Validation of the JPSS NOAA-Unique CrIS/ATMS Processing System (NUCAPS) Operational EDR

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Outline

- **JPSS Sounder EDR Cal/Val Overview**
  - JPSS EDR validation
  - CrIS/ATMS (CrIMSS) Sounder Operational EDR
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  - Validation Methodology
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  - JPSS S-NPP Validation Datasets
    - STAR Validation Archive (VALAR)
    - NOAA Products Validation System (NPROVS/NPROVS+)
- **NUCAPS EDR Product Validation**
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  - Trace Gas
    - Ozone profile EDR
  - Long-Term Monitoring (LTM)
- **Future Work**
  - SNPP ICV and LTM

Validation of NOAA-Unique Operational Sounder EDR

JPSS SOUNDER EDR CAL/VAL OVERVIEW

Intro: JPSS Sounder EDR Validation

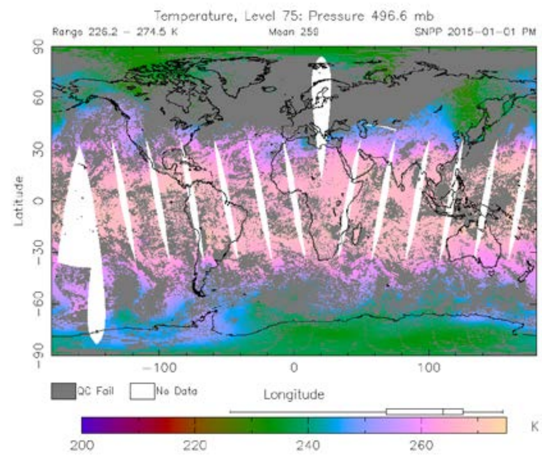
- **Validation** is "the process of ascribing uncertainties to these radiances and retrieved quantities through comparison with correlative observations" (*Fetzer et al.,* 2003).
  - EDR validation supports validation of SDRs and cloud-cleared radiances (a Level 2 product shown to have positive impact on NWP; e.g., *Le Marshall et al.,* 2008)
  - EDR validation enables development/improvement of algorithms
- **Users of sounder EDR observations** (AVTP, AVMP and trace gas) include
  - Weather Forecast Offices (AWIPS)
    - Nowcasting / severe weather
  - NOAA Data Centers (e.g., NGDC, CLASS)
  - Basic and applied science research/investigation (e.g., *Pagano et al.,* 2013)
- **JPSS Cal/Val Phases**
  - Pre-Launch / Early Orbit Checkout (EOC)
  - **Intensive Cal/Val (ICV)**
    - Validation of EDRs against multiple correlative datasets
  - **Long-Term Monitoring (LTM)**
    - Characterization of all EDR products and long-term demonstration of performance
- In accordance with the JPSS phased schedule, the **SNPP CrIMSS EDR cal/val plan** was devised to ensure the EDR would meet the mission **Level 1 requirements** (*Barnet,* 2009)
- The **EDR validation methodology** draws upon previous work with AIRS and IASI (*Nalli et al.,* 2013, *JGR Special Section on SNPP Cal/Val*)
  - Classification of various approaches into a "Validation Methodology Hierarchy"

CrIS/ATMS (CrIMSS) Sounder Operational EDR: NOAA Unique CrIS/ATMS Processing System (NUCAPS)

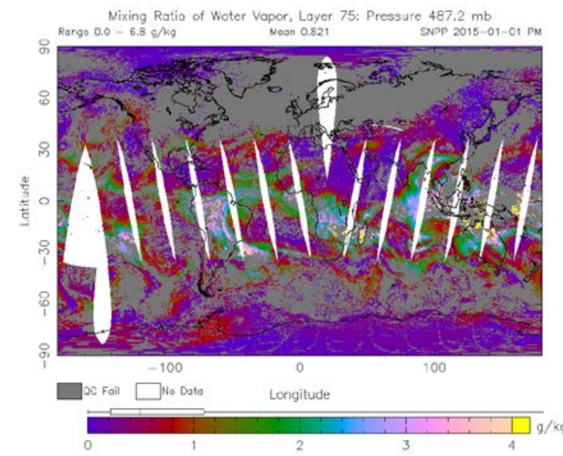
- **Original IDPS Algorithm**
  - Optimal Estimation (OE) algorithm originally developed by AER, LaRC and NGAS
  - CrIMSS operational product (MX7.1) validated through Beta and Provisional Maturities (*Divakarla et al.,* 2014)

- **NUCAPS Algorithm** (*Gambacorta et al.* 2014)
  - **Operational algorithm beginning Sep 2013**
    - Transition to NUCAPS validation
    - **Stage-1 Validated Maturity achieved in Sep 2014**
  - Line-for-line modular implementation of the iterative, multistep AIRS Science Team retrieval algorithm
  - Non-precipitating conditions (cloudy, partly cloudy, clear)
  - Atmospheric Vertical Temperature , Moisture (AVTP, AVMP) and trace gas profiles (O_3, CO, CO_2, CH_4)

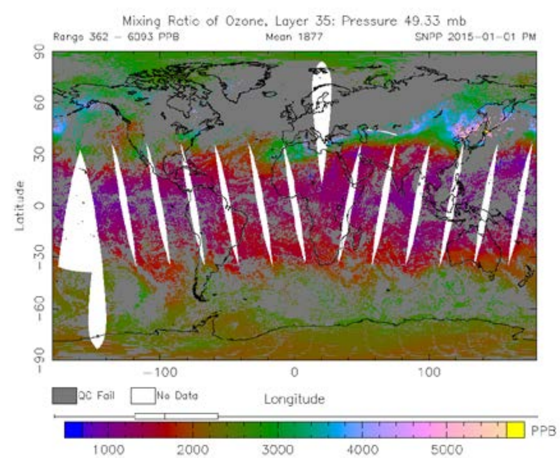
NUCAPS AVTP



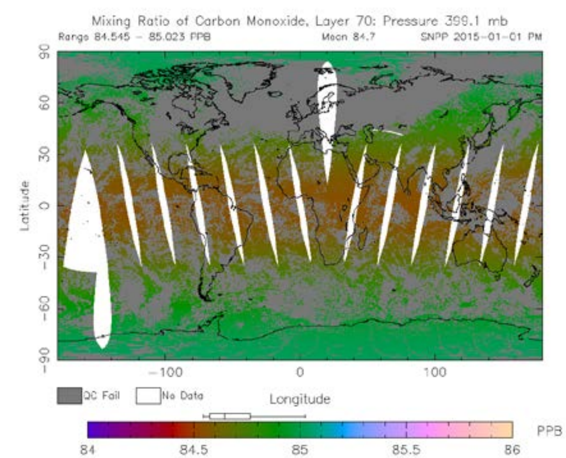
NUCAPS AVMP



NUCAPS O_3



NUCAPS CO



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

CrIS/ATMS Sounder EDR L1 Requirements

AVTP and AVMP EDR

CrIS/ATMS Atmospheric Vertical Temperature Profile (AVTP) Measurement Uncertainty – Layer Average Temperature Error	
PARAMETER	**THRESHOLD**
AVTP, Cloud fraction < 50%, surface to 300 hPa	1.6 K / 1-km layer
AVTP, Cloud fraction < 50%, 300–30 hPa	1.5 K / 3-km layer
AVTP, Cloud fraction < 50%, 30–1 hPa	1.5 K / 5-km layer
AVTP, Cloud fraction < 50%, 1–0.5 hPa	3.5 K / 5-km layer
AVTP, Cloud fraction ≥ 50%, surface to 700 hPa	2.5 K / 1-km layer
AVTP, Cloud fraction ≥ 50%, 700–300 hPa	1.5 K / 1-km layer
AVTP, Cloud fraction ≥ 50%, 300–30 hPa	1.5 K / 3-km layer
AVTP, Cloud fraction ≥ 50%, 30–1 hPa	1.5 K / 5-km layer
AVTP, Cloud fraction ≥ 50%, 1–0.5 hPa	3.5 K/ 5-km layer

