideally suited** given same orbit, retrieves the same constituents as NUCAPS, including total column CO and CH_4; offline v6 runs for CO_2 were made available courtesy of Ed Olsen
    - **OCO-2, MLS** (future plans)
    - Of high value for **inter-satellite stability**
  - **Total Carbon Column Observing Network (TCCON)** (*Wunch et al.* 2011) Cal/Val Method #3
    - Global network of ground-based FTS that accurately measure total column abundances of CO_2, CO, CH_4, N_2O trace gases
    - Provides "spot checks" for verifying NUCAPS and AIRS
- **Collocation Methodology**
  - 2-D linearly interpolated FOR – used for AIRS versus NUCAPS
  - "VALAR method" used for NUCAPS/AIRS versus TCCON
    - Include all FOR within threshold radius (150 km for 1 Focus Day; 100 km for 2 Focus Days); time window (±6 hours) versus mean TCCON
  - Quality assurance (QA)
    - NUCAPS IR+MW quality flag and AIRS trace gas quality flags
    - NUCAPS trace gas QA flags have not yet been developed, but possible criteria include DoF, Chi-Square and EDR thresholds

- **For NUCAPS CO_2**, stats are performed simply for atmospheric column averages (in PPMV)
- **For NUCAPS CO, CH_4,** profile EDRs on 100 RTA layers are integrated to obtain total column abundances (molecules/cm2) (e.g., *Nalli et al.* 2013)

$$\Sigma_x(z) \equiv \int_{z_t}^{z} N_x(z')\,\mathrm{d}z'$$

$$\Longrightarrow \quad \Sigma_x(z_s) \approx \mathcal{F}_{\mathrm{BL}}\,\overline{N}_{x,L_b}\,\delta z_{L_b} + \sum_{L}^{L_b-1} \overline{N}_{x,L}\,\delta z_L$$

- **TCCON CO, CH_4** (in dry mole fractions, ppm) are converted to total column abundance Σ_i (molecules/cm²) using the following formula

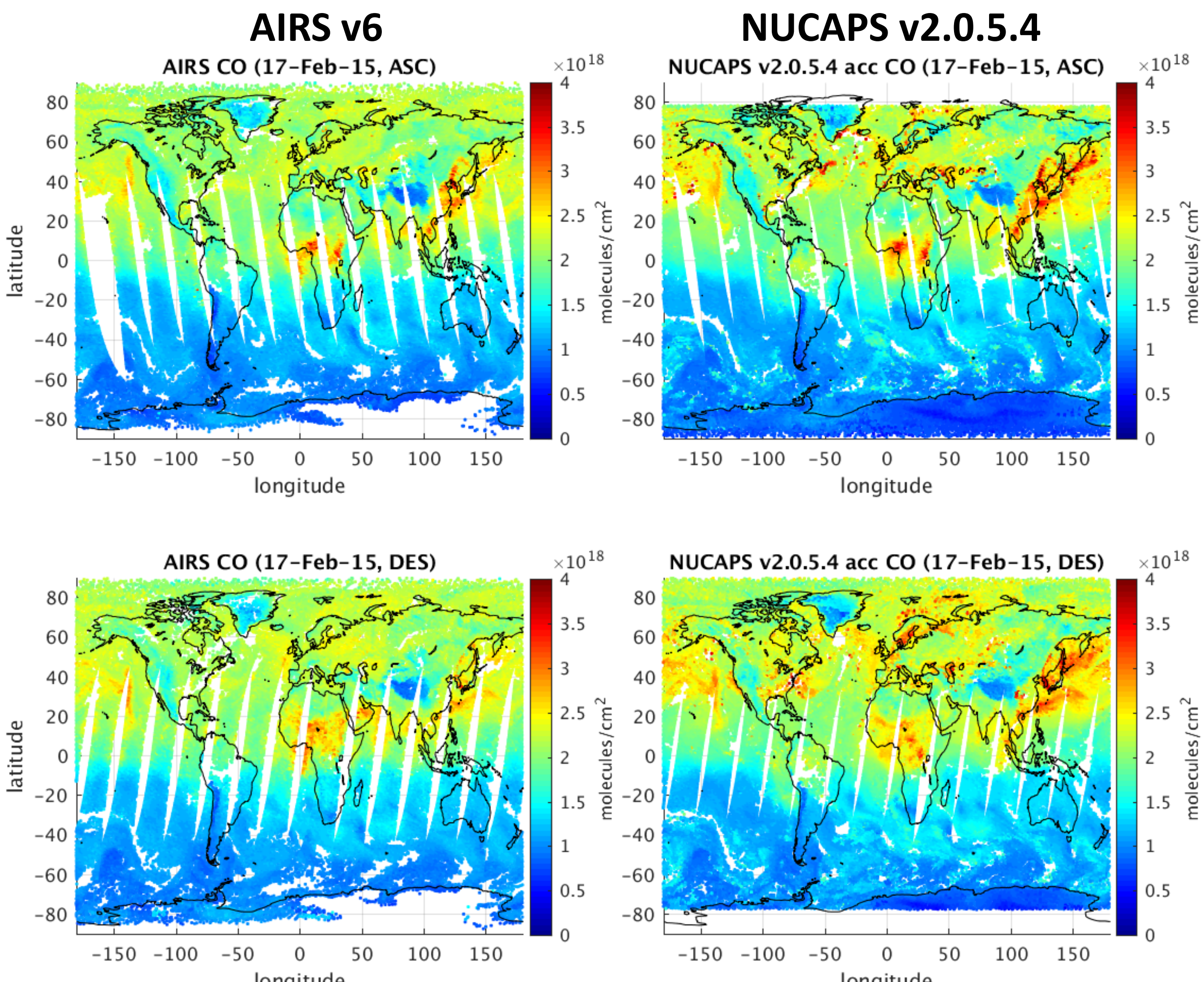
$$\Sigma_i(z_s) = x_i\left[\frac{N_A\, p_s}{g\, M_{dry}} - \varepsilon\,\Sigma_w(z_s)\right]$$

where x_i is the TCCON-measured dry mole fraction for species i, and Σ_w is the H_2O column abundance (provided by NUCAPS retrieval).

- A more rigorous methodology employing the **TCCON averaging kernels** is currently being researched and will be the subject of near-future work

