Validation and Long-Term Monitoring of the NOAA Unique CrIS/ATMS Processing System (NUCAPS) Operational Retrieval Products

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Outline

- **JPSS Sounder EDR Cal/Val Overview**
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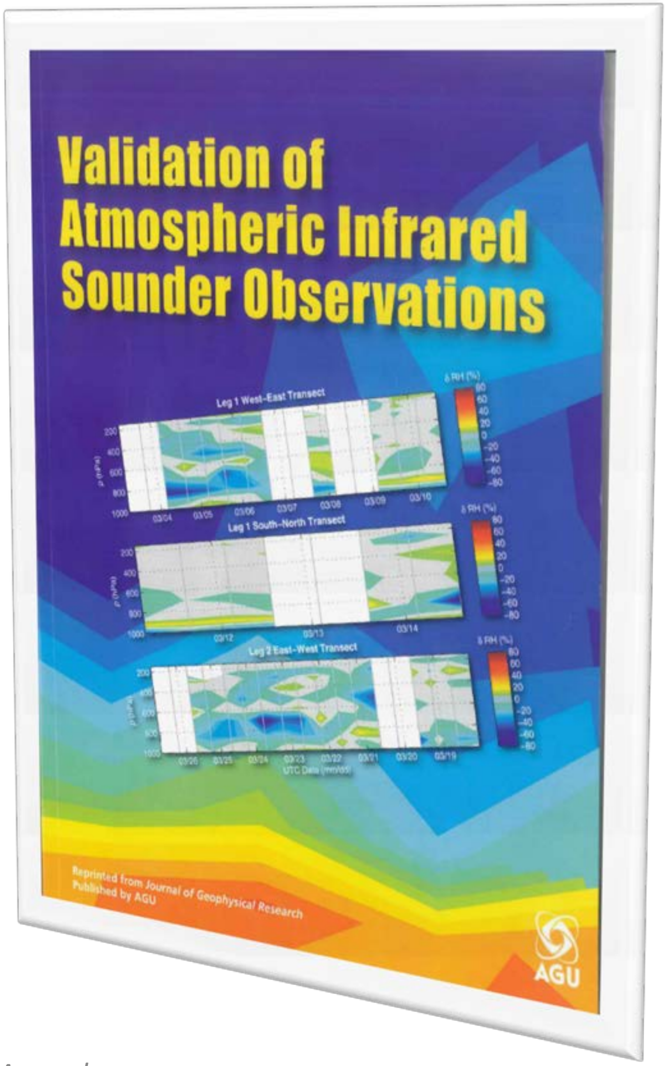
    - NOAA-Unique CrIS/ATMS Processing System (NUCAPS)
    - JPSS Level 1 Requirements
  - Validation Methodology
    - Validation Hierarchy
    - Statistical Metrics
  - JPSS SNPP Validation Datasets
    - STAR Validation Archive (VALAR)
    - NOAA Products Validation System (NPROVS/NPROVS+)
- **NUCAPS EDR Product Validation**
  - Temperature and Moisture (AVTP and AVMP) EDR
  - 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

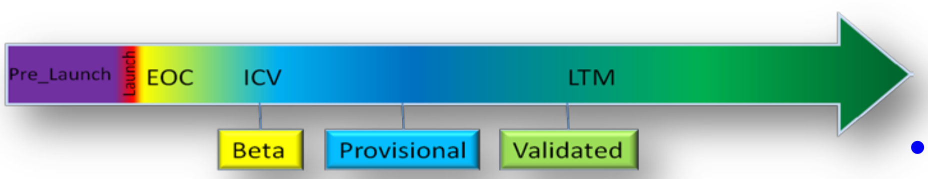
Intro: JPSS Sounder EDR Validation

- **Validation** is "the process of ascribing uncertainties to… radiances and retrieved quantities through comparison with correlative observations" (*Fetzer et al.,* 2003).
  - Sounder EDR validation supports validation of sounder 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



SNPP/JPSS Program Cal/Val

- **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)**
    - Routine characterization of all EDR products and long-term demonstration of performance



- In accordance with the JPSS phased schedule, the **SNPP CrIS/ATMS 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"

- The **J-1 CrIS/ATMS EDR Cal/Val Plan** was drafted during Jul–Aug 2015 and v1.0 was submitted on 20 August 2015

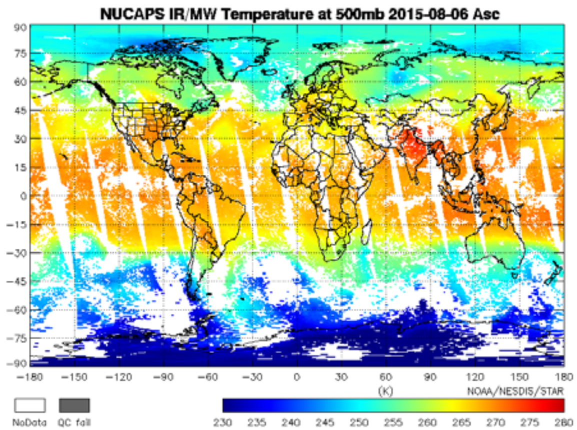
CrIS/ATMS Sounder Operational EDR:
NOAA Unique CrIS/ATMS Processing System (NUCAPS)

NUCAPS Algorithm

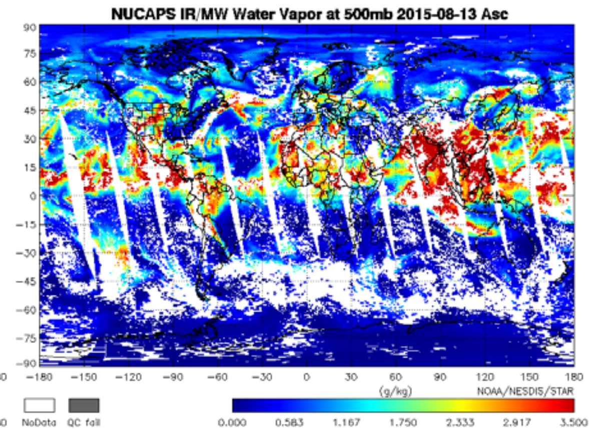
(*Susskind, Barnet and Blaisdell,* IEEE 2003; *Gambacorta et al.,* 2014)