CrIS/ATMS Atmospheric Vertical Moisture Profile (AVMP) Measurement Uncertainty – 2-km Layer Average Mixing Ratio % Error	
PARAMETER	**THRESHOLD**
AVMP, Cloud fraction < 50%, surface to 600 hPa	Greater of 20% or 0.2 g·kg^{-1} / 2-km layer
AVMP, Cloud fraction < 50%, 600–300 hPa	Greater of 35% or 0.1 g·kg^{-1} / 2-km layer
AVMP, Cloud fraction < 50%, 300–100 hPa	Greater of 35% or 0.1 g·kg^{-1} / 2-km layer
AVMP, Cloud fraction ≥ 50%, surface to 600 hPa	Greater of 20% of 0.2 g·kg^{-1} / 2-km layer
AVMP, Cloud fraction ≥ 50%, 600–400 hPa	Greater of 40% or 0.1 g·kg^{-1} / 2-km layer
AVMP, Cloud fraction ≥ 50%, 400–100 hPa	Greater of 40% or 0.1 g·kg^{-1} / 2-km layer

Source: L1RD (2014), pp. 41, 43

Trace Gas EDR

CrIS Infrared Trace Gases Specification Performance Requirements	
PARAMETER	**THRESHOLD**
CO (Carbon Monoxide) Total Column Precision	35%, or full res mode 15%
CO (Carbon Monoxide) Total Column Accuracy	±25%, or full res mode ±5%
CO_2 (Carbon Dioxide Total Column Precision	0.5% (2 ppmv)
CO_2 (Carbon Dioxide) Total Column Accuracy	±1% (4 ppmv)
CH_4 (Methane) Total Column Precision	1% (≈20 ppbv)
CH_4 (Methane) Total Column Accuracy	±4% (≈80 ppmv)
O_3 (Ozone) Profile Precision, 4–260 hPa (6 statistic layers)	20%
O_3 (Ozone) Profile Precision, 260 hPa to sfc (1 statistic layer)	20%
O_3 (Ozone) Profile Accuracy, 4–260 hPa (6 statistic layers)	±10%
O_3 (Ozone) Profile Accuracy, 260 hPa to sfc (1 statistic layer)	±10%
O_3 (Ozone) Profile Uncertainty, 4–260 hPa (6 statistic layers)	25%
O_3 (Ozone) Profile Uncertainty, 260 hPa to sfc (1 statistic layer)	25%

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

Global requirements defined for lower and upper atmosphere subdivided into 1-km and 2-km layers for AVTP and AVMP, respectively.

Validation Methodology Hierarchy

(e.g., *Nalli et al.,* 2013)

1. **Numerical Model (e.g., ECMWF, NCEP/GFS) Global *Comparisons***
   - Large, truly global samples acquired from Focus Days
   - Useful for early sanity checks, bias tuning and regression
   - However, not independent truth data

2. **Satellite EDR (e.g., AIRS, ATOVS, COSMIC) *Intercomparisons***
   - Global samples acquired from Focus Days (e.g., AIRS)
   - Consistency checks; merits of different retrieval algorithms
   - However, IR sounders have 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
   - Useful for representation of global zones and long-term monitoring
   - Large statistical samples acquired after a couple months' accumulation (e.g., *Divakarla et al.,* 2006)
   - NOAA Products Validation System (NPROVS) (*Reale et al.,* 2012)
   - Limitations:
     - Skewed distribution toward NH-continental sites
     - 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
     - Well-specified error characteristics and optimal accuracy
     - Minimal mismatch errors
     - Include atmospheric state "best estimates" or "merged soundings"
   - Reference sondes: CFH, corrected RS92
     - Traceable measurement
   - Detailed performance specification and regional characterization
   - Limitation: Small sample sizes and geographic coverage
   - E.g., **ARM sites** (e.g., *Tobin et al.,* 2006), AEROSE, ideally GRUAN

5. **Intensive Field Campaign *Dissections***
   - Include dedicated RAOBs, especially those *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; EDR "dissections"
   - E.g., **AEROSE**, **CalWater2**, JAIVEX, WAVES, AWEX-G, EAQUATE

Assessment Methodology: Statistical Metrics

- Level 1 AVTP and AVMP accuracy requirements are defined over **coarse layers**, roughly 1–5 km for tropospheric AVTP and 2 km for AVMP (Table, Slide 5).
- We have recently introduced rigorous **geographic surface area weighting** to these schemes for dedicated/reference RAOB samples

AVTP

$$\mathrm{RMS}(\Delta T_{\mathfrak{L}}) = \sqrt{\frac{1}{n_j}\sum_{j=1}^{n_j}(\Delta T_{\mathfrak{L},j})^2} \qquad \mathrm{BIAS}(\Delta T_{\mathfrak{L}}) \equiv \overline{\Delta T_{\mathfrak{L}}} = \frac{1}{n_j}\sum_{j=1}^{n_j}\Delta T_{\mathfrak{L},j}$$

$$\mathrm{STD}(\Delta T_{\mathfrak{L}}) \equiv \sigma(\Delta T_{\mathfrak{L}}) = \sqrt{[\mathrm{RMS}(\Delta T_{\mathfrak{L}})]^2 - [\mathrm{BIAS}(\Delta T_{\mathfrak{L}})]^2}$$

AVMP and O_3

- W2 weighting was used in determining Level 1 Requirements
- To allow compatible STD calculation, W2 weighting should be consistently used for both RMS and BIAS

$$\Delta q_{\mathfrak{L},j} \equiv \frac{\hat{q}_{\mathfrak{L},j} - q_{\mathfrak{L},j}}{q_{\mathfrak{L},j}} \qquad \mathrm{RMS}(\Delta q_{\mathfrak{L}}) = \sqrt{\frac{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}(\Delta q_{\mathfrak{L},j})^2}{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}}}\,,$$

water vapor weighting factor, $W_{\mathfrak{L},j}$,

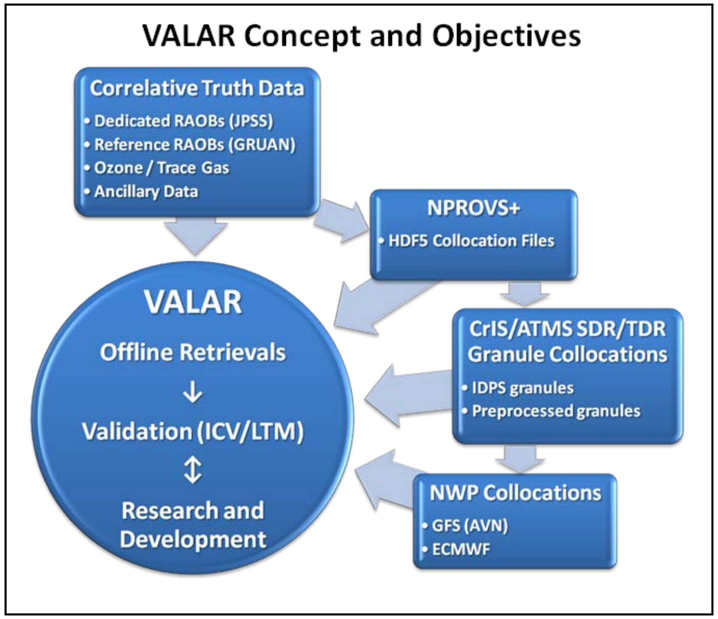
$$\mathrm{BIAS}(\Delta q_{\mathfrak{L}}) = \frac{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}\,\Delta q_{\mathfrak{L},j}}{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}}\,, \qquad W_{\mathfrak{L},j} = \begin{cases} 1 & , \mathrm{W}^0 \\ q_{\mathfrak{L},j} & , \mathrm{W}^1 \\ (q_{\mathfrak{L},j})^2 & , \mathrm{W}^2 \end{cases}$$

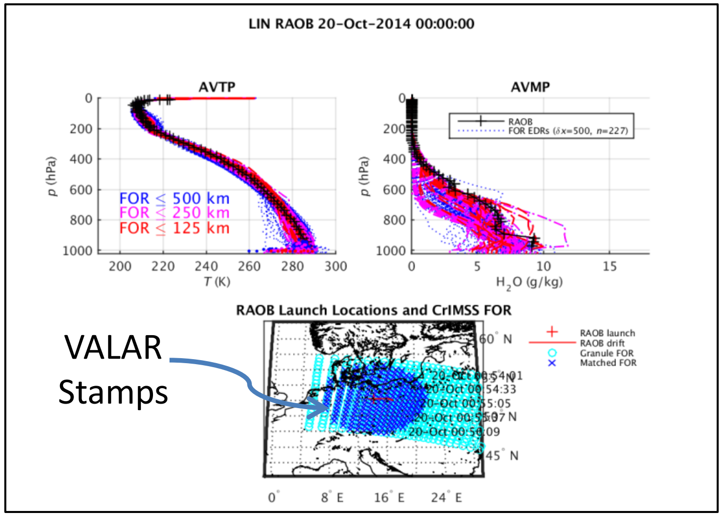
$$\mathrm{STD}(\Delta q_{\mathfrak{L}}) = \sqrt{[\mathrm{RMS}(\Delta q_{\mathfrak{L}})]^2 - [\mathrm{BIAS}(\Delta q_{\mathfrak{L}})]^2}$$