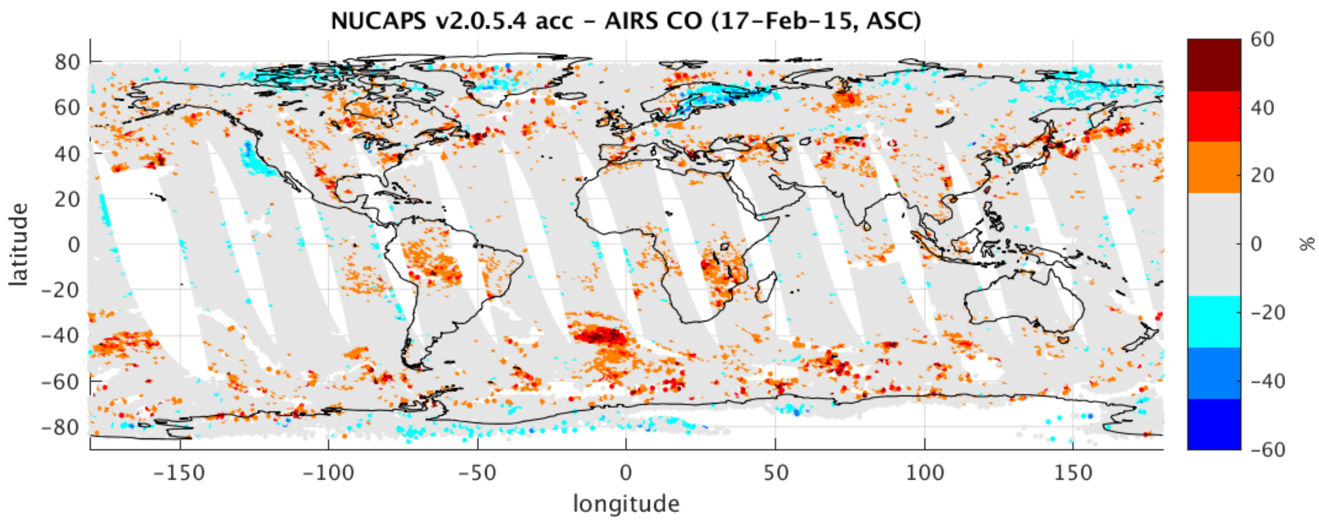
Total Column Carbon Monoxide (CO) EDRs

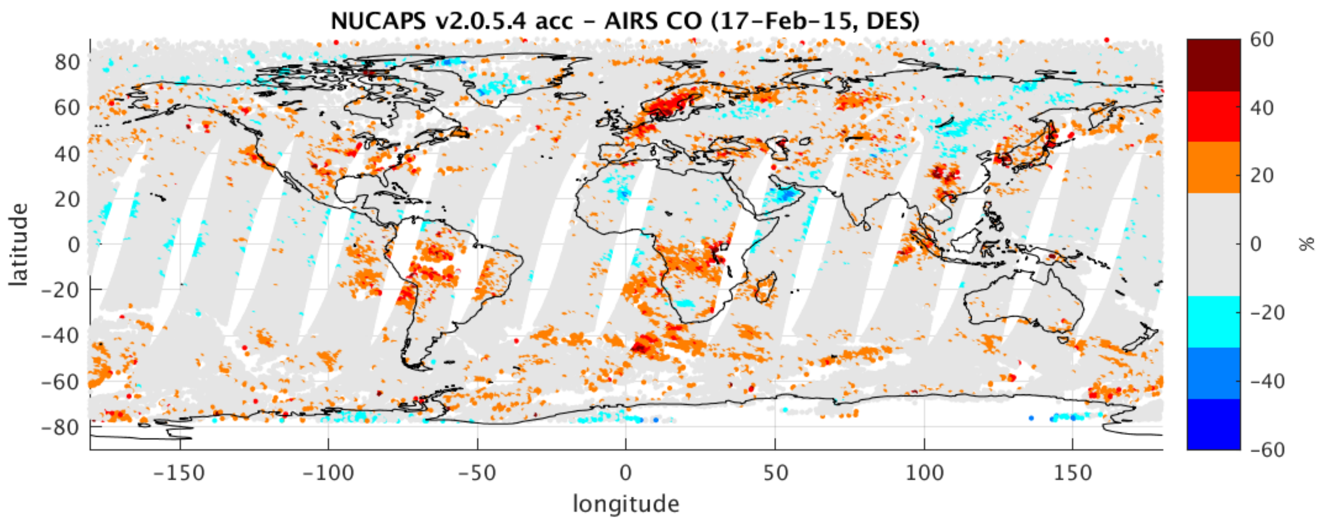
17 Feb 2015 Focus Day, All Cases



NUCAPS v2.0.5.4 CO – AIRS v6 CO

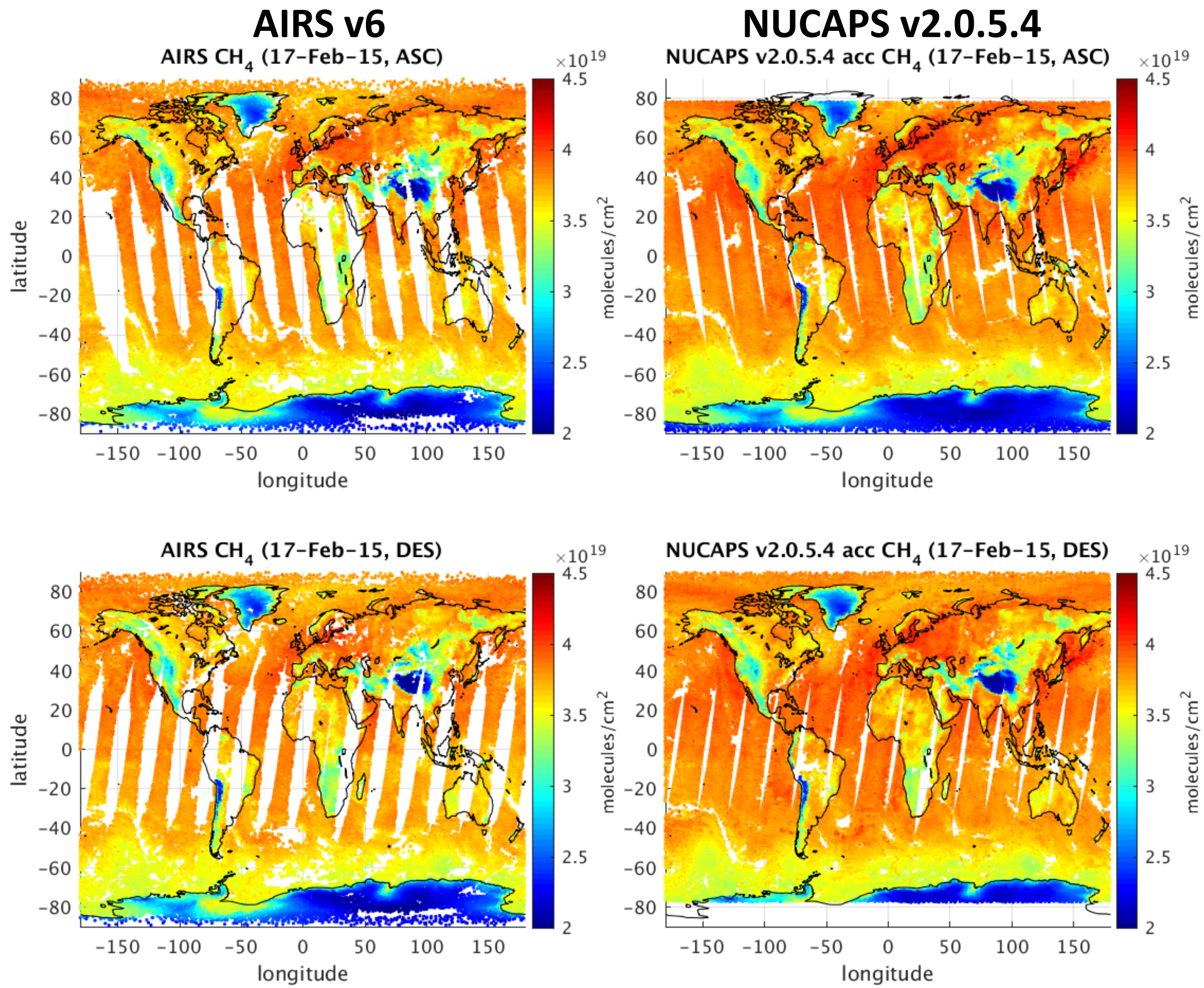
17 Feb 2015 Focus Day, Accepted Cases





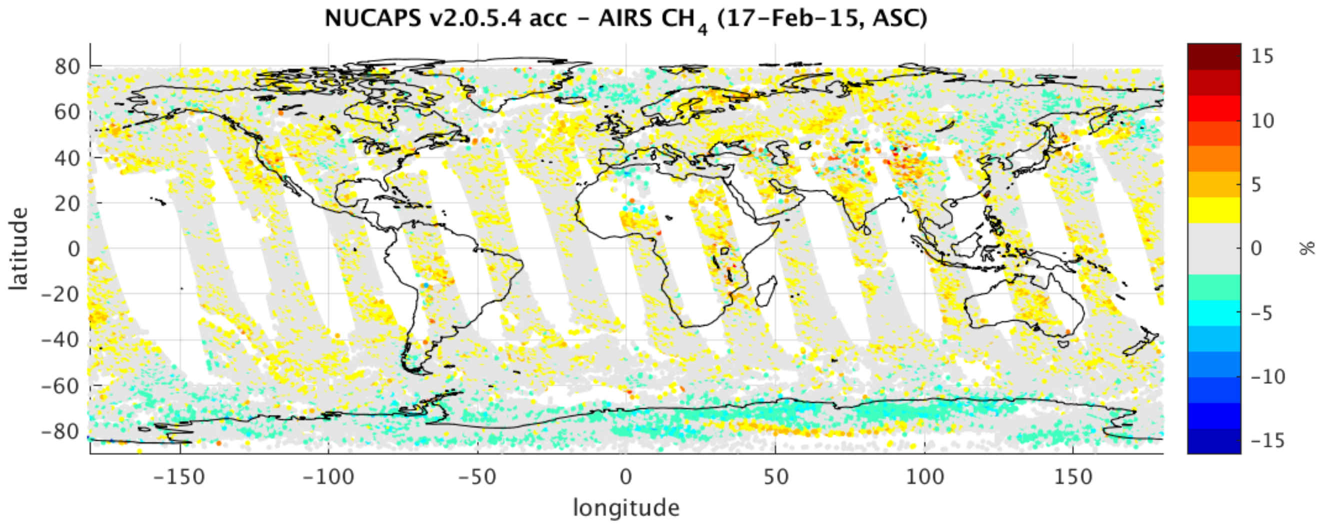
Total Column Methane (CH_4) EDRs

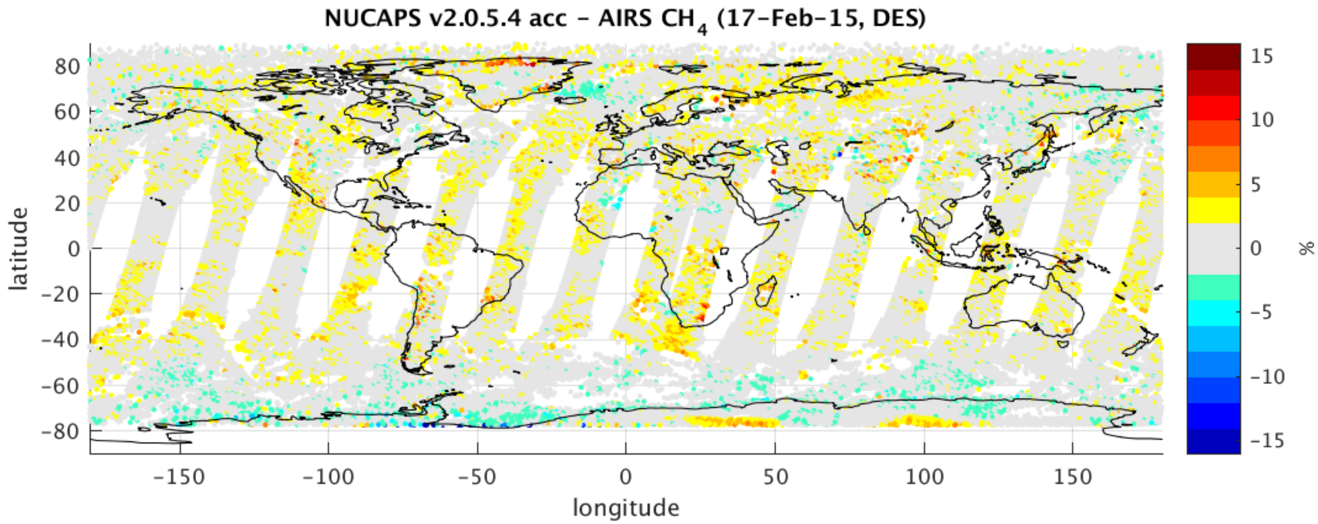