- **Operational algorithm**
  - Superseded original IDPS CrIMSS algorithm in Sep 2013
  - Unified Sounder Science Team (AIRS/IASI/CrIS) 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)
- **Stage-1 Validated Maturity achieved in Sep 2014**
  - Original IDPS CrIMSS EDR was validated through Beta and Provisional Maturities (*Divakarla et al.,* 2014)
- **Users** (Mark Liu's presentation, Thursday morning Users Session)
  - Weather Forecast Offices (AWIPS)
    - Nowcasting / severe weather
    - Alaska (cold core)
  - NOAA/CPC (OLR)
  - NOAA/ARL (IR ozone and trace gases)
  - TOAST (IR ozone)
  - Basic and applied science research (e.g., *Pagano et al.,* 2014)
    - Via NOAA Data Centers (e.g., NGDC, CLASS)
    - Universities, peer-reviewed pubs

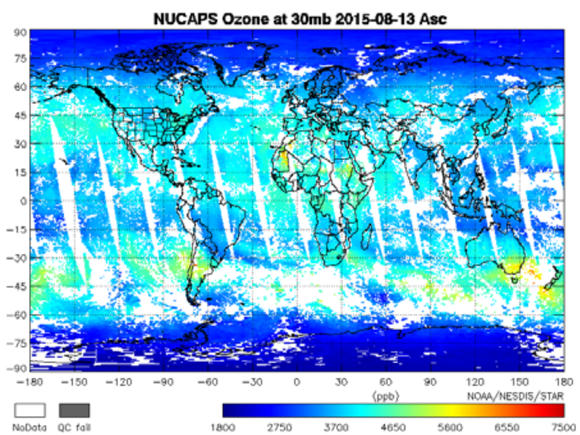
NUCAPS AVTP



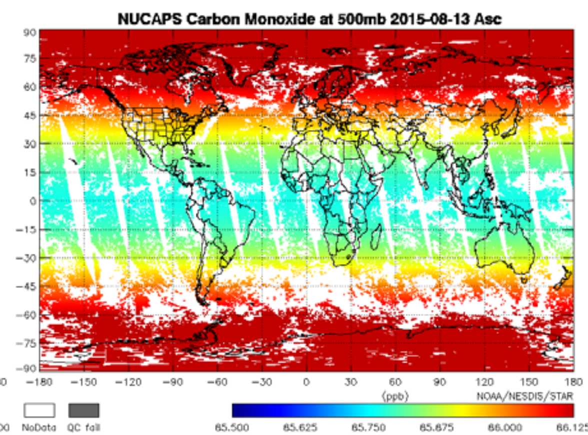
NUCAPS AVMP



NUCAPS O_3



NUCAPS CO



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

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 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction < 50%, 600–300 hPa	Greater of 35% or 0.1 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction < 50%, 300–100 hPa	Greater of 35% or 0.1 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction ≥ 50%, surface to 600 hPa	Greater of 20% of 0.2 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction ≥ 50%, 600–400 hPa	Greater of 40% or 0.1 $g \cdot kg^{-1}$ / 2-km layer
AVMP, Cloud fraction ≥ 50%, 400–100 hPa	Greater of 40% or 0.1 $g \cdot kg^{-1}$ / 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.

"Clear to Partly-Cloudy" (Cloud Fraction < 50%) ↔ **IR retrieval**
"Cloudy" (Cloud Fraction >= 50%) ↔ **MW-only retrieval**

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 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
     - 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 geographic coverage
   - E.g., **ARM sites** (e.g., *Tobin et al.,* 2006), BCCSO, PMRF, AEROSE

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; EDR "dissections"
   - E.g., **AEROSE**, **CalWater/ACAPEX**, **SNAP**, 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 6).
- We have recently introduced rigorous **zonal/land/sea surface area weighting** capabilities 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, $W_{\mathfrak{L},j}$,

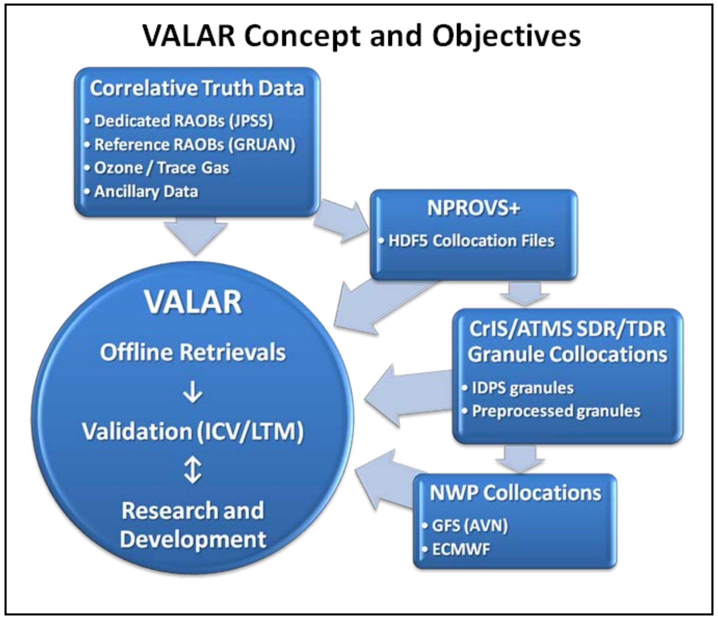
$$\mathrm{BIAS}(\Delta q_{\mathfrak{L}}) = \frac{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}\,\Delta q_{\mathfrak{L},j}}{\sum_{j=1}^{n_j} W_{\mathfrak{L},j}}, \qquad W_{\mathfrak{L},j} = \begin{cases} 1 & , \mathrm{W}^0 \\ q_{\mathfrak{L},j} & , \mathrm{W}^1 \\ (q_{\mathfrak{L},j})^2 & , \mathrm{W}^2 \end{cases}$$

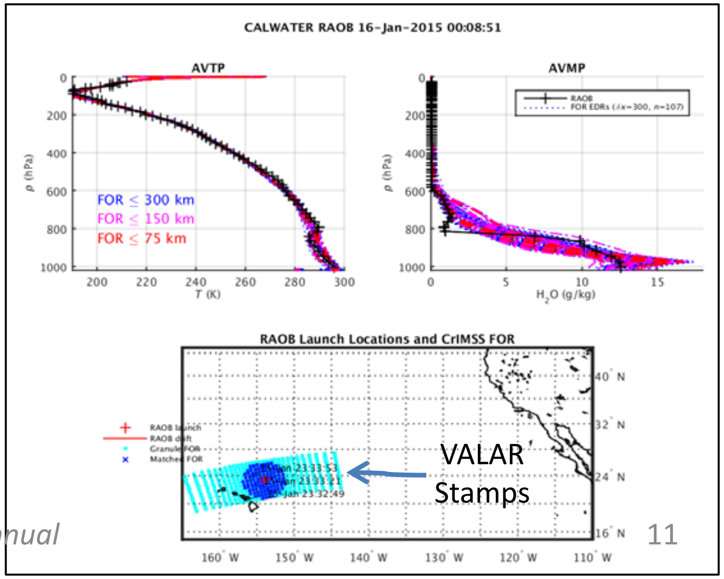
$$\mathrm{STD}(\Delta q_{\mathfrak{L}}) = \sqrt{[\mathrm{RMS}(\Delta q_{\mathfrak{L}})]^2 - [\mathrm{BIAS}(\Delta q_{\mathfrak{L}})]^2}$$