JPSS SNPP Validation Datasets and Tools

- **STAR Validation Archive (VALAR)** (*Nalli et al.*, 2014)
  - Low-level research archive designed to meet needs of Cal/Val Plan
  - Dedicated/reference and intensive campaign RAOBs
  - SDR/TDR granule-based collocations ("stamps") within 500 km radius acquired off SCDR (past 90 days) or CLASS (older than 90 days)
  - Basis for Trace Gas EDR validation
  - Offline retrievals / retrospective reprocessing
  - MATLAB and IDL statistical codes and visualization software tools for monitoring
  - Rigorous coarse-layer (1-km, 2-km) product performance measures based on statistical metrics corresponding to Level 1 Requirements detailed in *Nalli et al.* (2013)

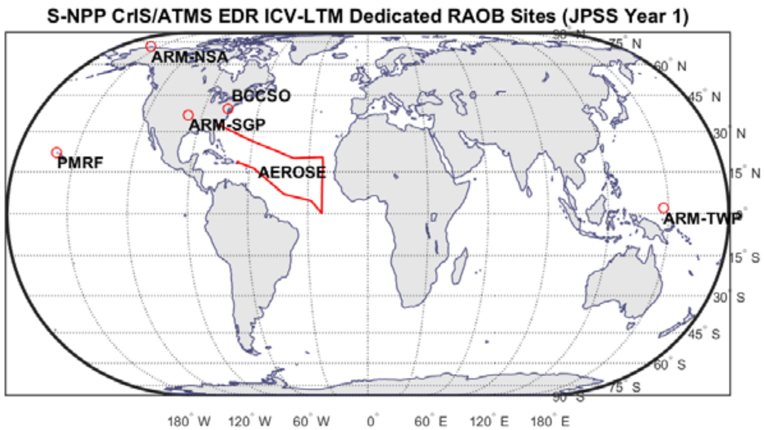
- **NOAA Products Validation System (NPROVS)** (*Reale et al.,* 2012)
  - Conventional RAOBs (NPROVS+ dedicated/reference), "single closest FOR" collocations
  - HDF5-formatted Collocation Files facilitates GRUAN RAOB matchups within VALAR
  - NRT monitoring capability
  - Satellite EDR intercomparison (e.g., *Nalli et al.* 2013) capability
  - Java based graphical user interface tools for monitoring
    - Profile Display (PDISP)
    - NPROVS Archive Summary (NARCS)

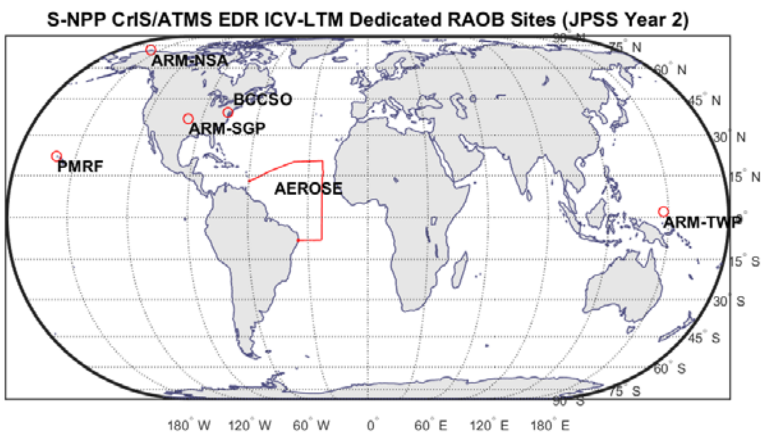




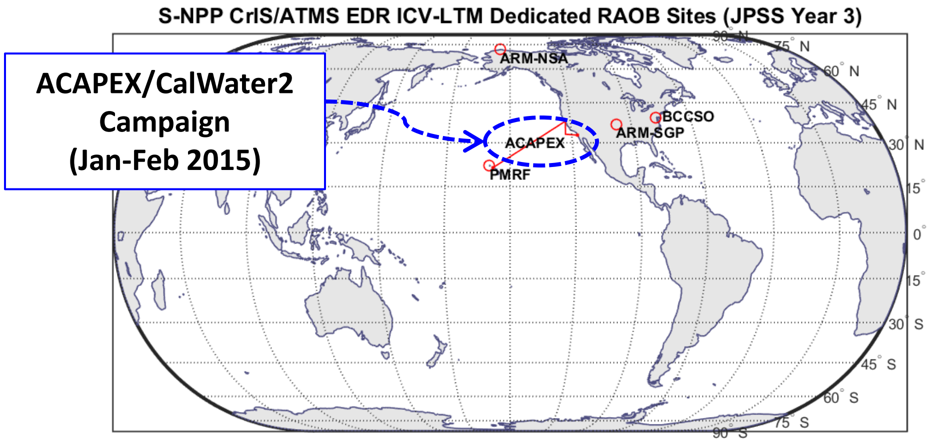
VALAR Dedicated and Reference RAOBs

JPSS S-NPP Dedicated Years 1 and 2 (2012-2014)

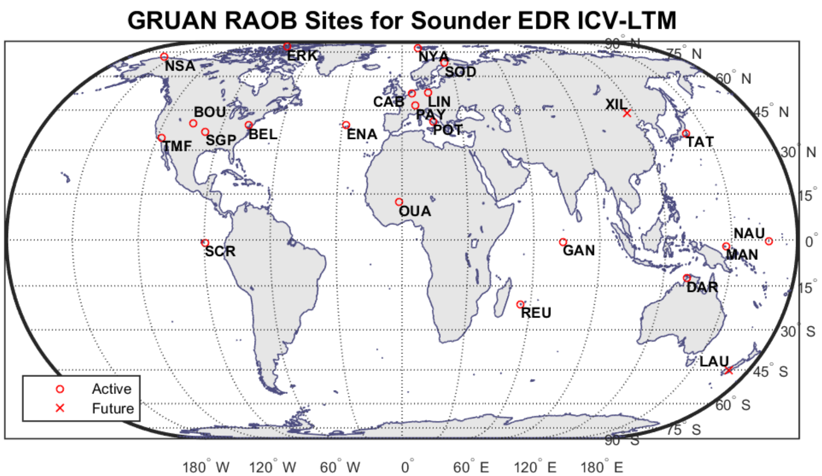




JPSS S-NPP Dedicated Year 3 (2014-2015)



GRUAN Reference Sites (NPROVS+ Collocation)