17 Feb 2015 Focus Day, All Cases



NUCAPS v2.0.5.4 CH_4 – AIRS v6 CH_4

17 Feb 2015 Focus Day, Accepted Cases

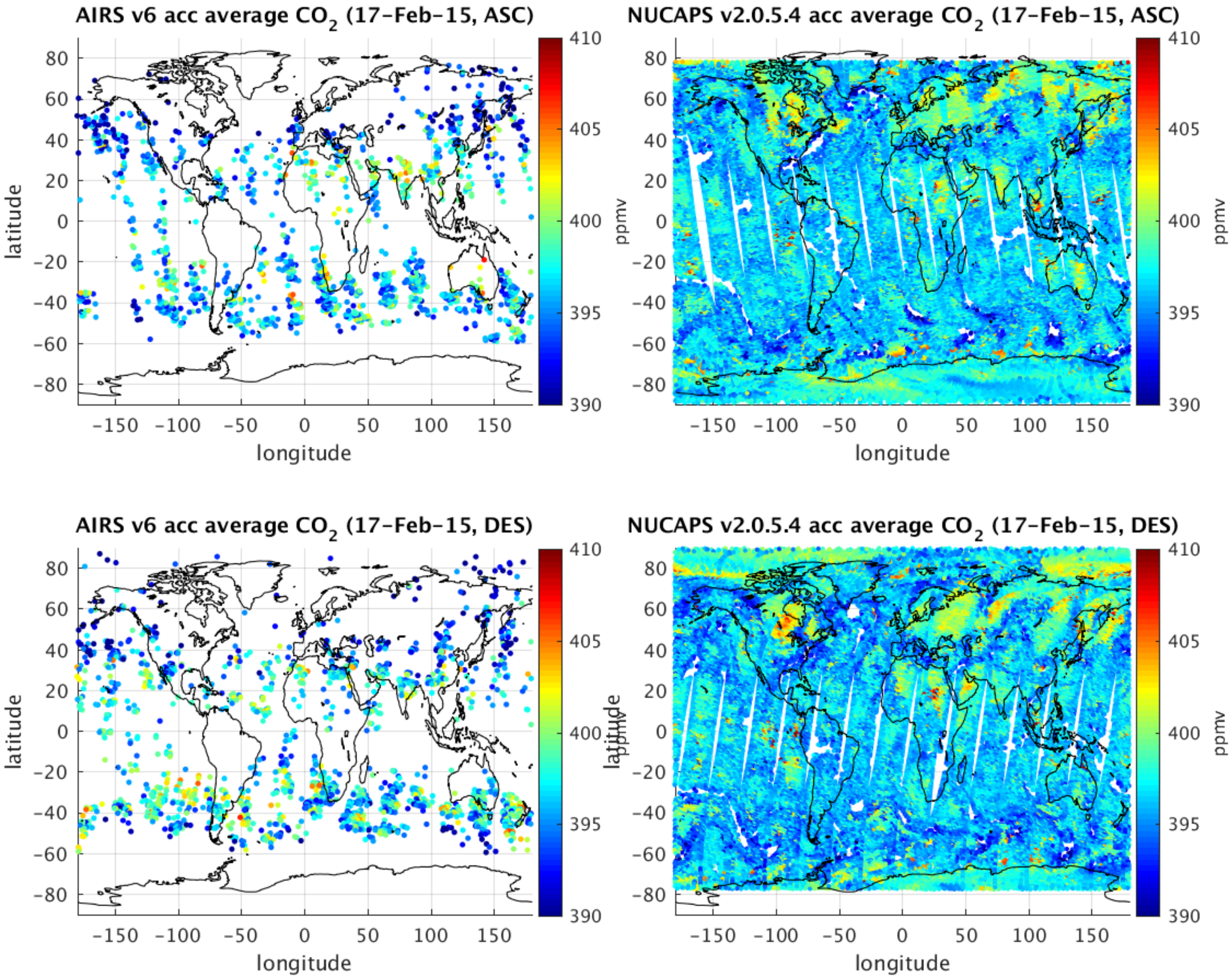




Total Column Carbon Dioxide (CH_2) EDRs

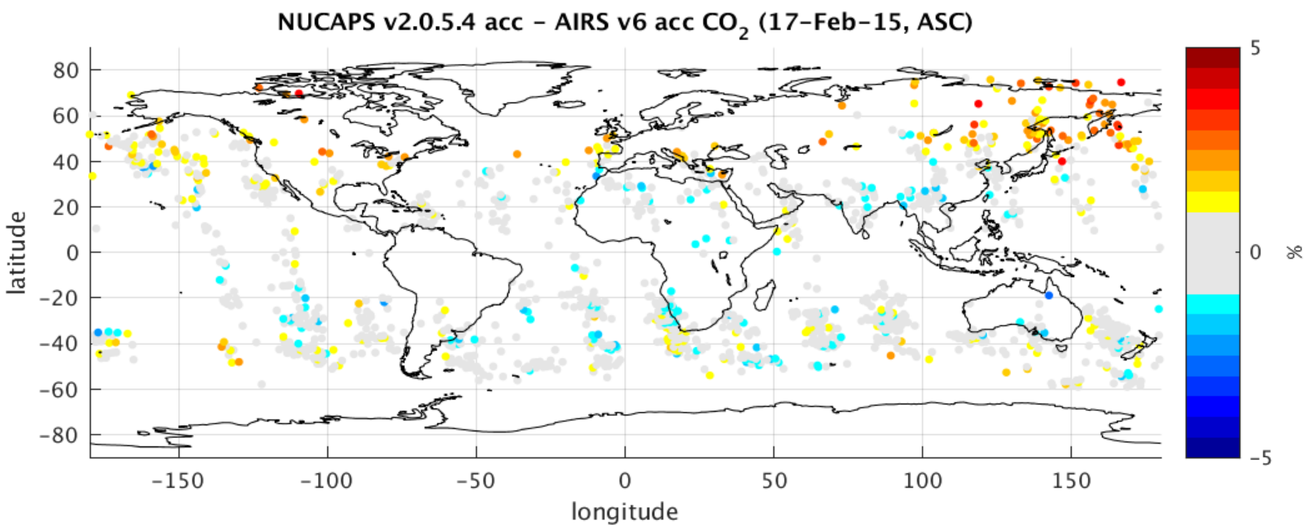
17 Feb 2015 Focus Day, All Cases

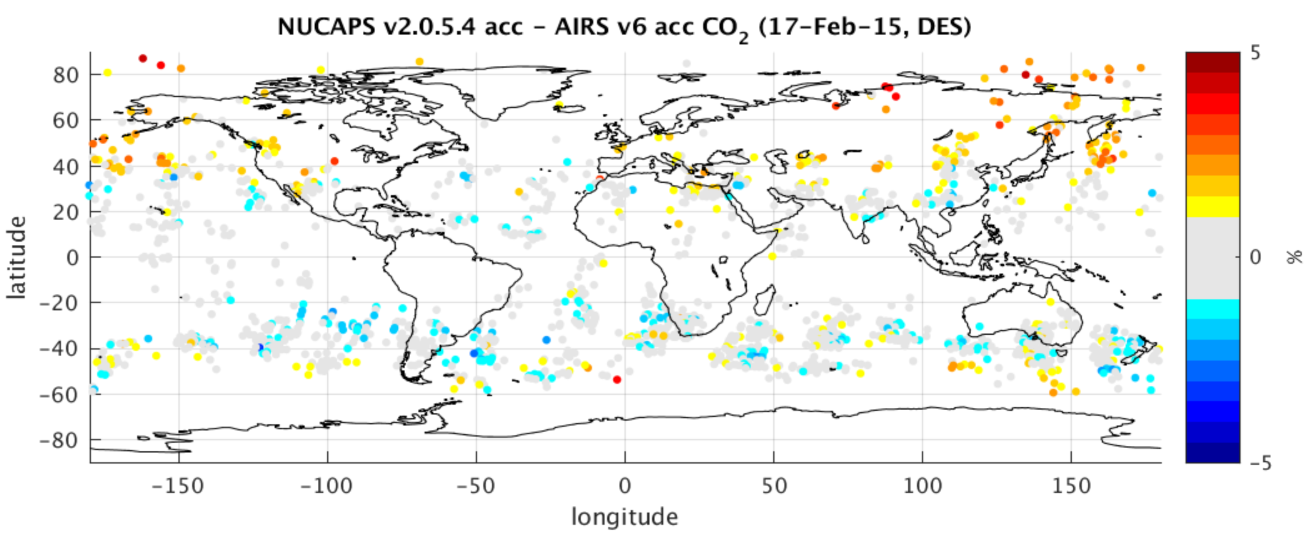
AIRS v6 **NUCAPS v2.0.5.4**



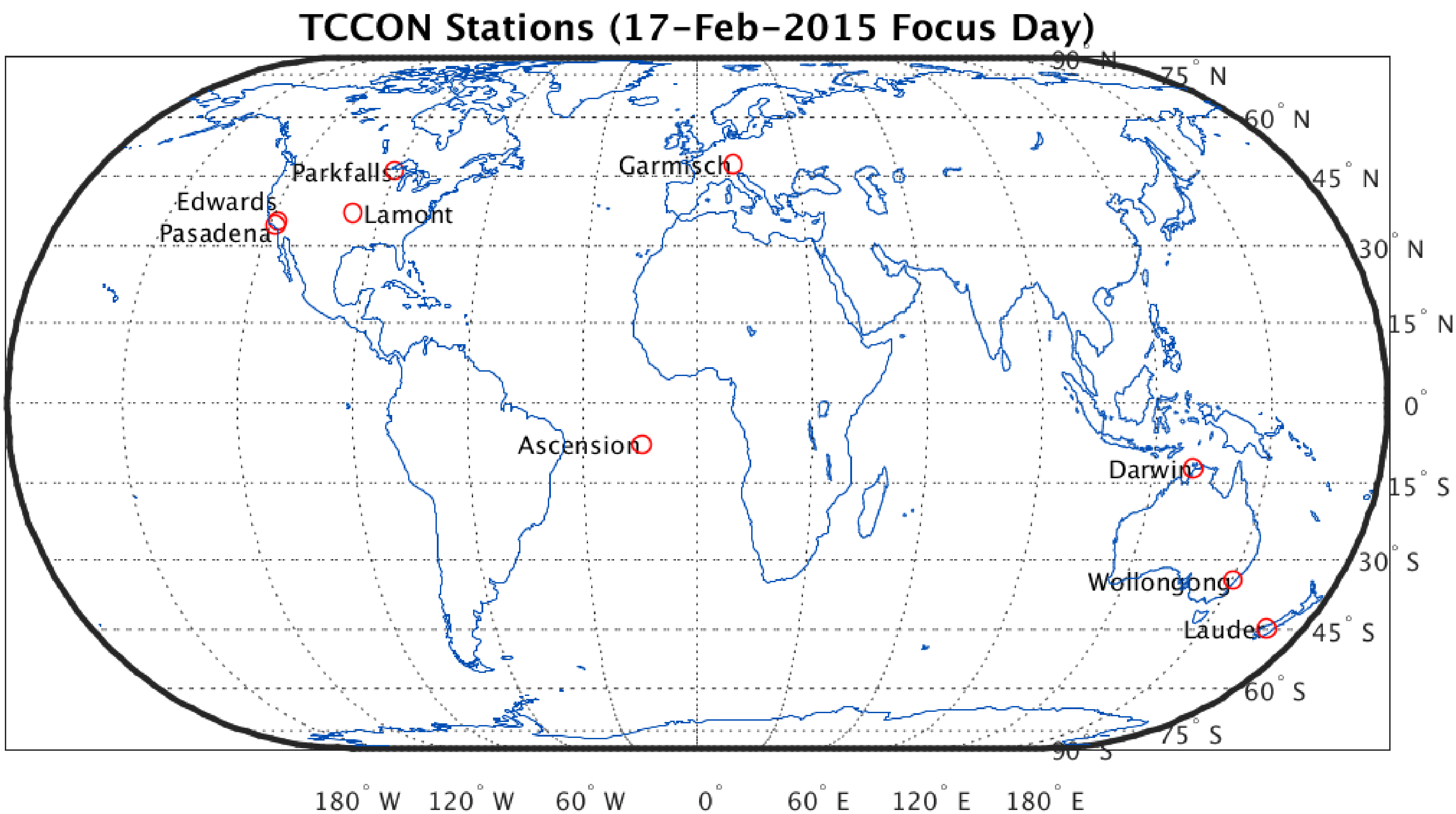