JPSS SNPP Validation Datasets and Tools

- **STAR Validation Archive (VALAR)** (*Nalli et al.,* 2014)
  - Low-level research data 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)
  - 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)

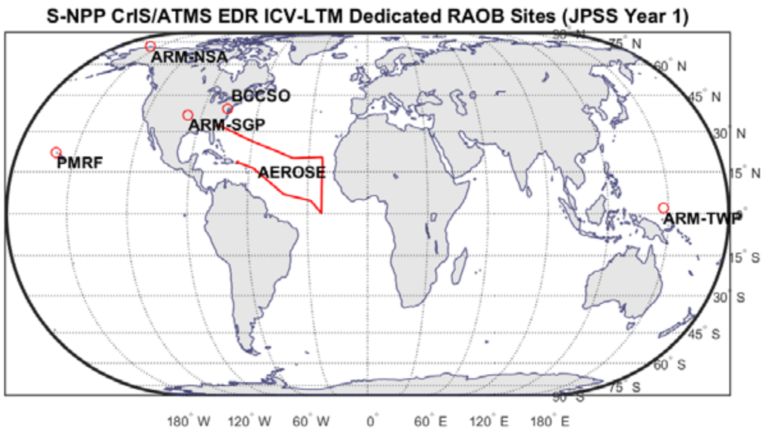
- **NOAA Products Validation System (NPROVS)** (*Reale et al.,* 2012)
  - Conventional RAOBs (NPROVS+ dedicated/reference), "single closest FOR" collocations
  - HDF5-formatted Collocation Files facilitates GRUAN RAOB matchups within VALAR
  - NRT monitoring capability
  - Satellite EDR intercomparison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

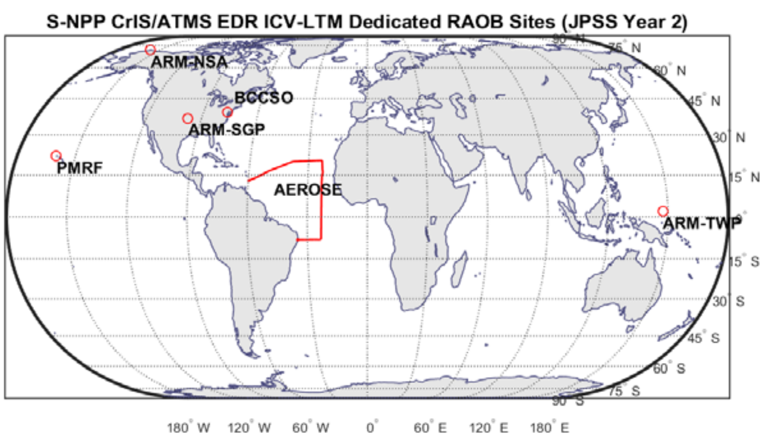




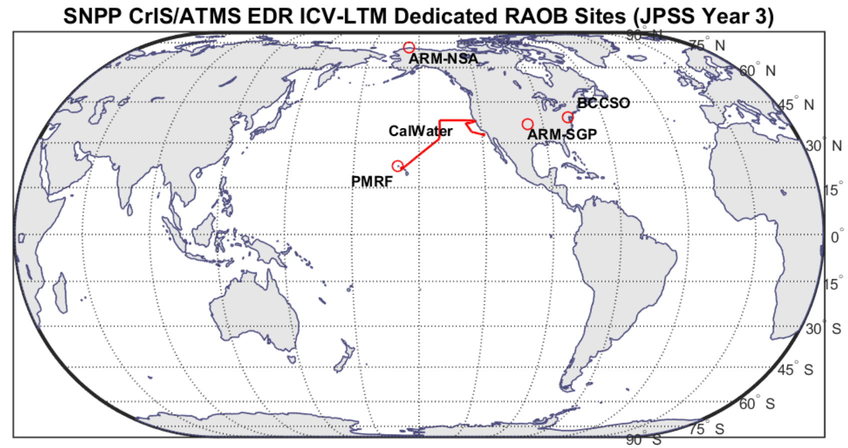
VALAR/NPROVS+ Dedicated and Reference RAOBs

JPSS SNPP Dedicated Years 1 and 2 (2012-2014)

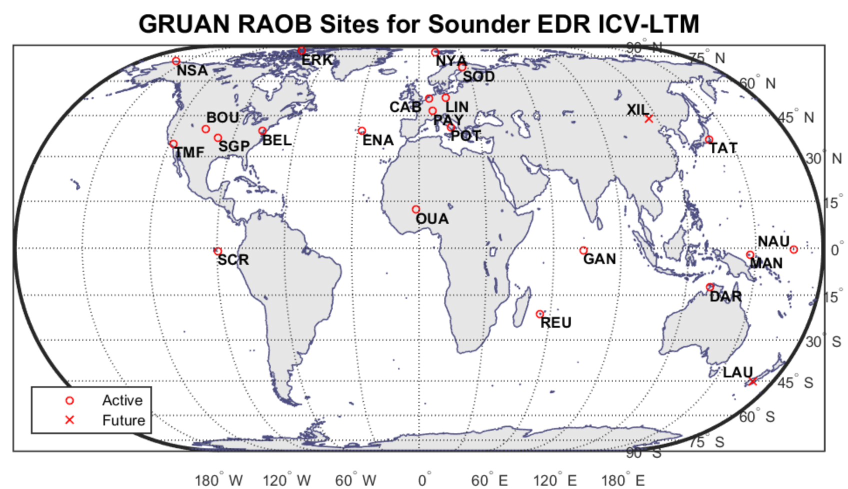




JPSS SNPP Dedicated Year 3 (2014-2015)