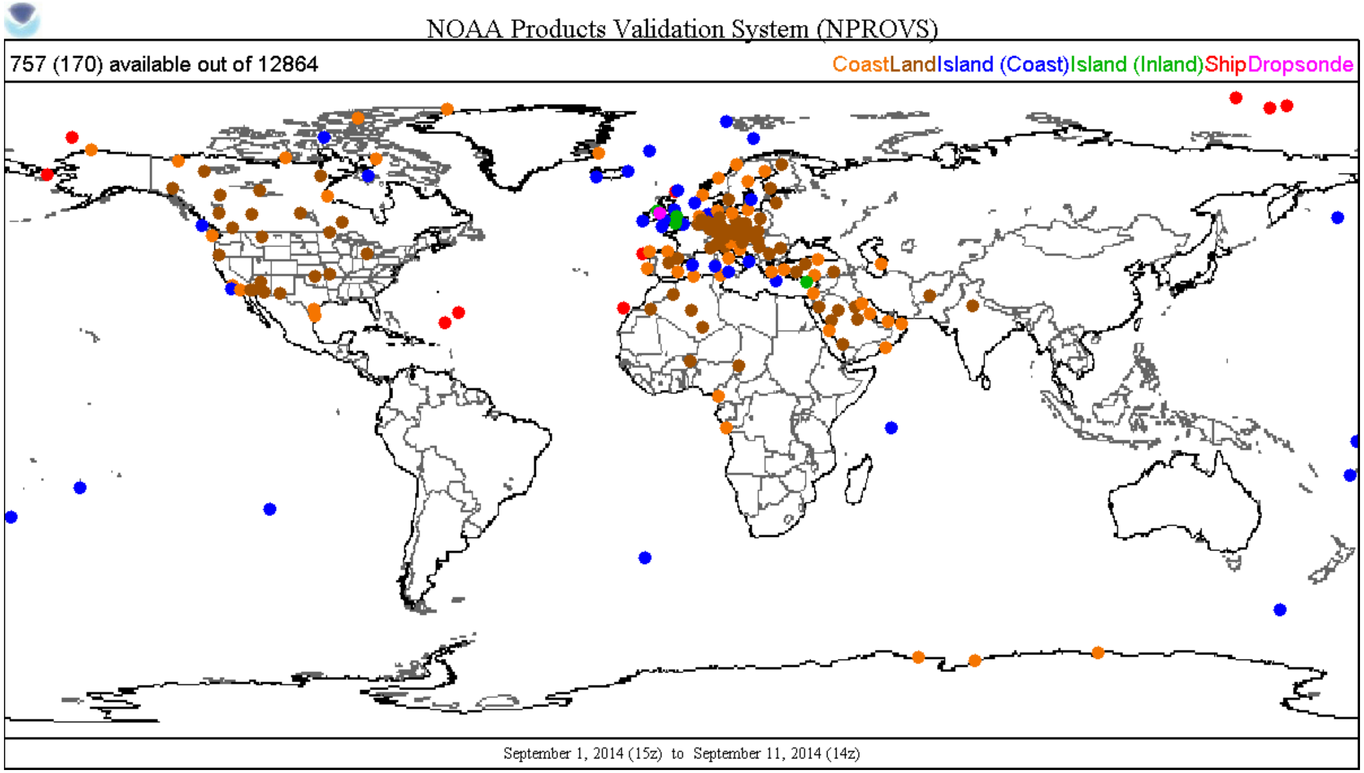


Validation of NOAA-Unique Operational Sounder EDR

NUCAPS EDR PRODUCT VALIDATION

NPROVS Conventional RAOB Collocations

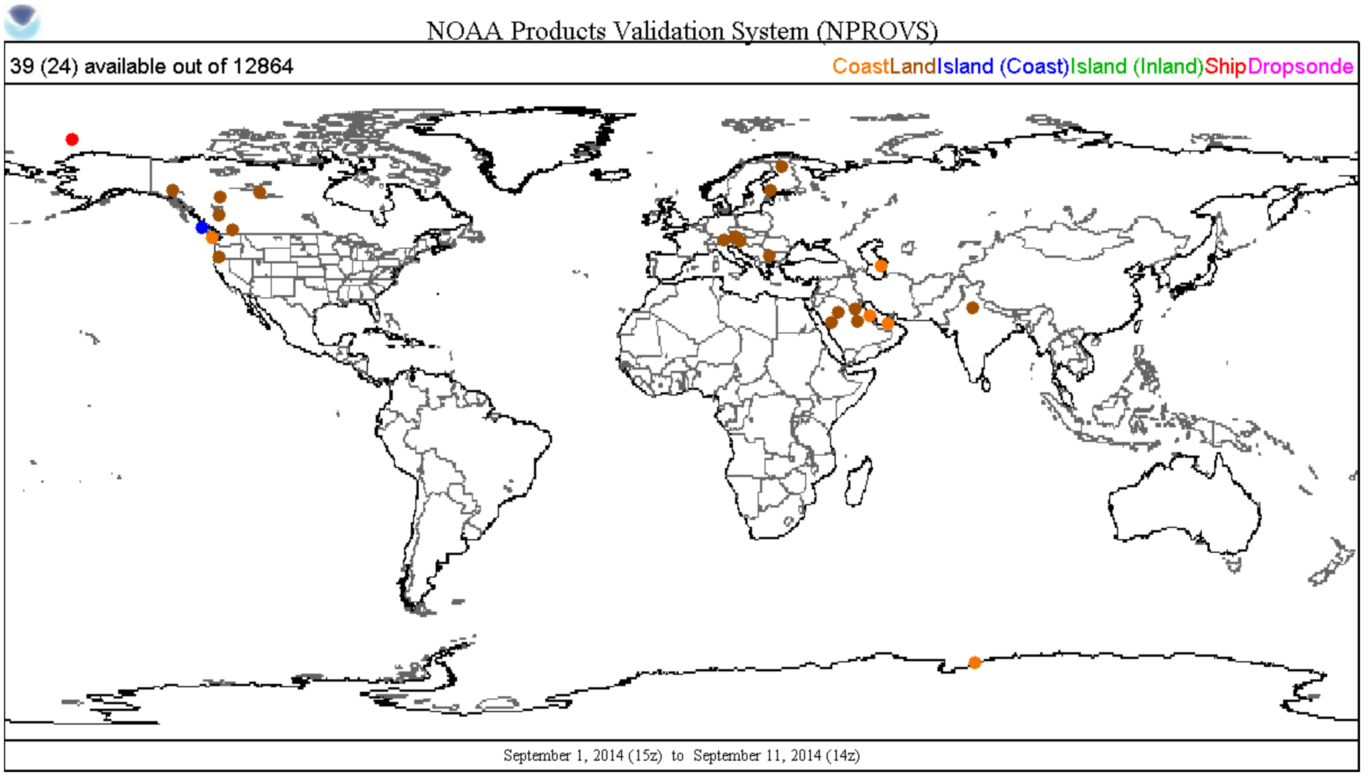
Single Closest FOR (*Reale et al.*, 2012)



- 1–11 Sep 2014
- **RS92 and RS41 sondes**
- Single-closest FOR
- **Space-time window 1**
  - **±3 h before/after overpass**
  - **75 km**
- **Sample size 1 *N* = 757**

NPROVS Conventional RAOB Collocations

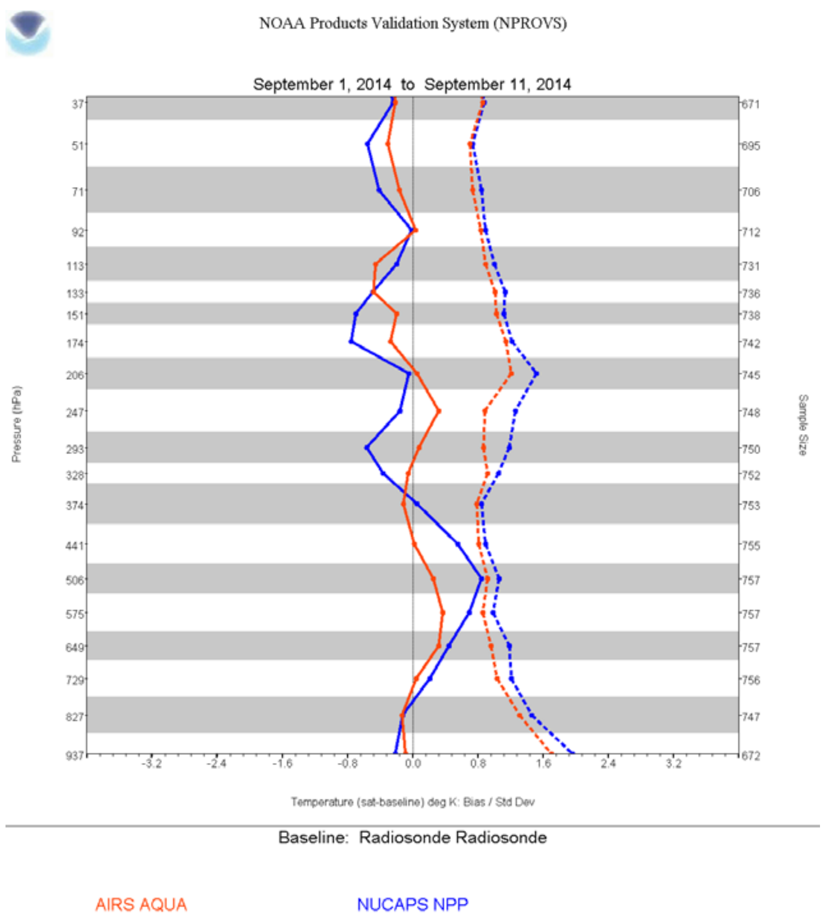
Single Closest FOR (*Reale et al.*, 2012)