NUCAPS v2.0.5.4 CO_2 – AIRS v6 CO_2

17 Feb 2015 Focus Day, Accepted Cases





Total Carbon Column Observing Network (TCCON)
17 Feb 2015 Focus Day

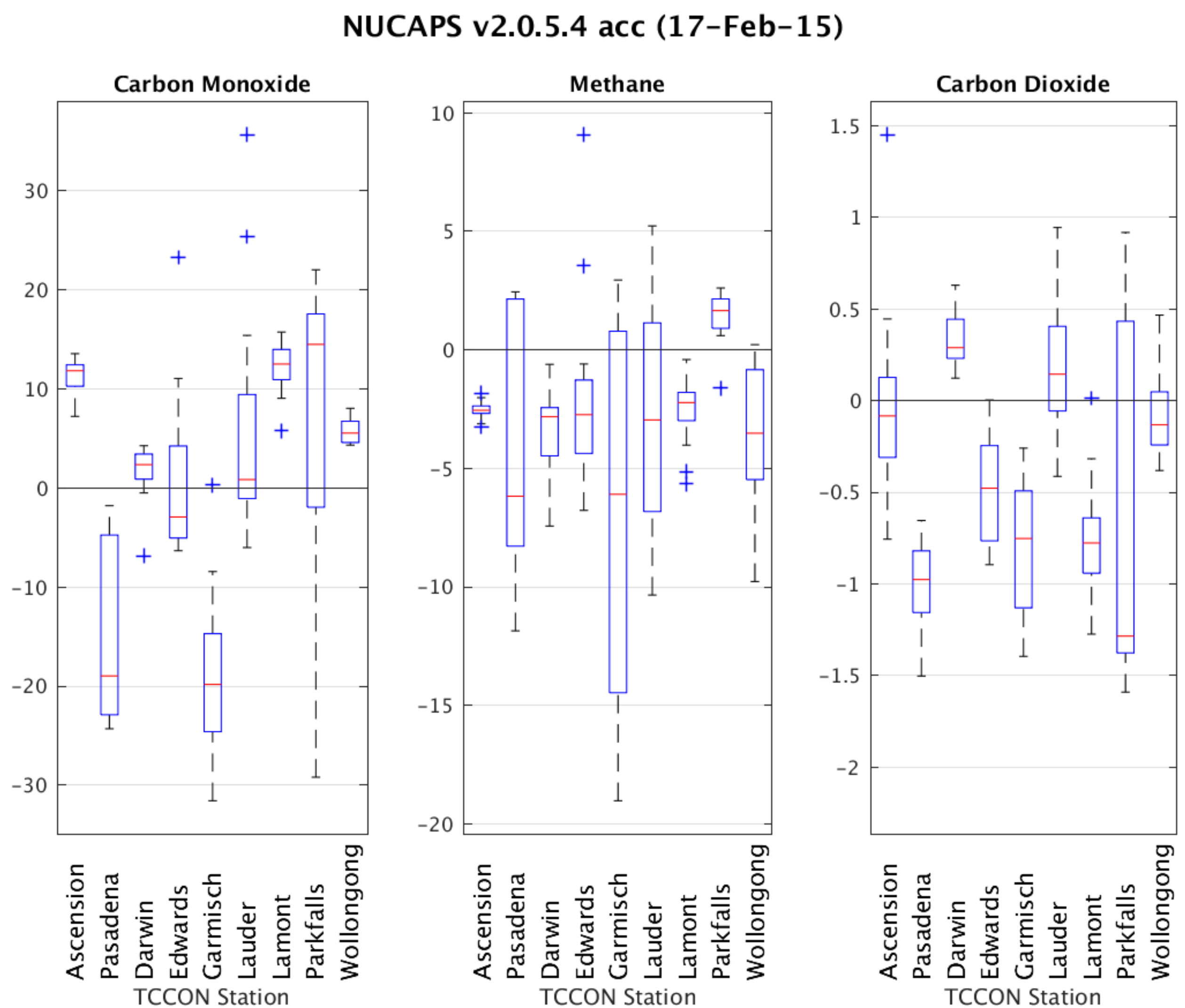


TCCON (*Wunch et al.* 2011)

NUCAPS-AIRS vs TCCON Box Plots
17 Feb 2015 Focus Day

All FOR within threshold radius (150 km)

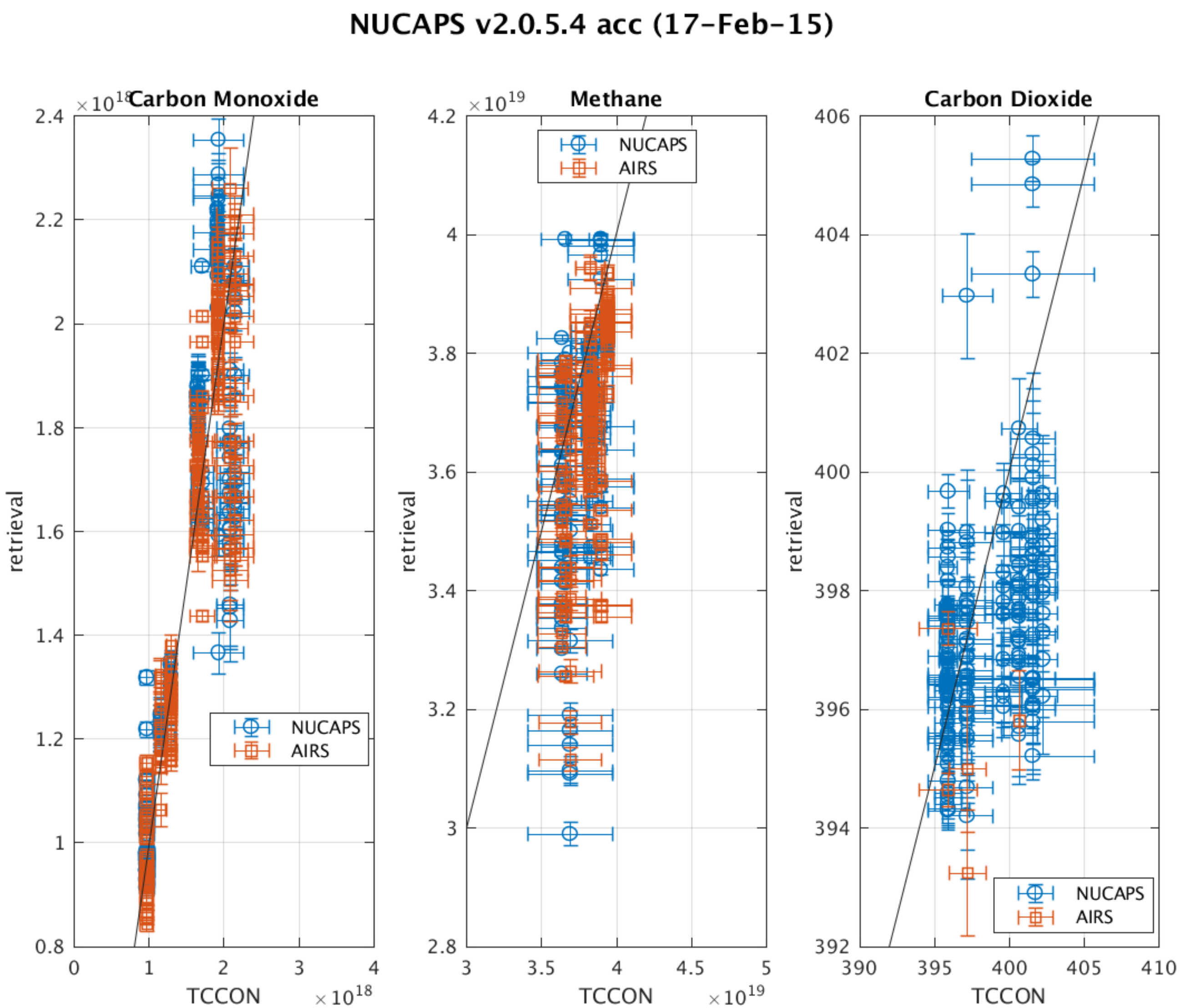
Time window (±6 hours) versus mean TCCON