GRUAN Reference Sites

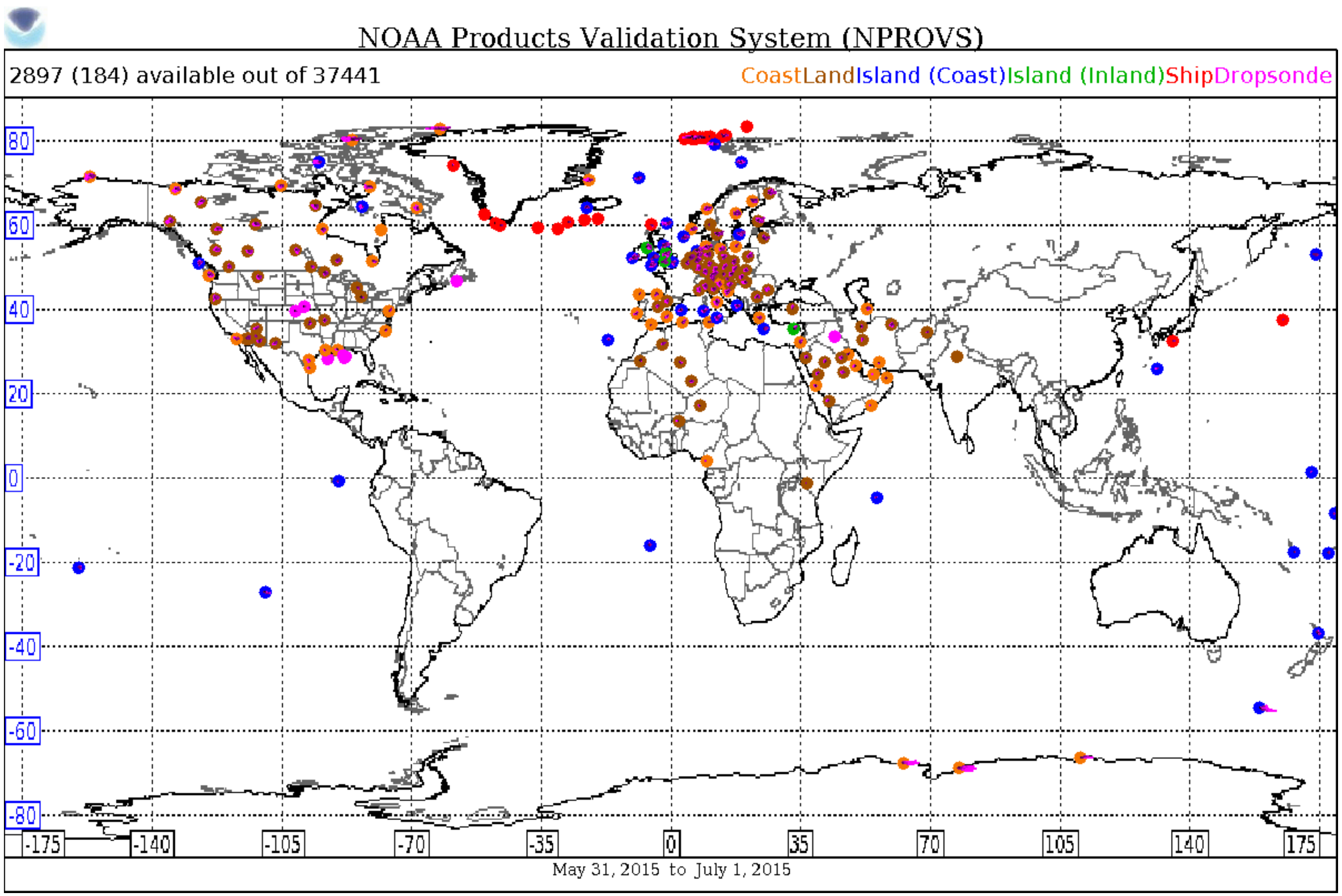


Validation of NOAA-Unique Operational Sounder EDR

NUCAPS EDR PRODUCT VALIDATION

NPROVS Conventional RAOB Collocations

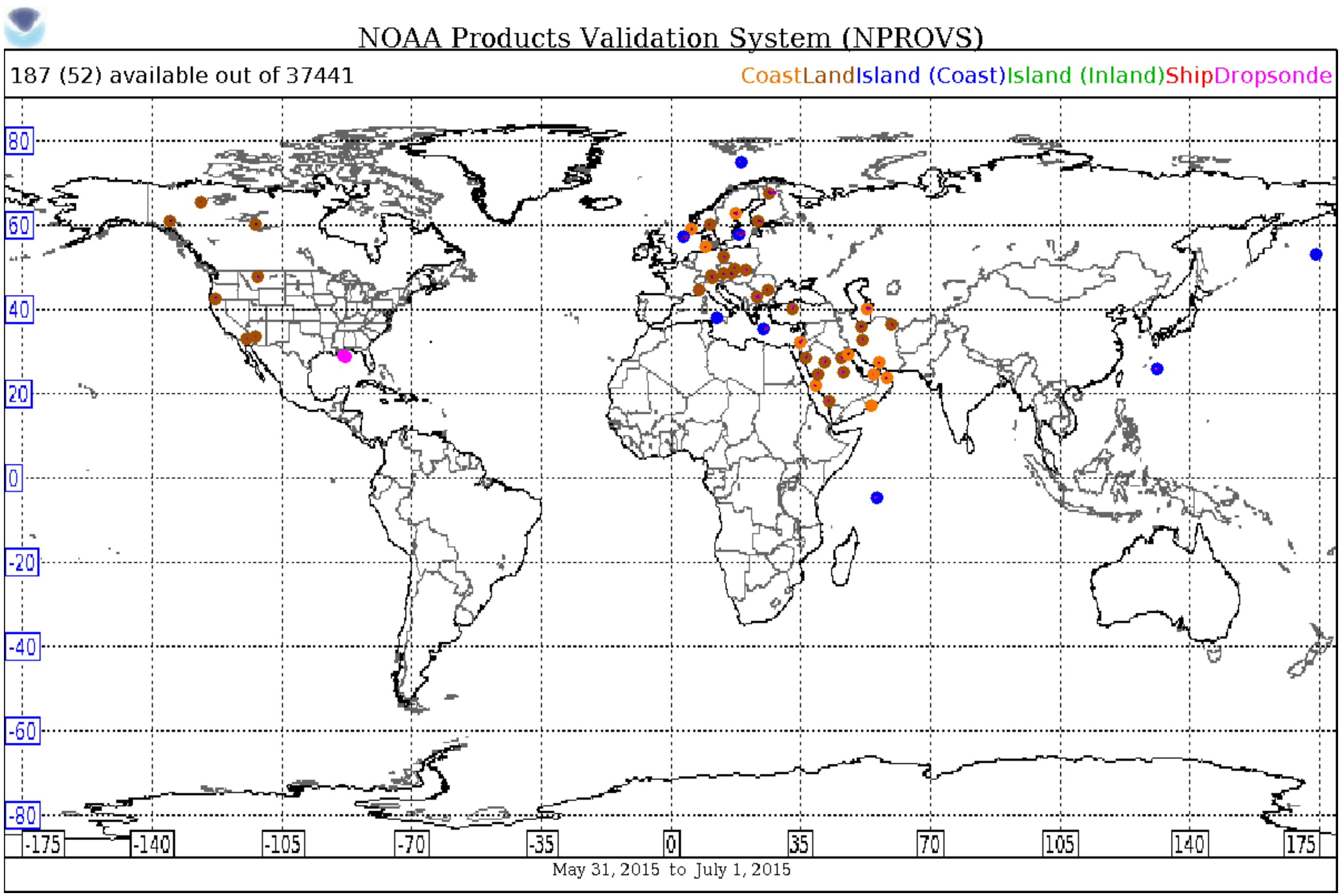
Single Closest FOR



- June 2015
- **RS92 and RS41 sondes**
- Single-closest FOR
- **Space-time window [1]**
  - **±3 h before/after overpass**
  - **75 km**
- **Sample size [1] *N* = 2897**