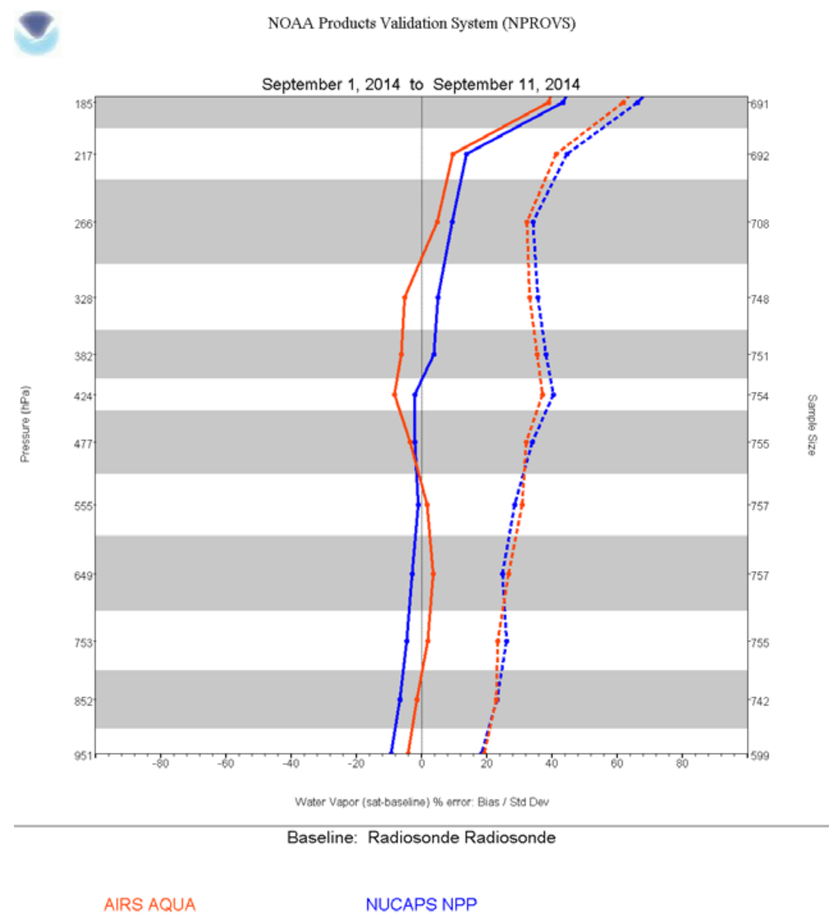
- 1–11 Sep 2014
- **RS92 and RS41 sondes**
- Single-closest FOR
- **Space-time window 2**
  - **−1–0 h before overpass**
  - **75 km**
- **Sample size 2 *N* = 39**

NDE-OPS NUCAPS and AIRS versus NPROVS Collocated Conventional RAOB: Sample 1

AVTP (BIAS and RMS)

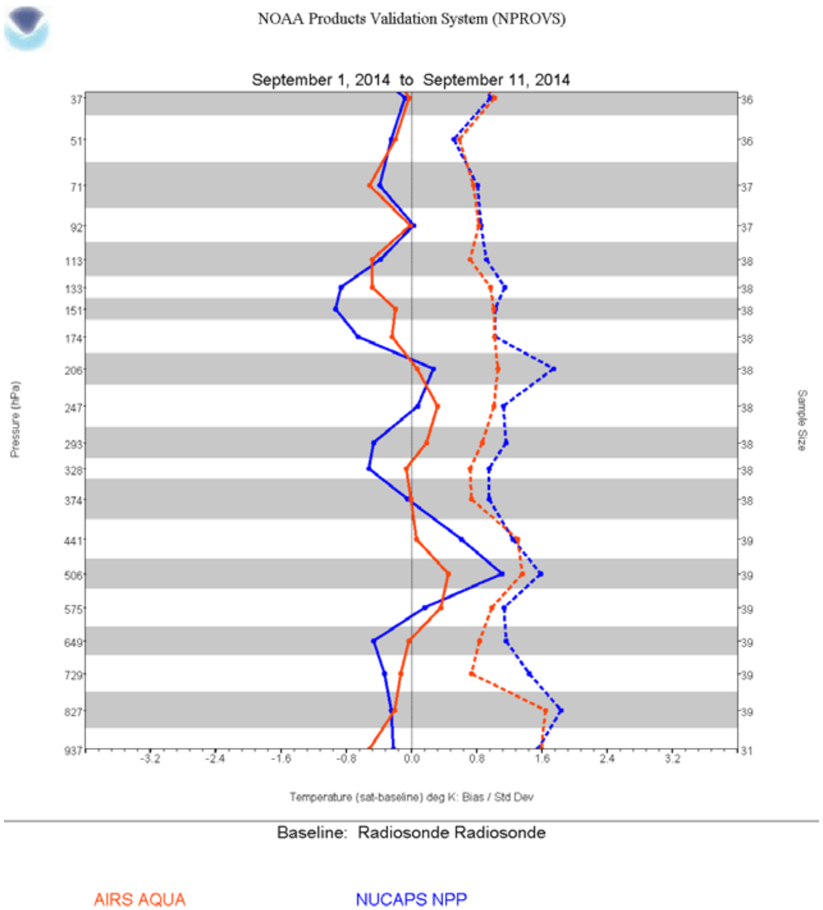


AVMP (BIAS and RMS)

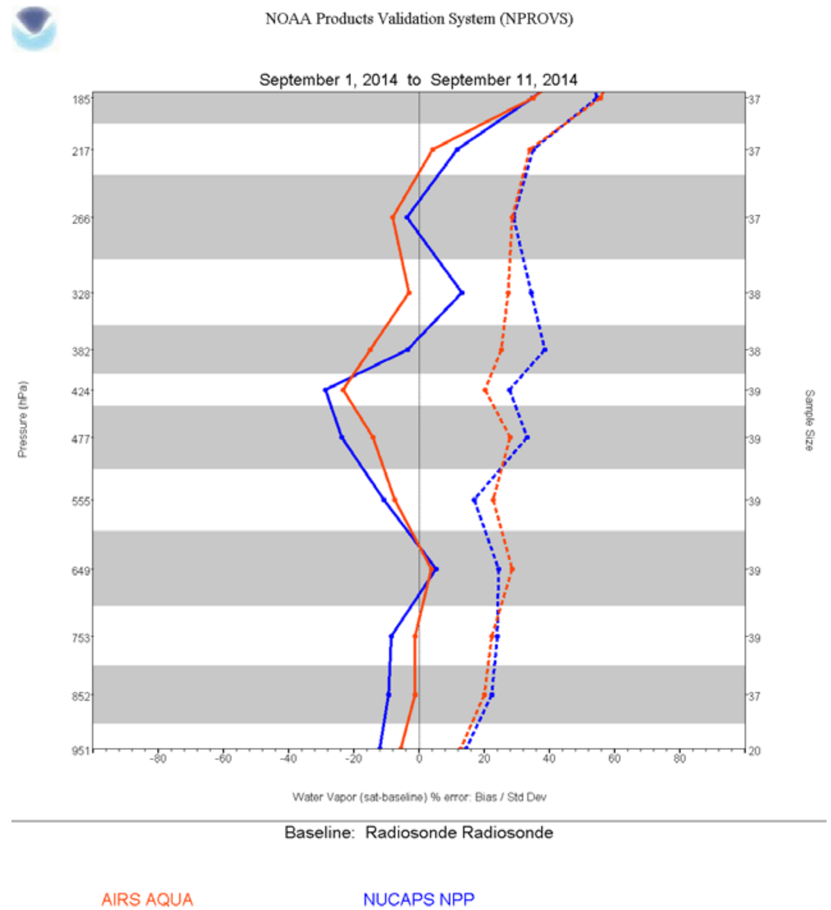


NDE-OPS NUCAPS and AIRS versus NPROVS Collocated Conventional RAOB: Sample 2

AVTP (BIAS and RMS)