NUCAPS-AIRS vs TCCON Box Plots
17 Feb 2015 Focus Day

All FOR within threshold radius (150 km)

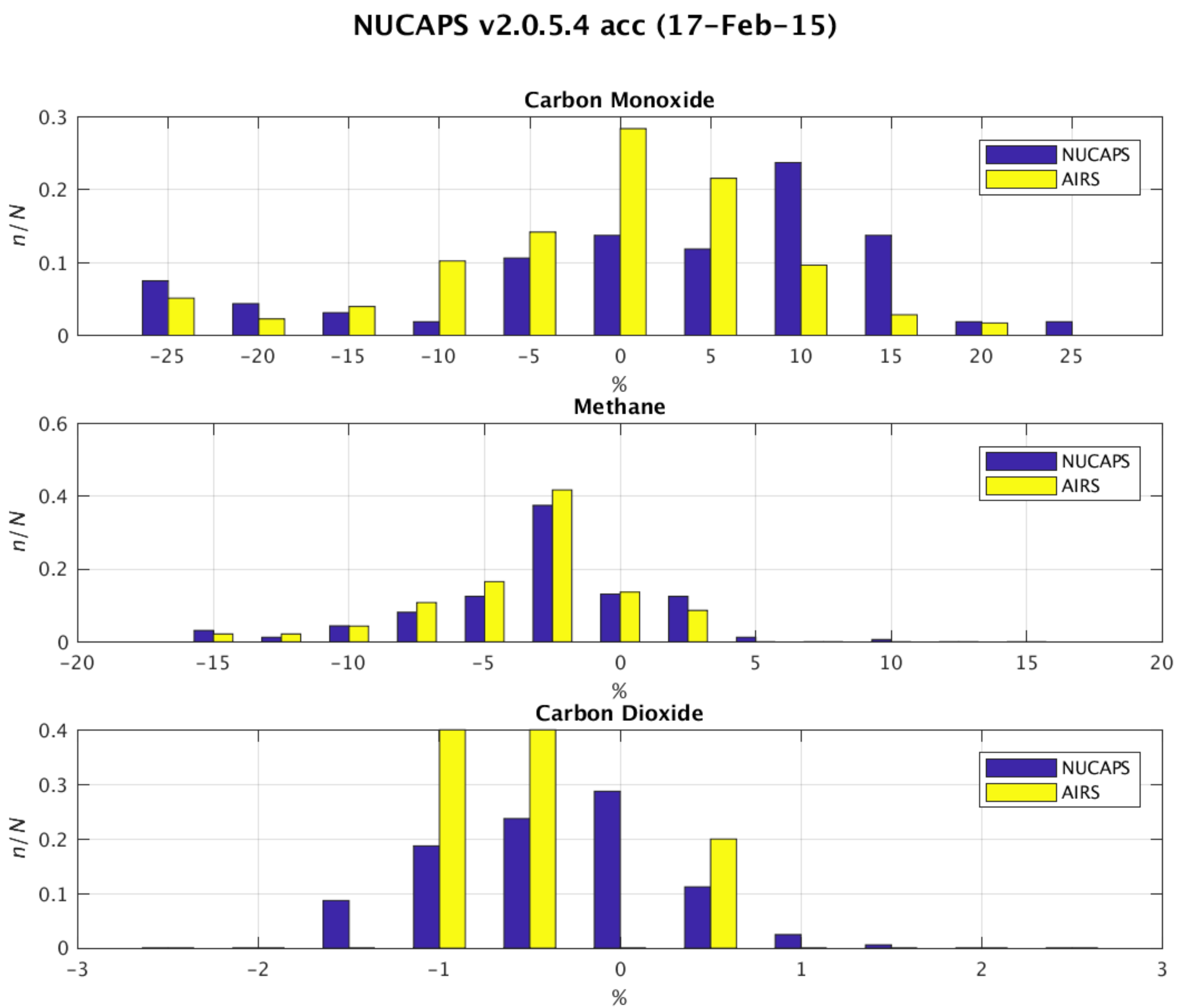
Time window (±6 hours) versus mean TCCON



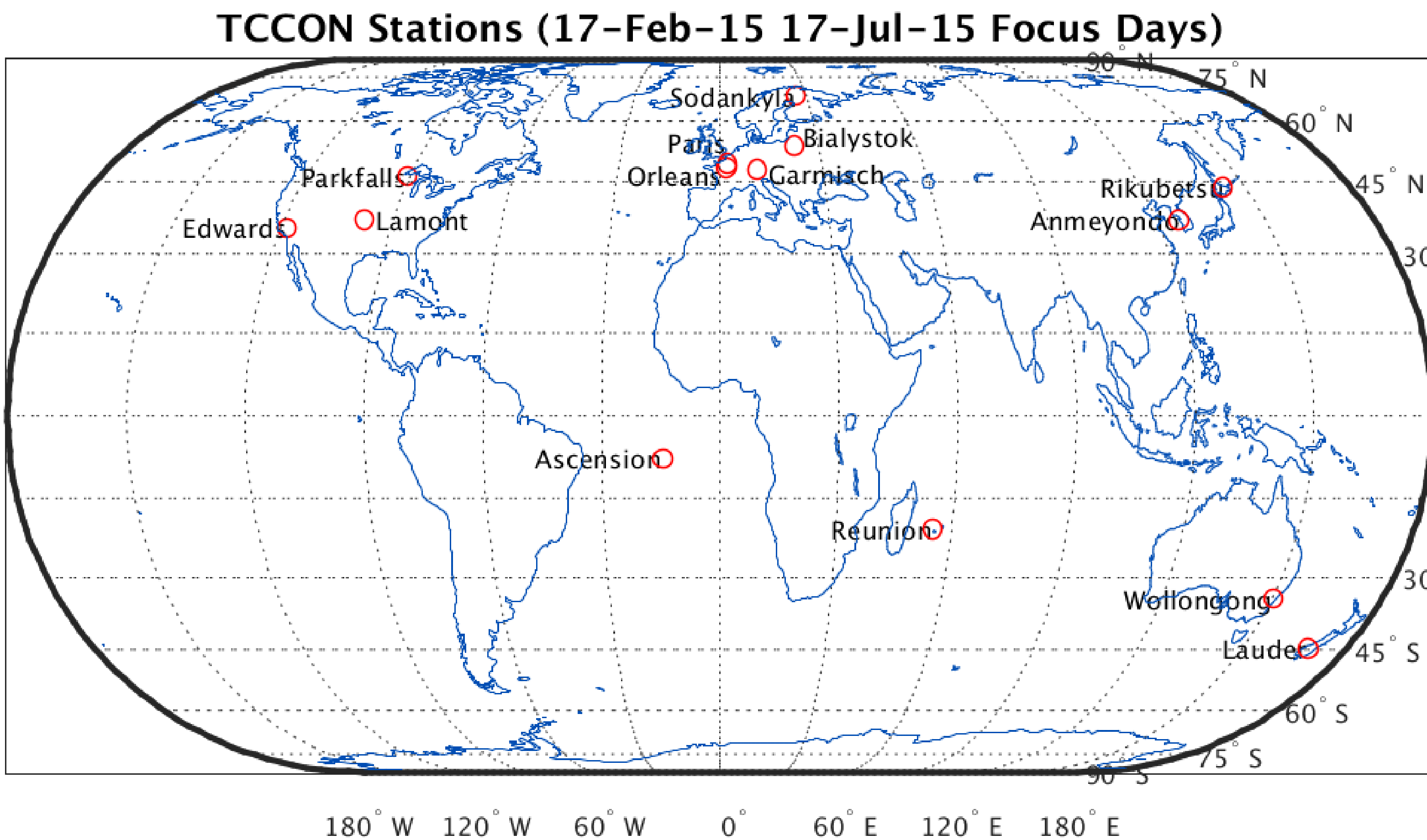
NUCAPS-AIRS vs TCCON Histograms
17 Feb 2015 Focus Day

All FOR within threshold radius (150 km)

Time window (±6 hours) versus mean TCCON



Total Carbon Column Observing Network (TCCON)
17 Feb 2015 and 17 Jul 2015 Focus Days