NPROVS Conventional RAOB Collocations

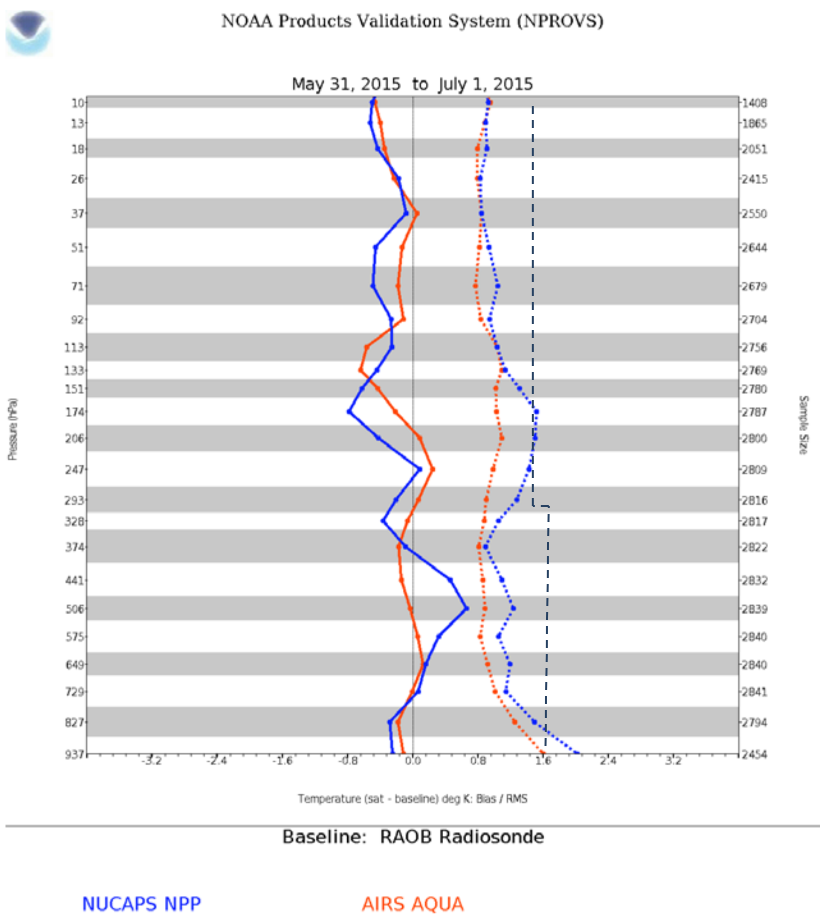
Single Closest FOR



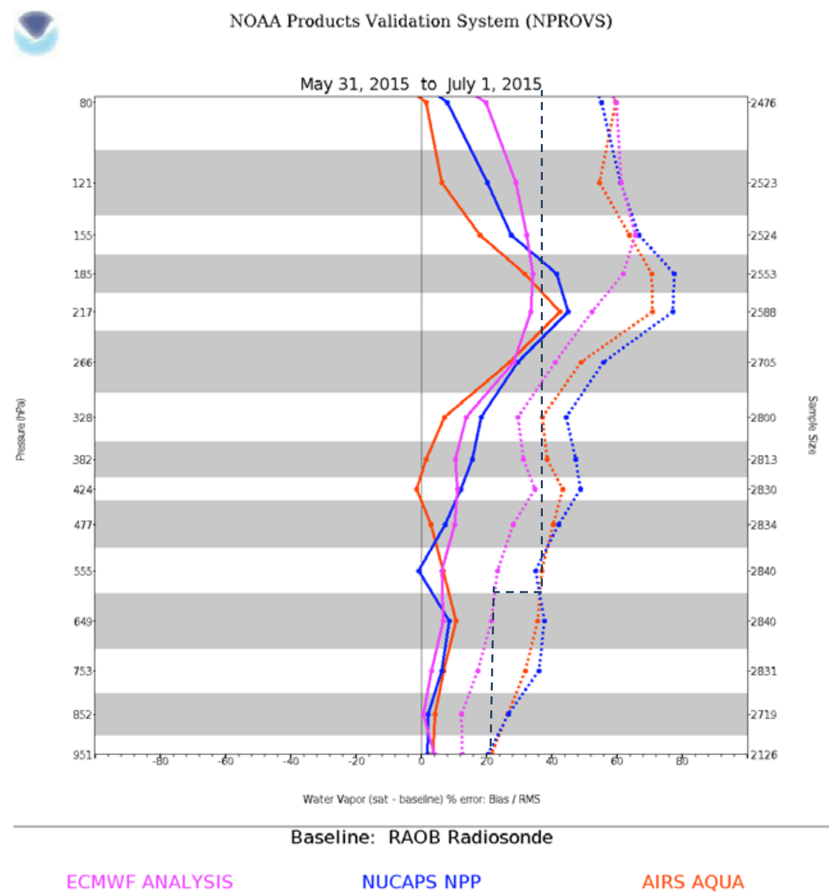
- June 2015
- **RS92 and RS41 sondes**
- Single-closest FOR
- **Space-time window [2]**
  - **−2 to +0.5 h before/after overpass**
  - **75 km**
- **Sample size [2] *N* = 187**

NUCAPS OPS-EDR and AIRS versus NPROVS Collocated Conventional RAOB: Sample [1]

AVTP (BIAS and RMS)