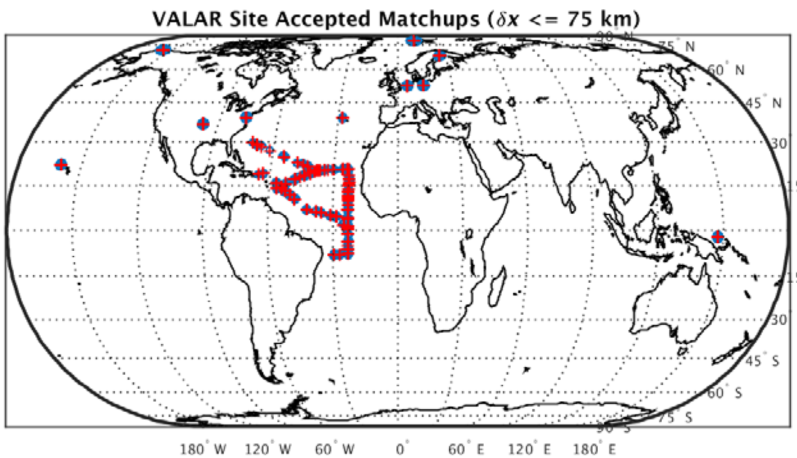


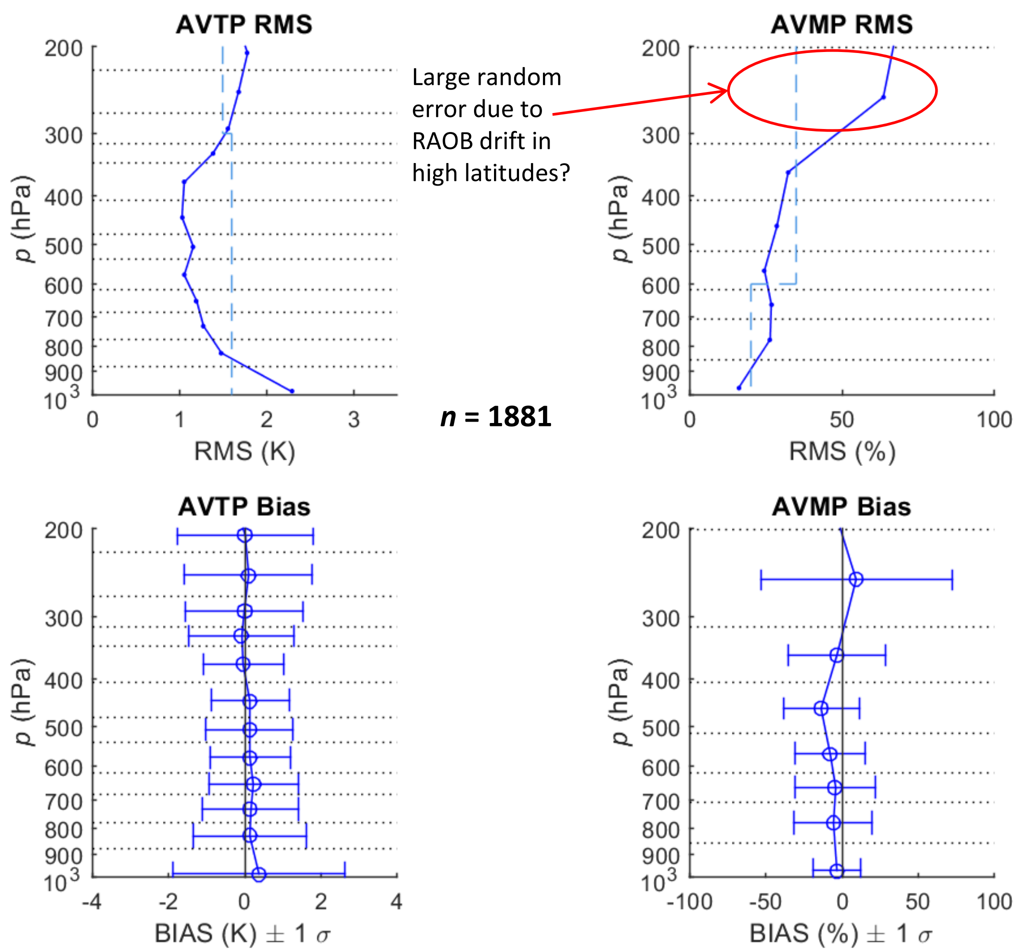
AVMP (BIAS and RMS)



NUCAPS AVTP/AVMP (NDE-OPS) versus Dedicated/Reference RAOB Day and Night

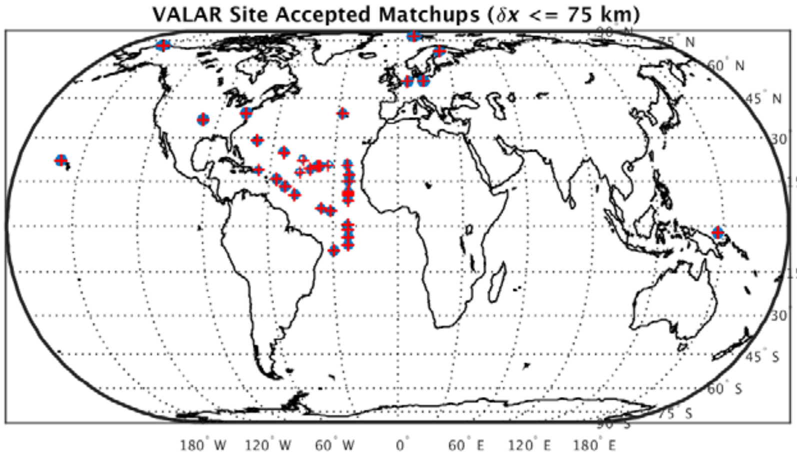
VALAR RAOB sample weighted by zonal surface areas