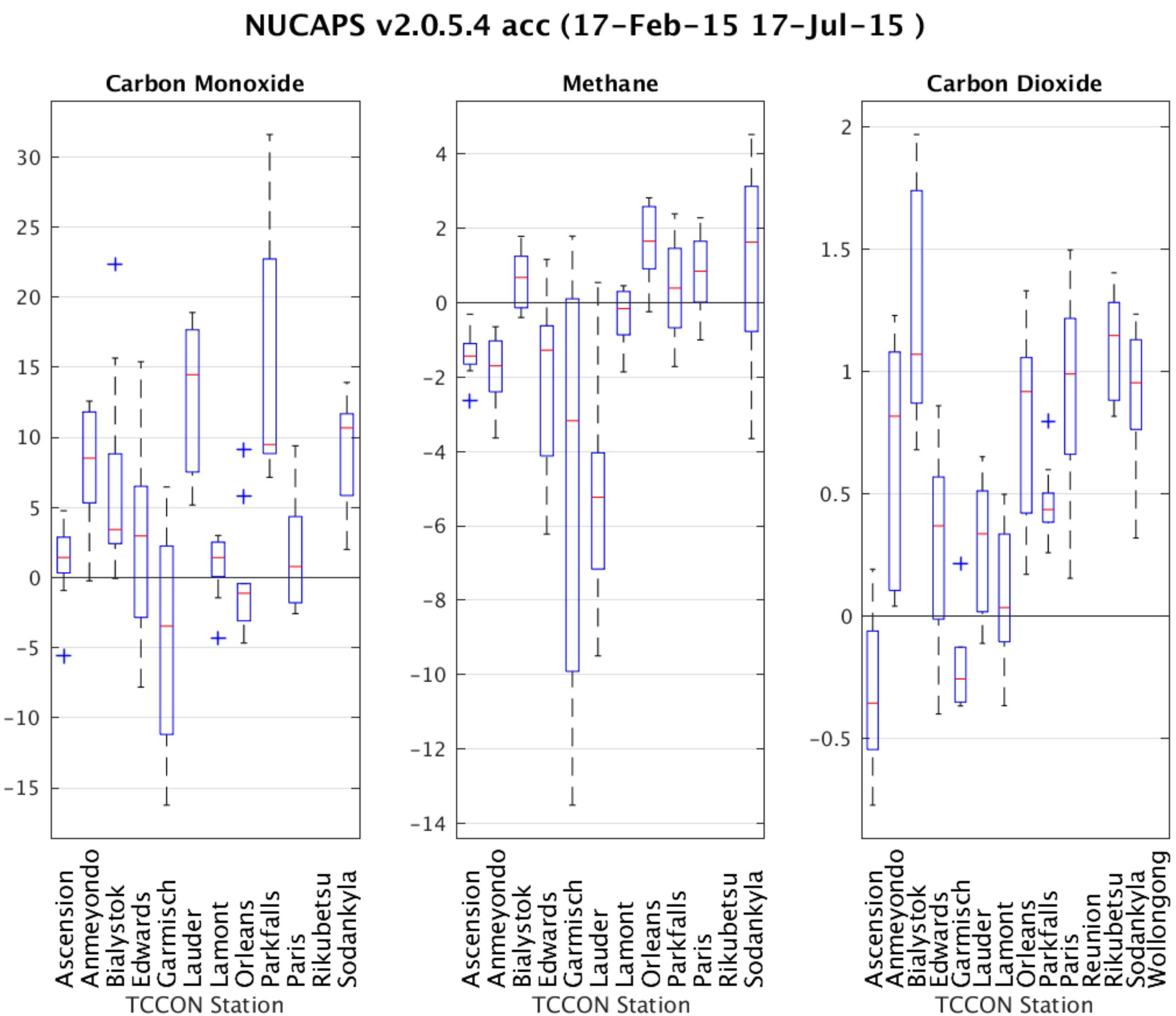


TCCON (*Wunch et al.* 2011)

NUCAPS vs TCCON Boxplots
17 Feb 2015 and 17 Jul 2015 Focus Days

All FOR within threshold radius (100 km)

Time window (±6 hours) versus mean TCCON

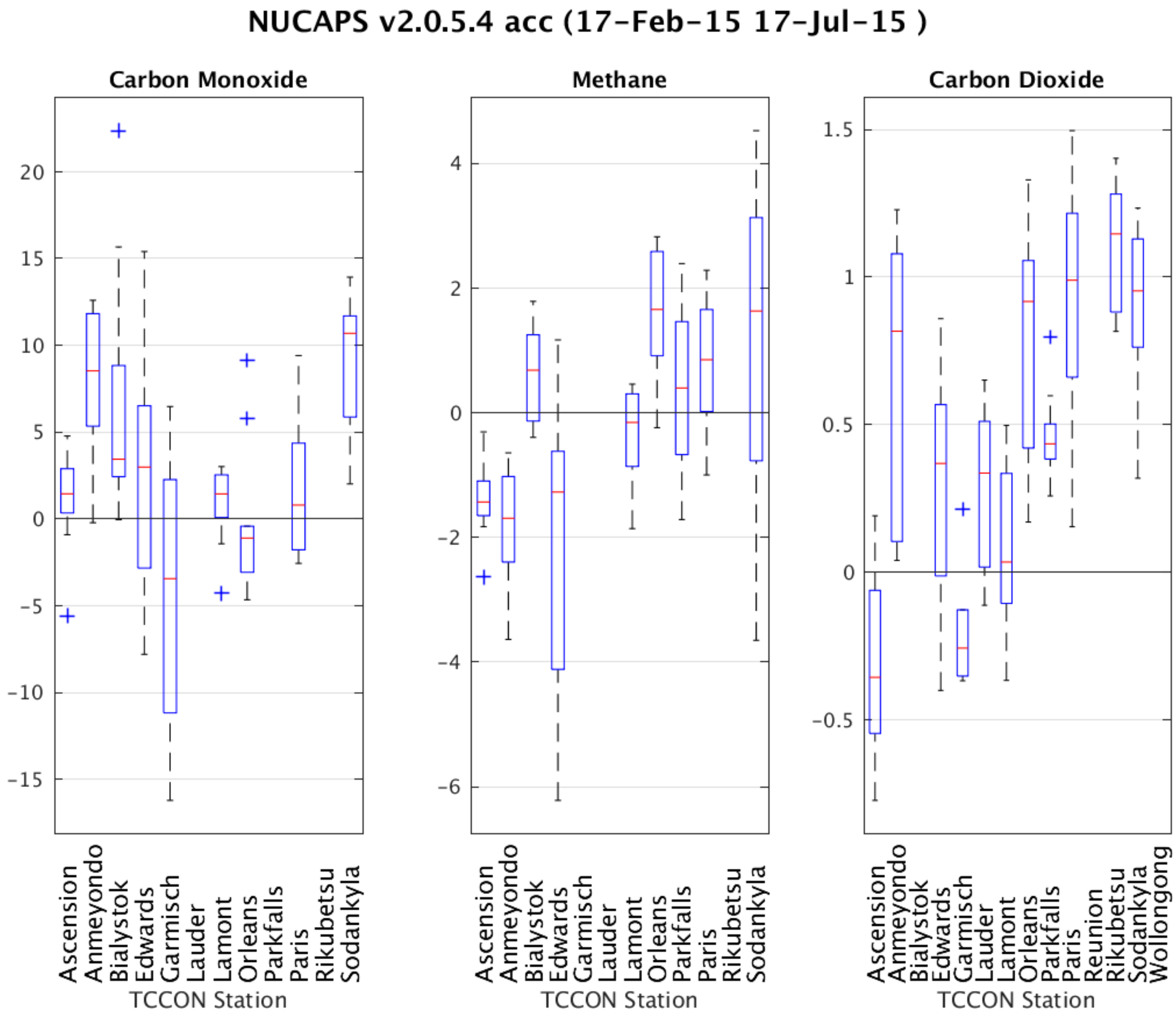


NUCAPS vs TCCON Boxplots
17 Feb 2015 and 17 Jul 2015 Focus Days

All FOR within threshold radius (100 km)