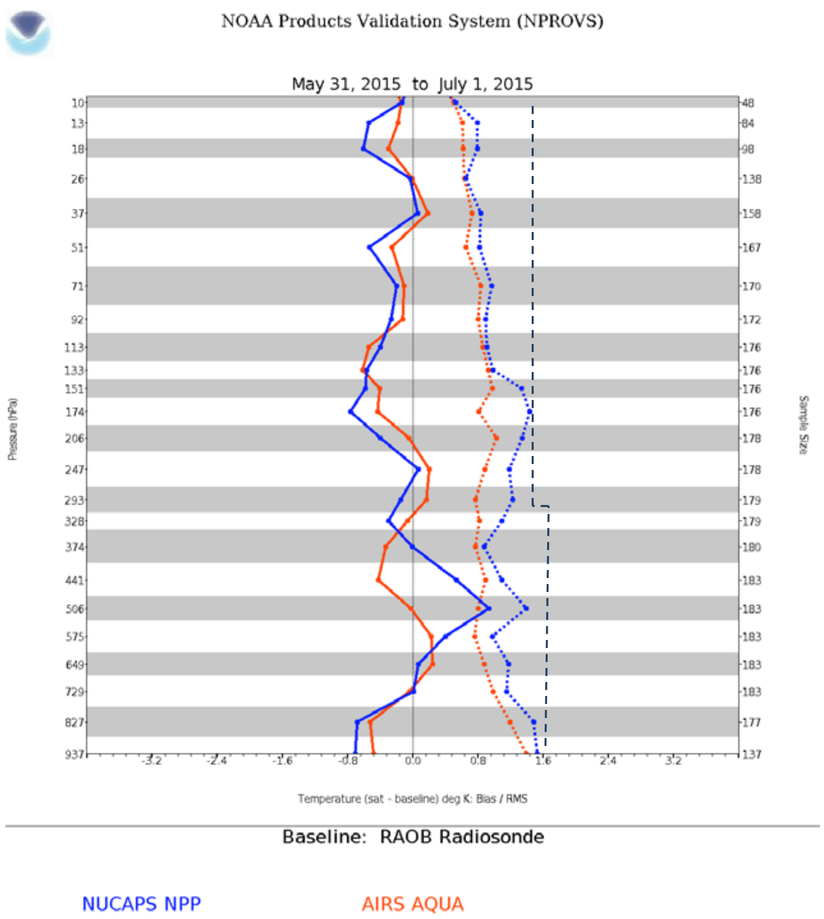


AVMP (BIAS and RMS)

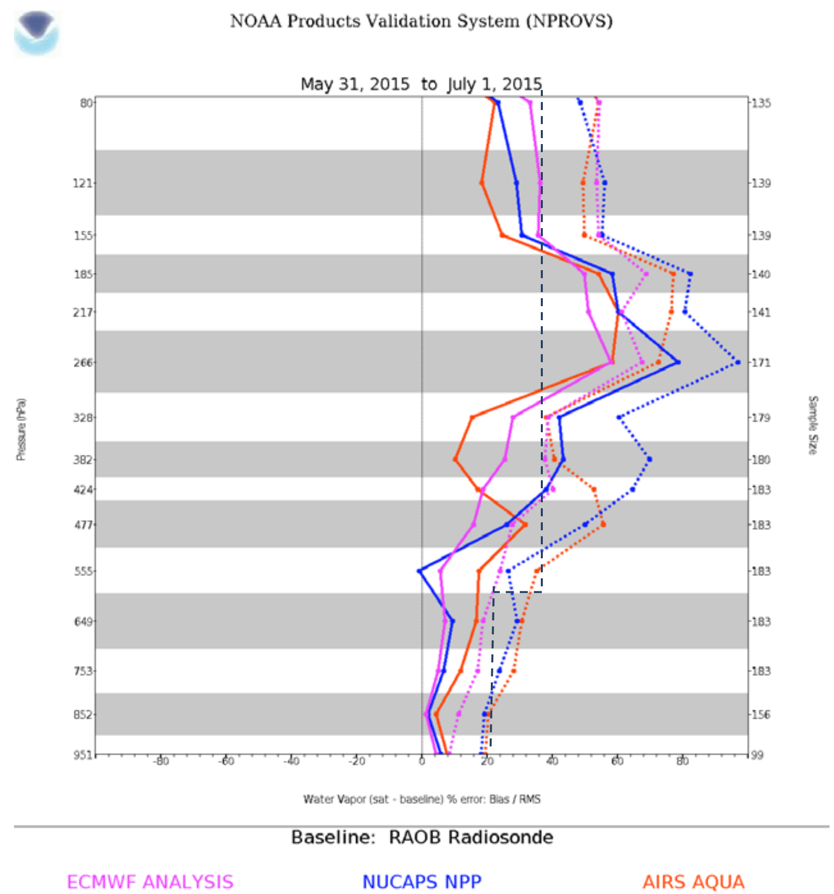


NUCAPS OPS-EDR and AIRS versus NPROVS Collocated Conventional RAOB: Sample [2]

AVTP (BIAS and RMS)



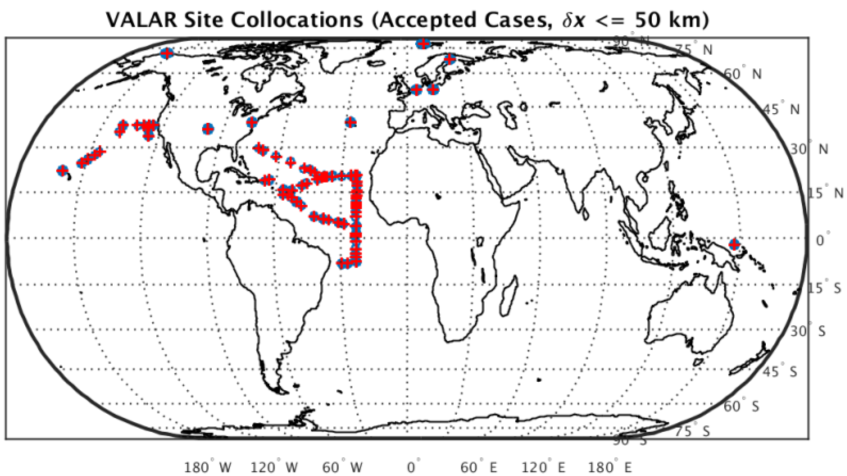
AVMP (BIAS and RMS)