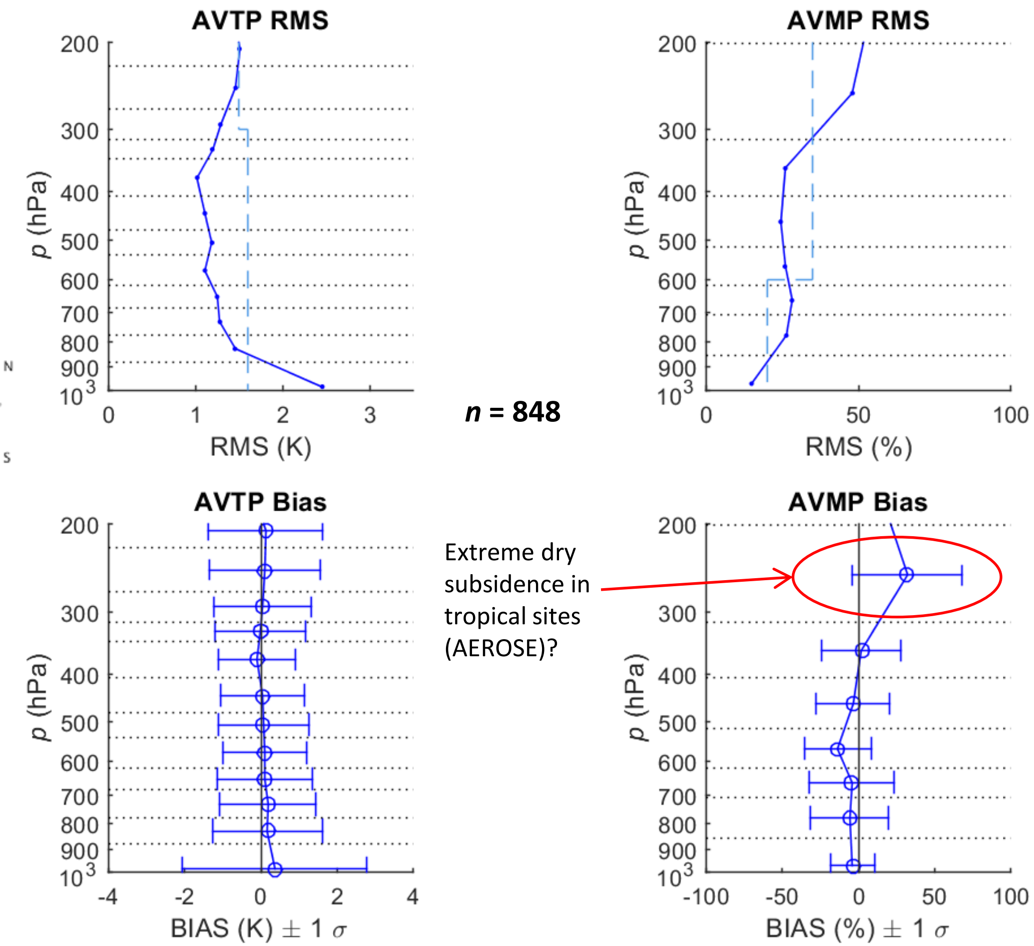




NUCAPS AVTP/AVMP (NDE-OPS) versus Dedicated/Reference RAOB Nighttime Only

VALAR RAOB sample weighted by zonal surface areas

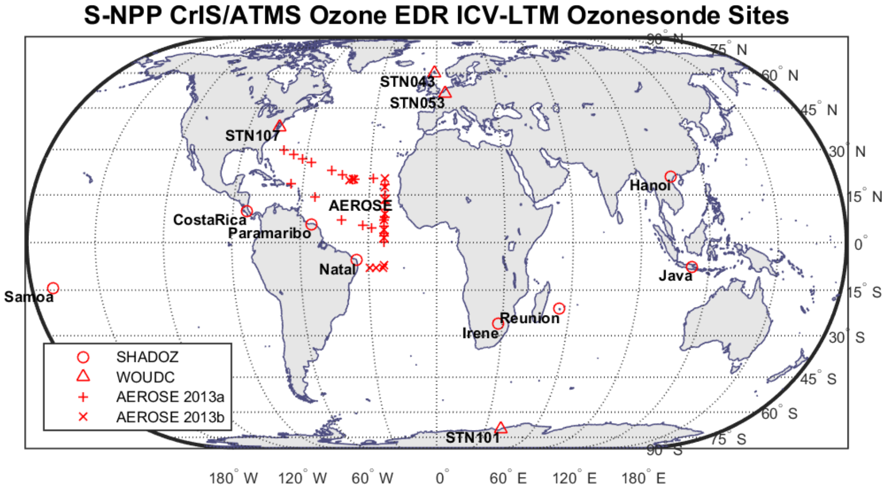


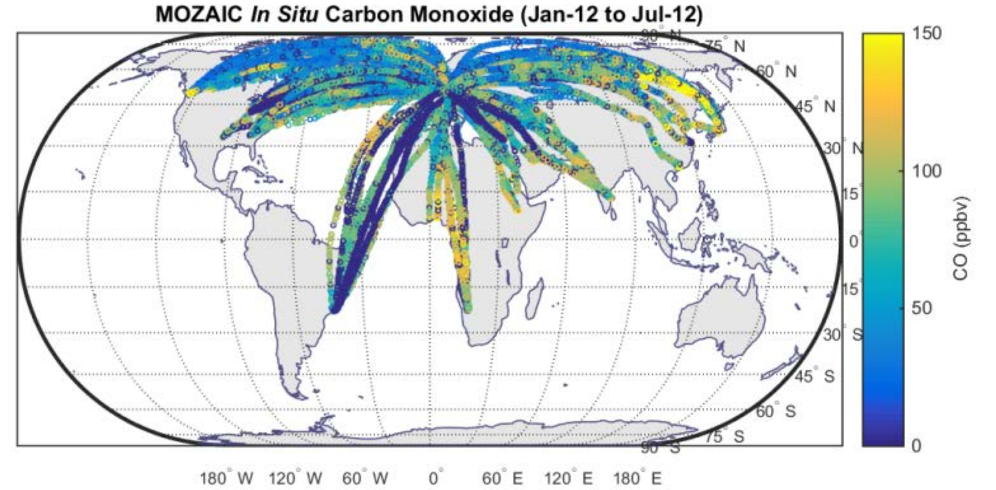


NUCAPS Trace Gas Validation

- **Validation of NUCAPS Trace Gases**
  - Available ***in situ*** **truth** datasets
  - **Collocated ozonesondes** for O_3 **(ozone) profile EDR**
    - **SHADOZ sites**
    - **WOUDC** currently being acquired
    - **AEROSE** and **CalWater2** dedicated ozonesondes
  - **Collocated aircraft** data for **CO, CO_2, O_3**
    - **MOZAIC**
    - Additional data currently being sought

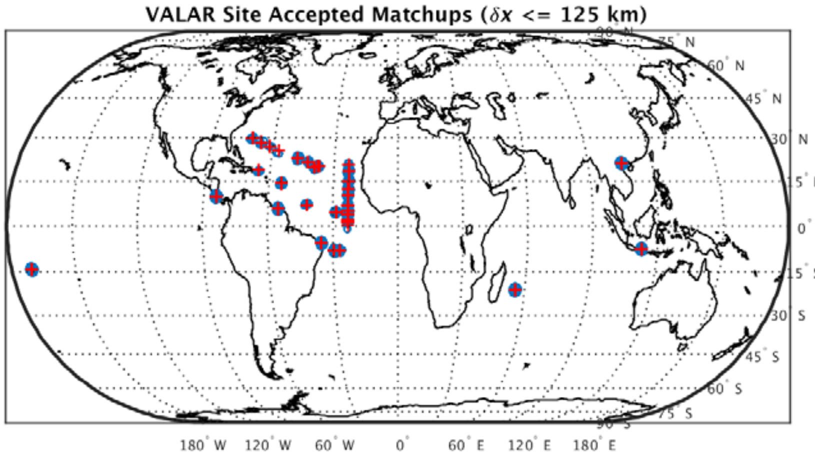
- **Comparisons of NUCAPS CO and O_3** can also be performed against models (i.e., Step 1 of Validation Hierarchy; e.g., WRF-CHEM Model, *Smith and Nalli,* 2014)