Time window (±6 hours) versus mean TCCON

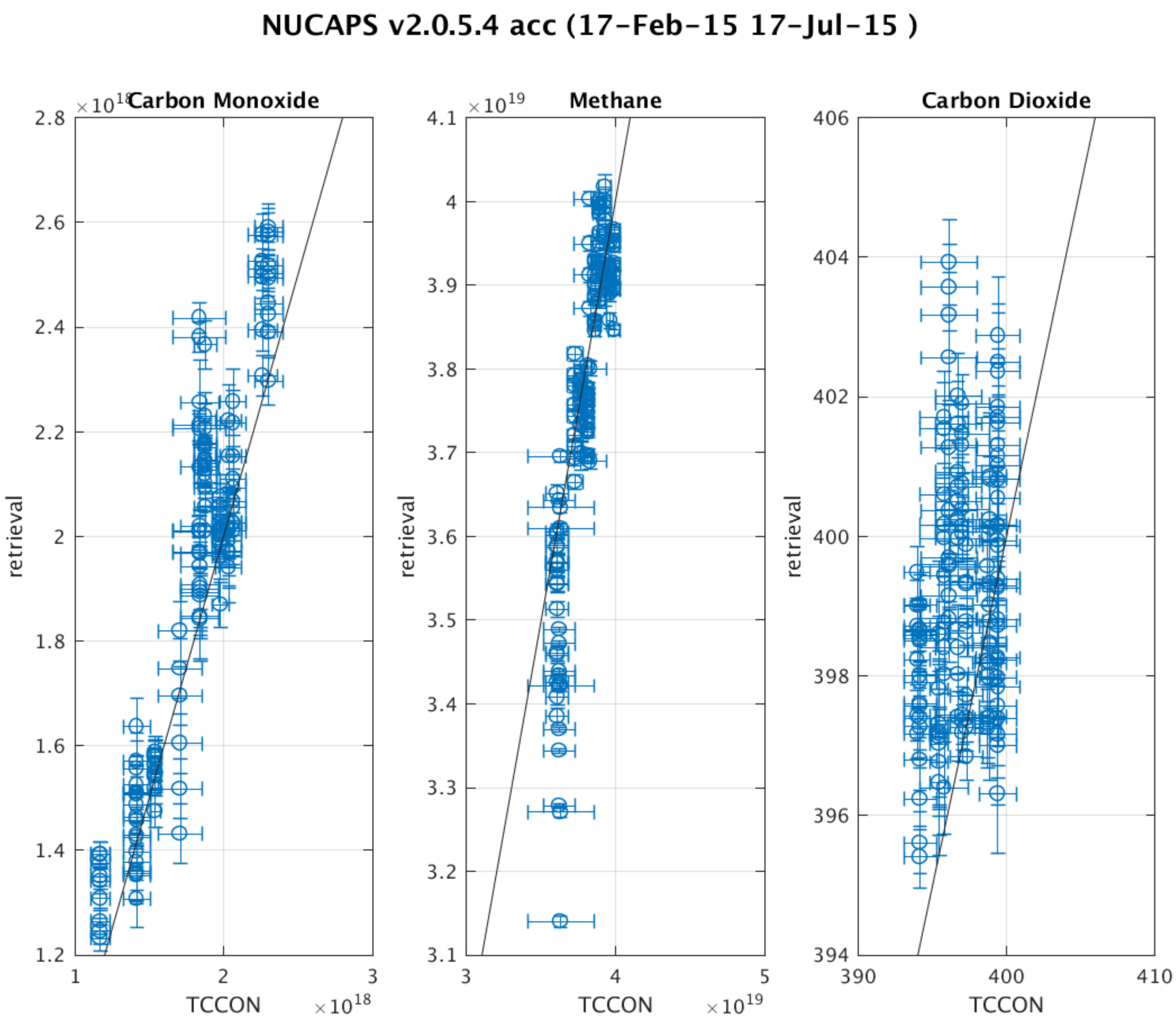
Outlier sites removed



NUCAPS vs TCCON Scatterplots
17 Feb 2015 and 17 Jul 2015 Focus Days

All FOR within threshold radius (100 km)

Time window (±6 hours) versus mean TCCON

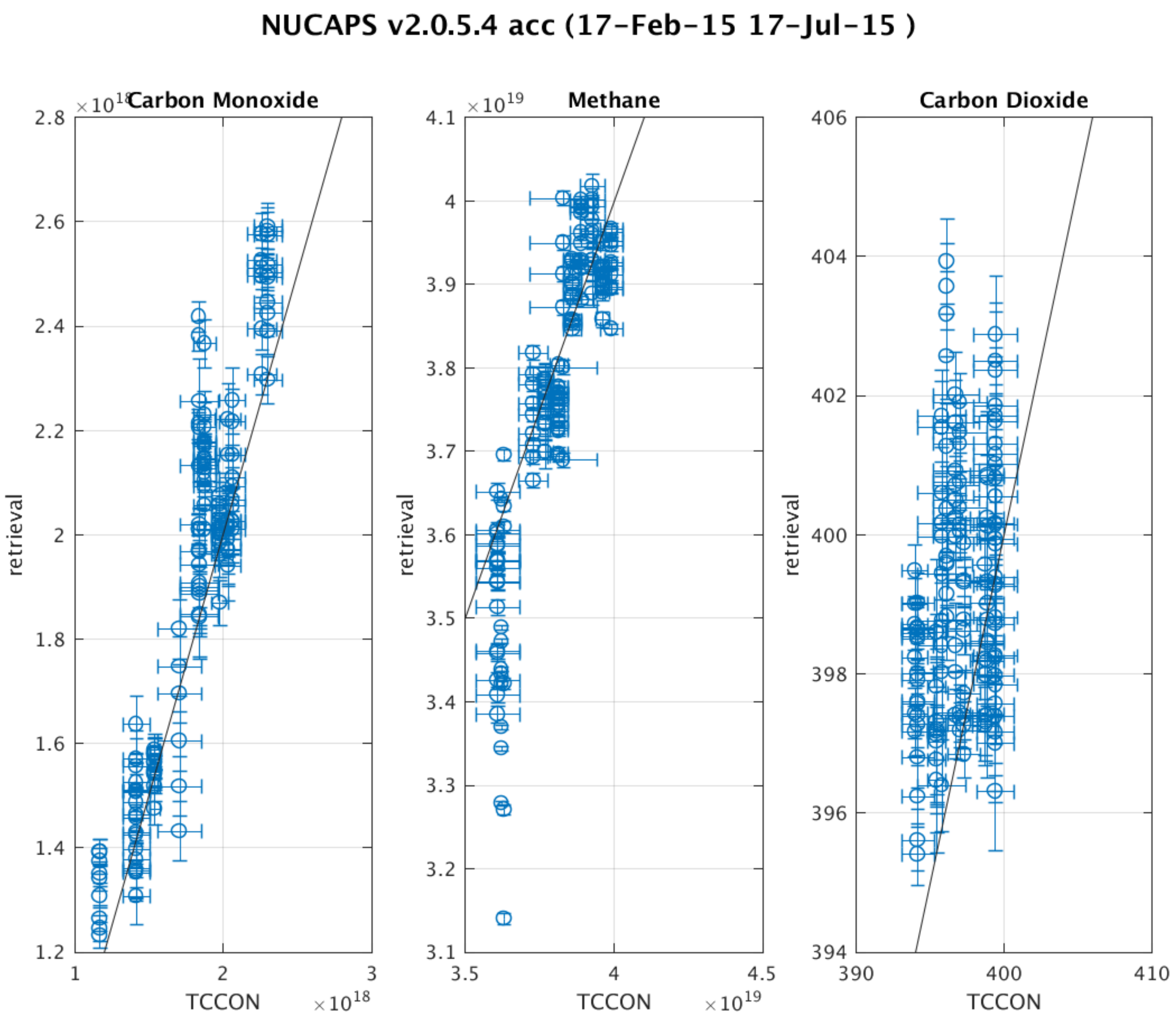


NUCAPS vs TCCON Scatterplots
17 Feb 2015 and 17 Jul 2015 Focus Days

All FOR within threshold radius (100 km)

Time window (±6 hours) versus mean TCCON

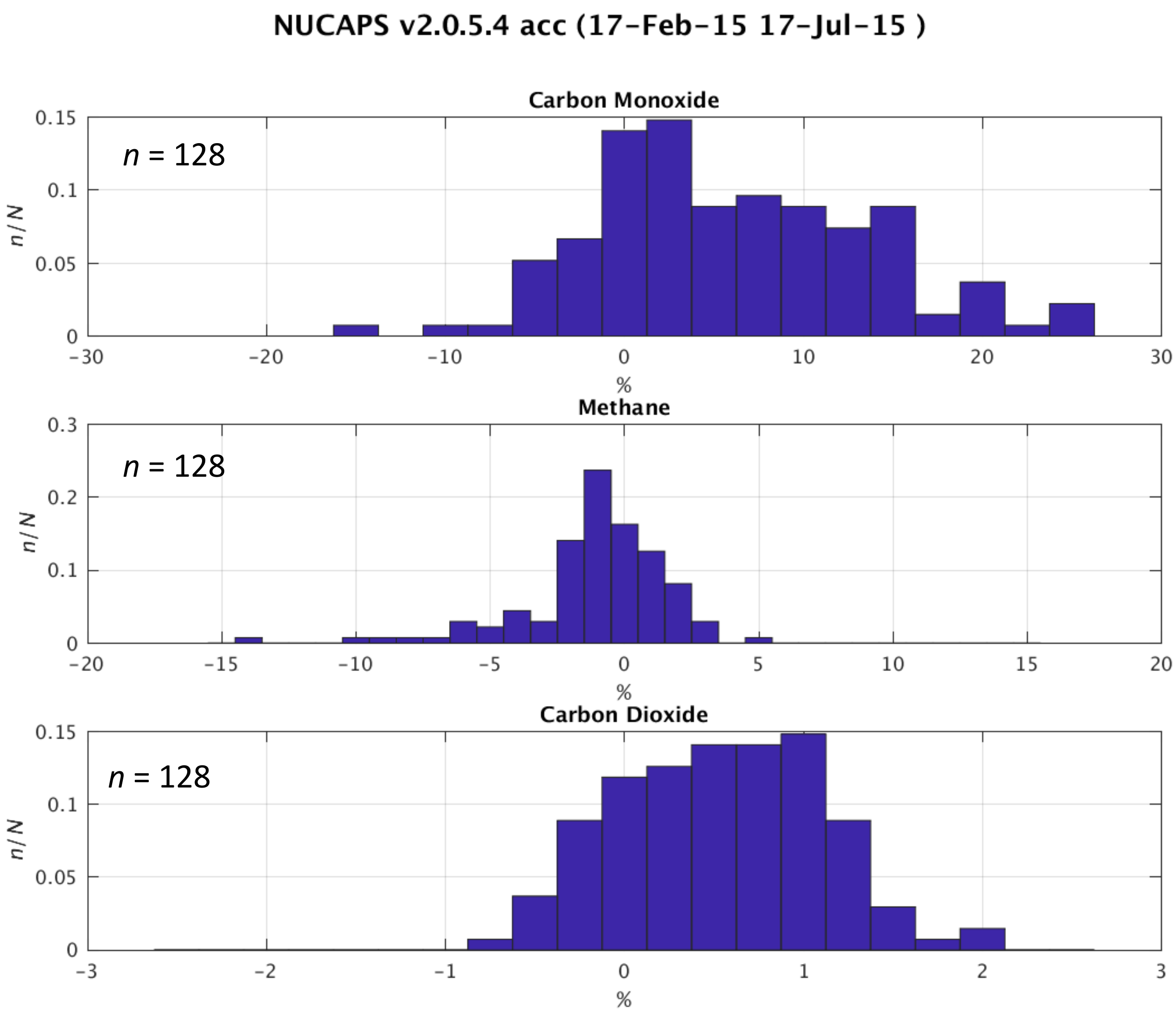
Outlier sites removed



NUCAPS vs TCCON Histograms
17 Feb 2015 and 17 Jul 2015 Focus Days

All FOR within threshold radius (100 km)