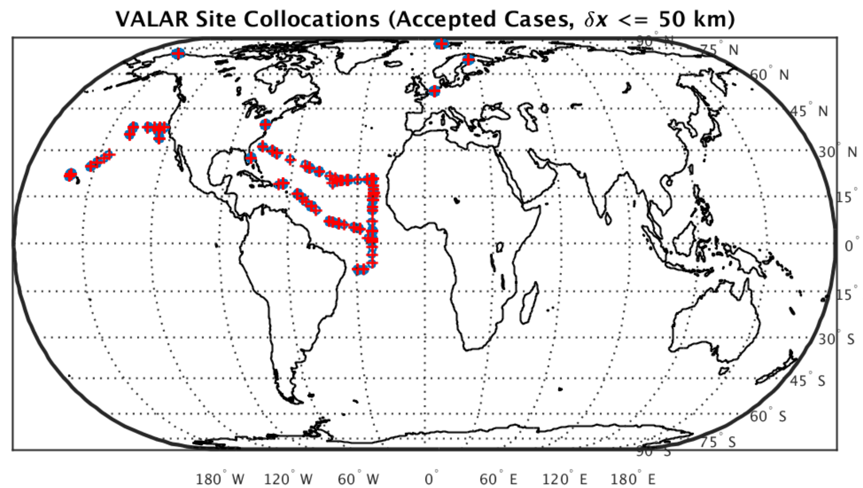
VALAR Dedicated/Reference RAOB Collocations