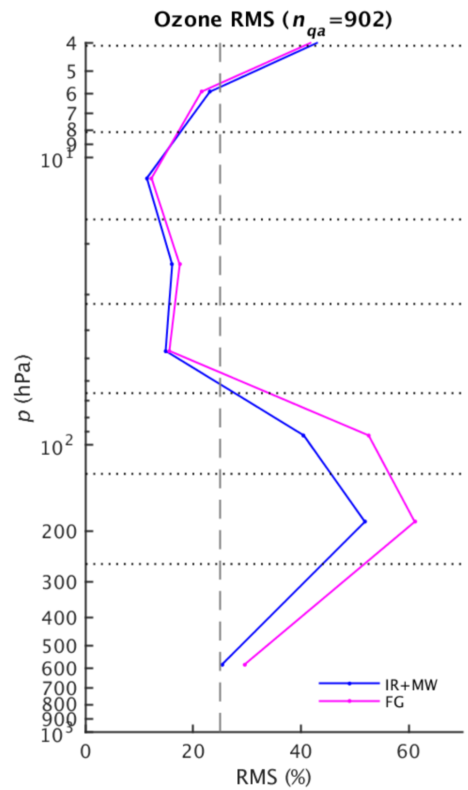


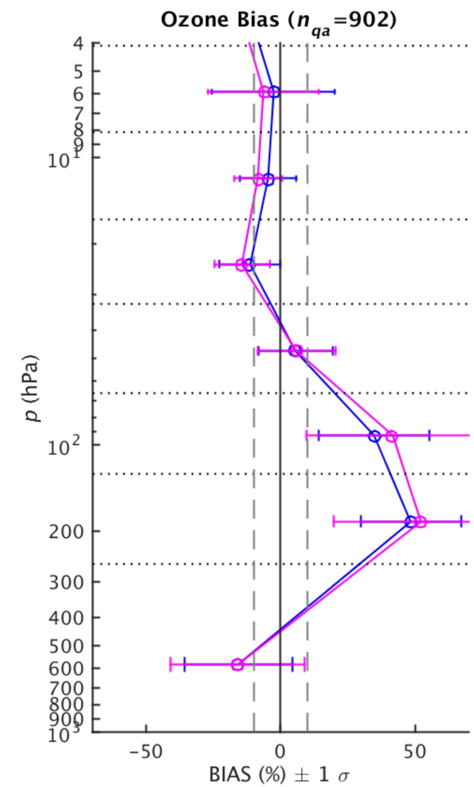


Preliminary Ozone Profile Validation

VALAR AEROSE Dedicated and SHADOZ Ozonesonde Sample

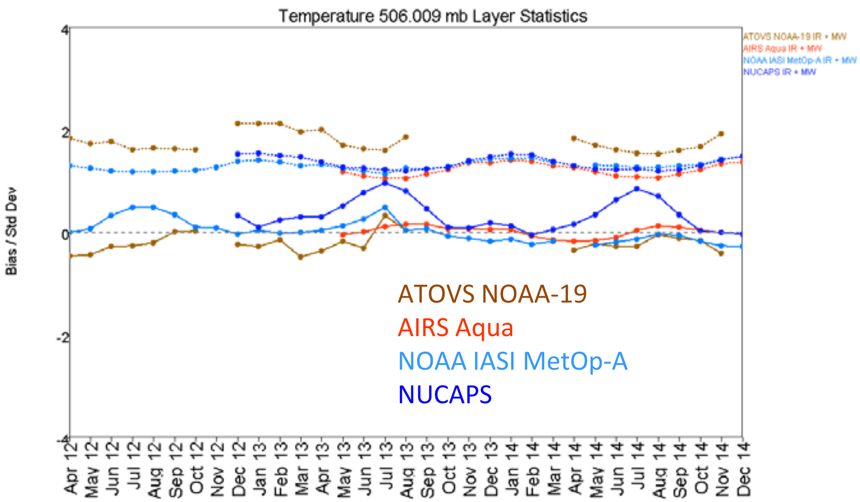


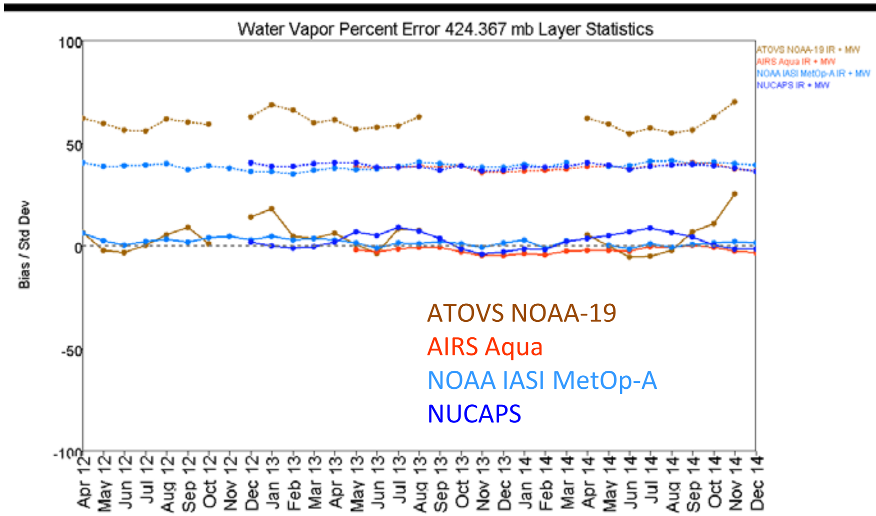




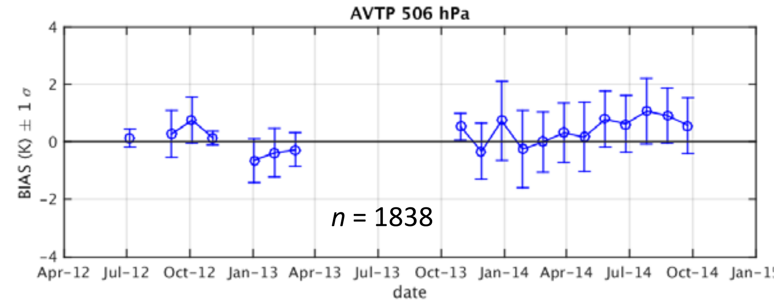
Long-Term Monitoring (LTM)

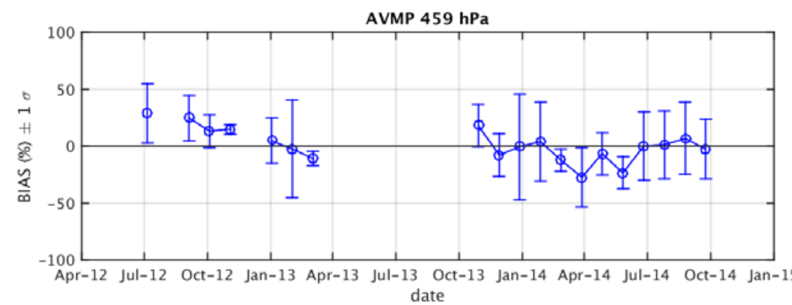
NPROVS NARCS Conventional RAOB Collocation

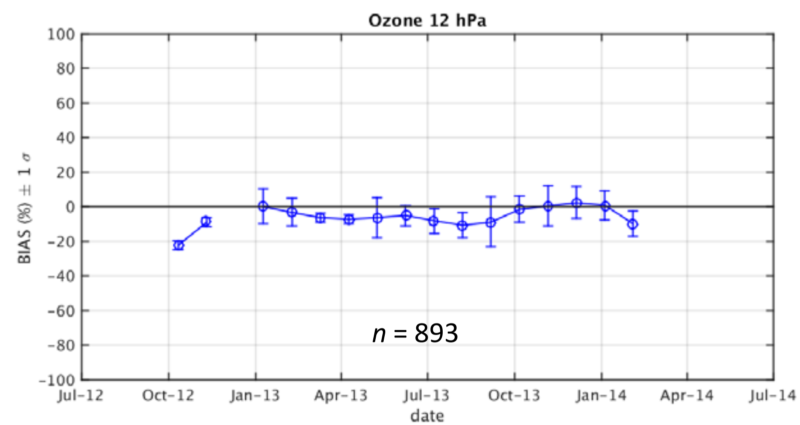




VALAR Dedicated/GRUAN/Ozonesonde Collocation







Future Work: SNPP ICV and LTM

- **NUCAPS Stages 2-3 Validated Maturities**
  - **AVTP/AVMP, Trace Gas validation** for operational and offline code versions
    - Global coarse-layer ensemble statistical analyses versus dedicated, reference and conventional RAOB truth
    - Geographic surface area weighting
    - **Apply averaging kernels** in NUCAPS error analyses, including ozone profile EDR
  - **VALAR growth, development and enhancements**
    - Support **ACAPEX/CalWater2 (Pacific Ocean, Jan-Feb 2015)** and future **AEROSE** campaigns
    - Support ARM and PMRF dedicated RAOBs (including dual-launches, "best estimates")
    - Leverage GRUAN reference RAOBs
    - Trace gas (O_3, CO, CO_2) datasets
    - **GRUAN reprocessing** of RS92 RAOB data (viz., entire AEROSE data record)
  - Support short- and long-term NUCAPS EDR algorithm development, updates, improvements

- **Other Related Work**
  - Collocation uncertainty estimates
  - calc − obs analyses for different forward models (CRTM, LBLRTM, SARTA, etc.)
  - Support skin SST EDR validation
  - Support EDR applications (AWIPS, atmospheric chemistry users)

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EXTRA SLIDES

Assessment Methodology: Reducing Truth to Correlative Layers

- The **measurement equation** (e.g., *Taylor and Kuyatt,* 1994) for retrieval includes forward and inverse operators (*Rodgers*, 1990) to estimate the measurand, $\mathbf{x}$, on forward model layers:

$$\hat{\mathbf{x}} = I[F(\mathbf{x}, \mathbf{b}), \mathbf{b}, \mathbf{c}]$$

- **Rigorous validation** therefore requires high-resolution truth measurements (e.g., dedicated RAOB) be **reduced to correlative RTA layers** (*Nalli et al.,* 2013, *JGR Special Section on SNPP Cal/Val*)
- **Radiative transfer approach** is to integrate quantities over the atmospheric path (e.g., number densities → column abundances), interpolate to RTA (arbitrary) levels, then compute RTA layer quantities, e.g.,

$$\Sigma_x(z) = \int_{z_t}^{z} N_x(z')\,dz'$$

NUCAPS AVTP/AVMP (NDE-OPS) versus VALAR Dedicated RAOB Ocean Only Day and Night

RAOB sample weighted by zonal surface areas