Time window (±6 hours) versus mean TCCON

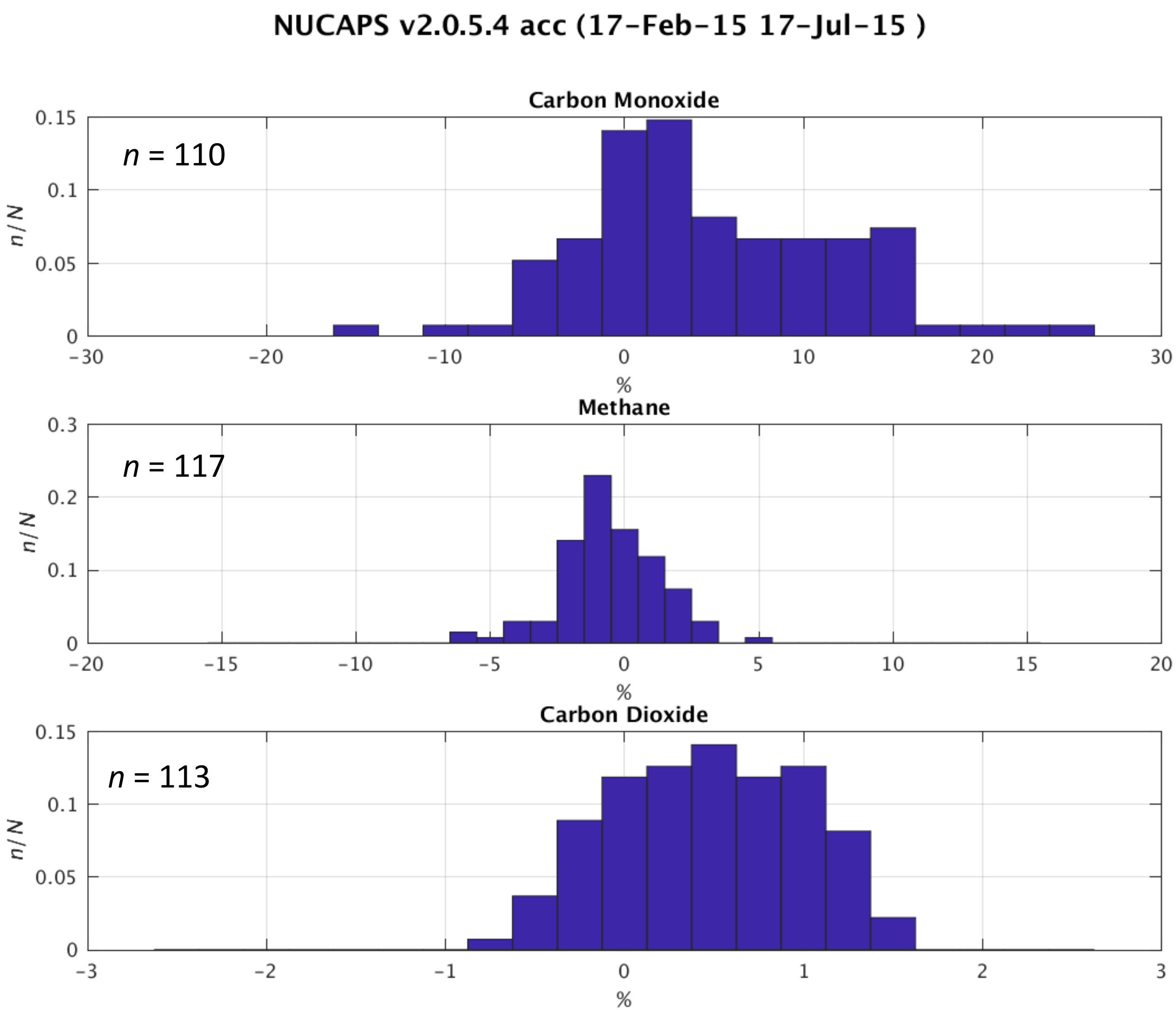


NUCAPS vs TCCON Histograms
17 Feb 2015 and 17 Jul 2015 Focus Days

All FOR within threshold radius (100 km)

Time window (±6 hours) versus mean TCCON

Outlier sites removed



NUCAPS v2.0 FSR Trace Gas Summary Stats

	TCCON Baseline One Focus Day *N* = 151			TCCON Baseline Two Focus Days *N* = 128			AIRS Baseline One Focus Day *N* = *O*(100,000)		
Trace Gas EDR	**BIAS (%)**	**STD (%)**	**RMS (%)**	**BIAS (%)**	**STD (%)**	**RMS (%)**	**BIAS (%)**	**STD (%)**	**RMS (%)**
CO	**+2.1** (±5.0)	**12.9** (15.0)	13.1	**+6.0** (±5.0)	**8.0** (15.0)	10.0	**+3.0** **+3.3** **(±5.0)**	**9.2** **8.9** (15.0)	9.7 9.5
CO_2	**−0.3** (±1.0)	**0.6** (0.5)	0.7	**+0.5** (±1.0)	**0.6** (0.5)	0.8	**+0.2** **+0.1** **(±1.0)**	**0.9** **1.0** (0.5)	0.9 1.0
CH_4	**−3.0** (±4.0)	**4.4** (1.0)	5.3	**−1.1** (±4.0)	**2.6** (1.0)	2.9	**+0.6** **+0.8** (±4.0)	**1.7** **1.6** (1.0)	1.8 1.8

Yield = 83.4% | Yield = 83.7% | Yield = 83.4%

NUCAPS v2.0 FSR Trace Gas Summary Stats

Trace Gas EDR	TCCON Baseline One Focus Day *N* = 151			TCCON Baseline Two Focus Days Outlier Sites Removed			AIRS Baseline One Focus Day *N* = *O*(100,000)		
	BIAS (%)	STD (%)	RMS (%)	BIAS (%)	STD (%)	RMS (%)	BIAS (%)	STD (%)	RMS (%)
CO	**+2.1** (±5.0)	**12.9** (15.0)	13.1	**+4.7** (±5.0)	**7.1** (15.0)	8.5	**+3.0** **+3.3** **(±5.0)**	**9.2** **8.9** (15.0)	9.7 9.5
CO_2	**−0.3** (±1.0)	**0.6** (0.5)	0.7	**+0.5** (±1.0)	**0.5** (0.5)	0.7	**+0.2** **+0.1** **(±1.0)**	**0.9** **1.0** (0.5)	0.9 1.0
CH_4	**−3.0** (±4.0)	**4.4** (1.0)	5.3	**−0.6** (±4.0)	**1.8** (1.0)	1.9	**+0.6** **+0.8** (±4.0)	**1.7** **1.6** (1.0)	1.8 1.8

Yield = 83.4% Yield = 83.7% Yield = 83.4%

NUCAPS EDR Maturity Status

Slide courtesy of Lihang Zhou, STAR/JPSS

S-NPP EDR Validated Maturity Oct. 2016-Current: NUCAPS

Sensor	Product	Priority	Validated Maturity Review Date & Status		Review Panel Recommendations
CrIS/ATMS	Atm. Vertical Moisture Profile (AVMP)	3	*	✓ V	September 2014
CrIS/ATMS	Atm. Vertical Temperature Profile (AVTP)	3	*	✓ V	September 2014
CrIS/ATMS	Ozone Profile EDR	3	Oct-2016	✓ V	Panel recommended the following: (1) Work with EMC and NWS on user applications (2) Validate against OMPS NP data (3) Extend validation to more ozonesondes
CrIS	Outgoing Longwave Radiation	3	Oct-2016	✓ V	Panel recommended the following: (1) Investigate the use of VIIRS for helping to understand the differences between OLR from CrIS and CERES. (2) Compare anomaly events from CERES OLR (e.g. ENSO, MJO) to CrIS OLR data (3) Provide information about how algorithm will be updated to utilize CrIS FS data
CrIS/ATMS	Carbon Monoxide	4	&	✓ P	Validated Maturity Review for Fall 2017
CrIS/ATMS	Carbon Dioxide	4	&	✓ P	Validated Maturity Review for Fall 2017
CrIS/ATMS	Methane	4	&	✓ P	Validated Maturity Review for Fall 2017

*Product reached validated maturity in September 2014.

&Product reached provisional maturity in January 2013. NUCAPS Phase IV/Part II ARR completed on July 6, 2017.

✓ Validated ✓ Provisional

5

O_3, CO, CH_4, CO_2 Trace Gas Summary

- **NUCAPS IR ozone (O_3) profile EDR products generally meet JPSS Level 1 requirements**
  - **NUCAPS (v1.5 NSR)** 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)
    - Statistics are comparable to those reported by *Divakarla et al.* (2008) for the AIRS Version 5 ozone product
  - **NUCAPS Phase 4 v2.0 FSR also meets Level 1 requirements** and have reached **Provisional Maturity** based upon coarse/broad layer statistical analyses versus global **Focus Day ECMWF**
    - Statistics are comparable to the ozonesonde-validated NUCAPS v1.5

- **Carbon trace gas EDR validation** versus program-established uncertainty specifications was a new task beginning with the transition to the FSR CrIS NUCAPS. Preliminary validation versus AIRS and TCCON truth datasets show the products are reasonably close to meeting JPSS Level 1 requirements

- **Next Steps / Future Work**
  - **Acquire additional Focus Days** to increase the TCCON data sample
    - Currently collecting 2 additional days for Spring and Autumn seasons
  - **Apply TCCON AKs**
  - Develop objective methods for eliminating TCCON "outlier sites"
    - **Check for altitude gradients** within collocation radii
    - **Check for land/sea boundaries** within collocation radii
  - **Develop Trace Gas EDR quality flags**
  - **Acquire field campaign datasets** (e.g., ATom)
  - **Further optimization of NUCAPS trace gas *a priori*** (viz., O_3, CH_4 and CO_2)

Status of NUCAPS FSR Trace Gas EDR Validation

THANK YOU! QUESTIONS?