50 km radius

NUCAPS OPS-EDR Sample

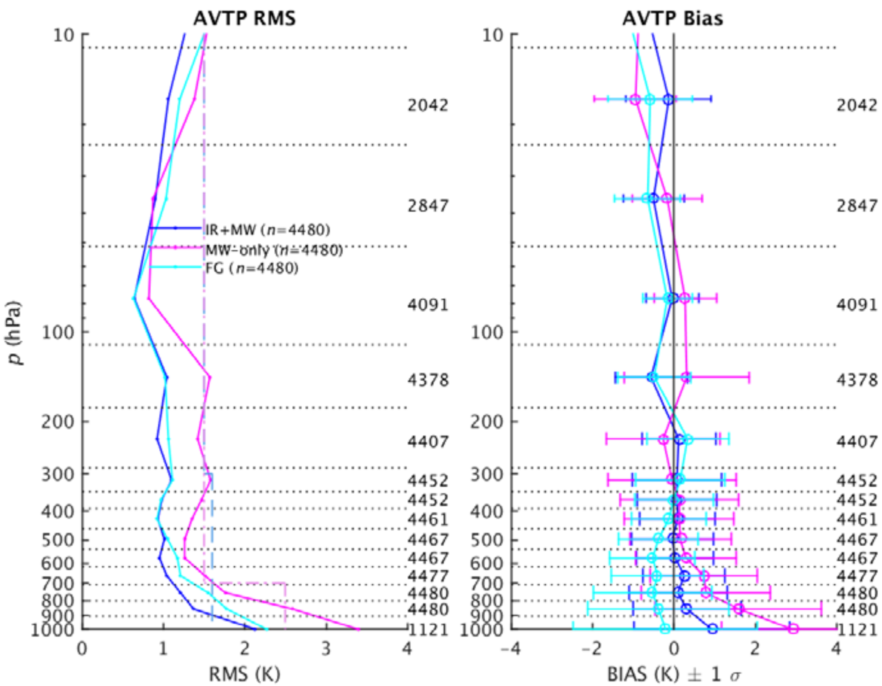


NUCAPS Offline (v1.5) Prelim Sample

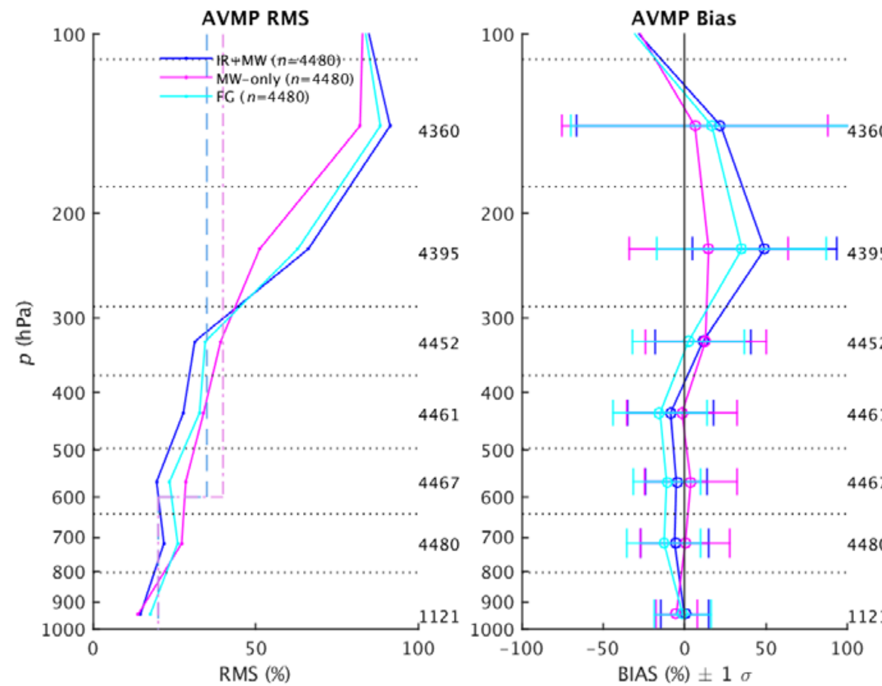


NUCAPS OPS-EDR
VALAR Dedicated/Reference RAOB Sample

AVTP

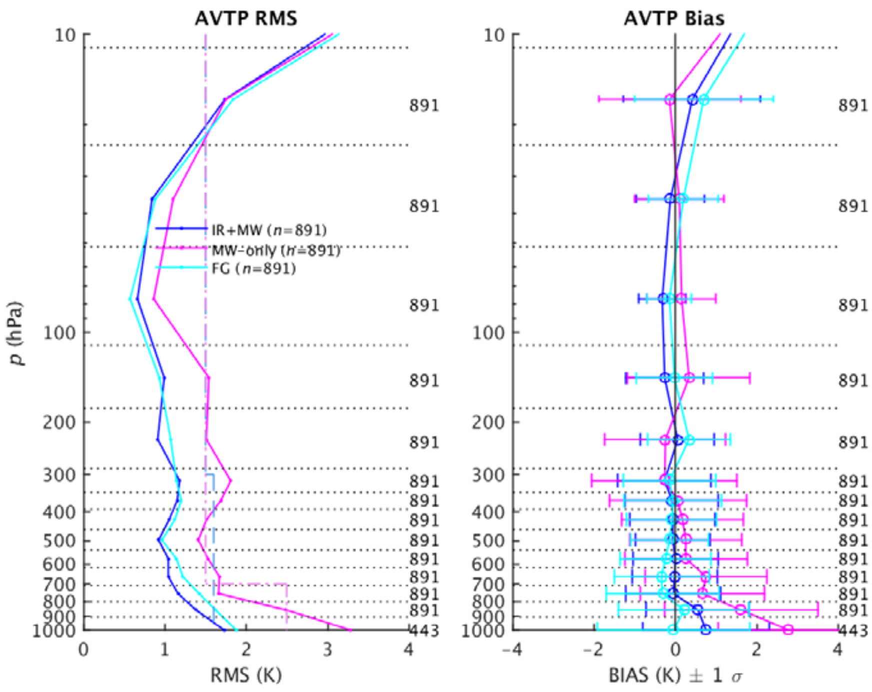


AVMP

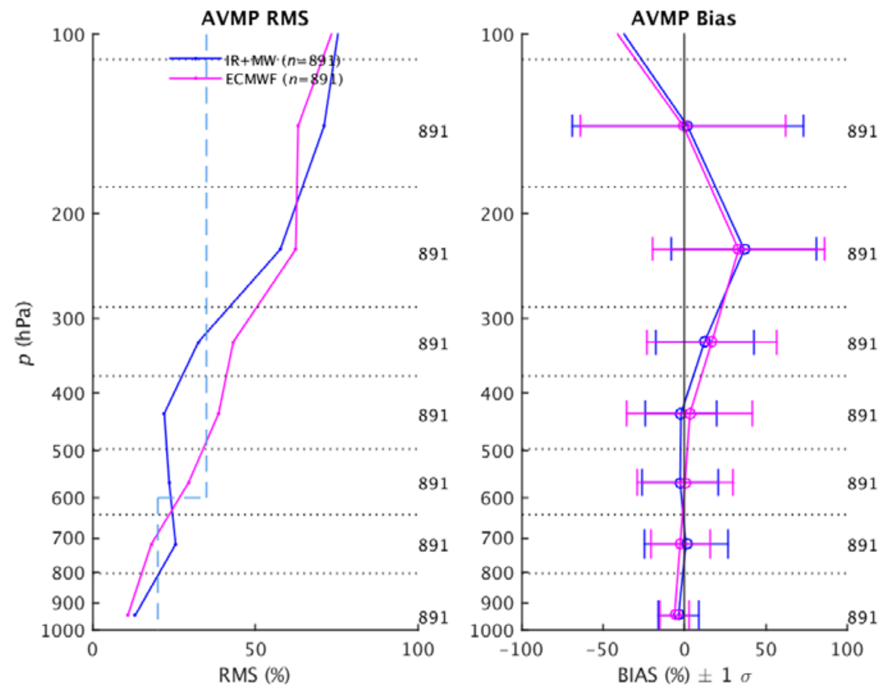


NUCAPS Offline (v1.5) EDR
VALAR Dedicated/Reference RAOB Prelim Sample

AVTP



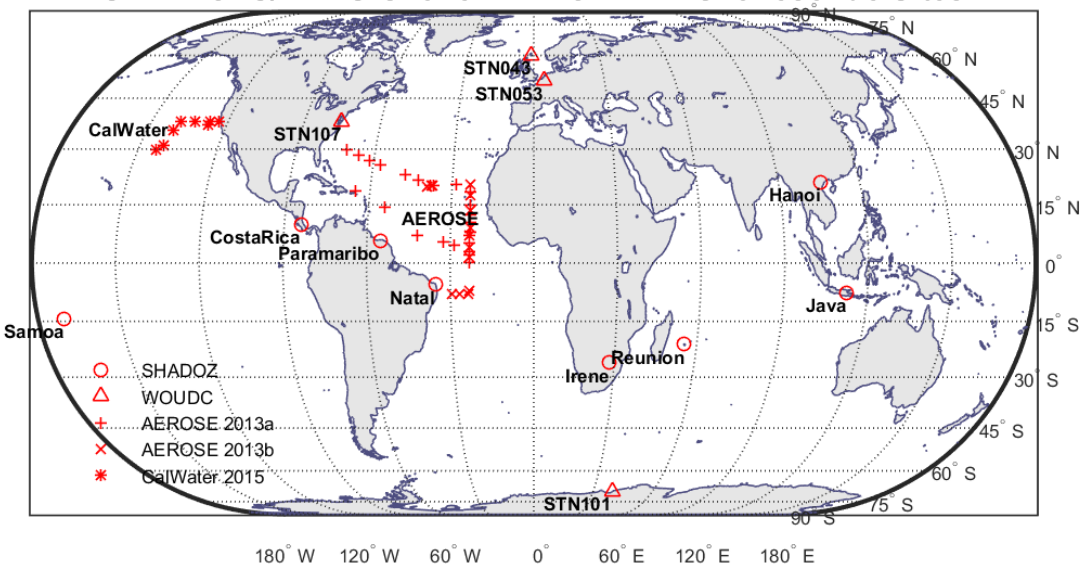
AVMP



NUCAPS Trace Gas Validation *In Situ* Truth Datasets

- **Collocated ozonesondes** for **O_3 (ozone) profile EDR**
  - **Dedicated Ozonesondes**
    - **NOAA AEROSE** (*Nalli et al.* 2011)
    - **CalWater/ACAPEX 2015**
  - **Sites of Opportunity**
    - **SHADOZ**
      - Costa Rica
      - Hanoi
      - Irene
      - Java
      - Natal
      - Paramaribo
      - Reunion
      - American Samoa
    - **WOUDC**
      - STN043
      - STN053
      - STN107
      - STN101
- Data suitable for carbon product CO, CO_2, CH_4 are currently being identified
  - MOZAIC aircraft (CO)
  - NOAA ESRL flask data (CO)
  - Satellite data (MLS, OCO-2, etc.)
  - Additional data currently being sought

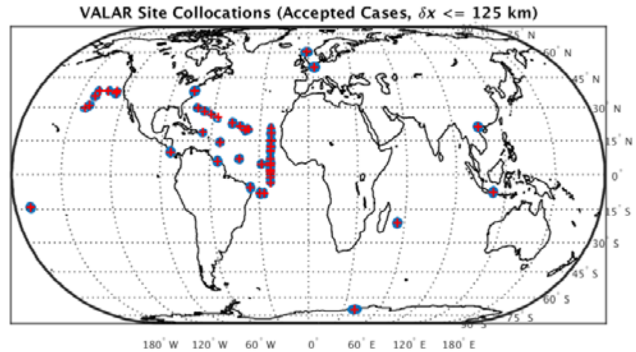
S-NPP CrIS/ATMS Ozone EDR ICV-LTM Ozonesonde Sites



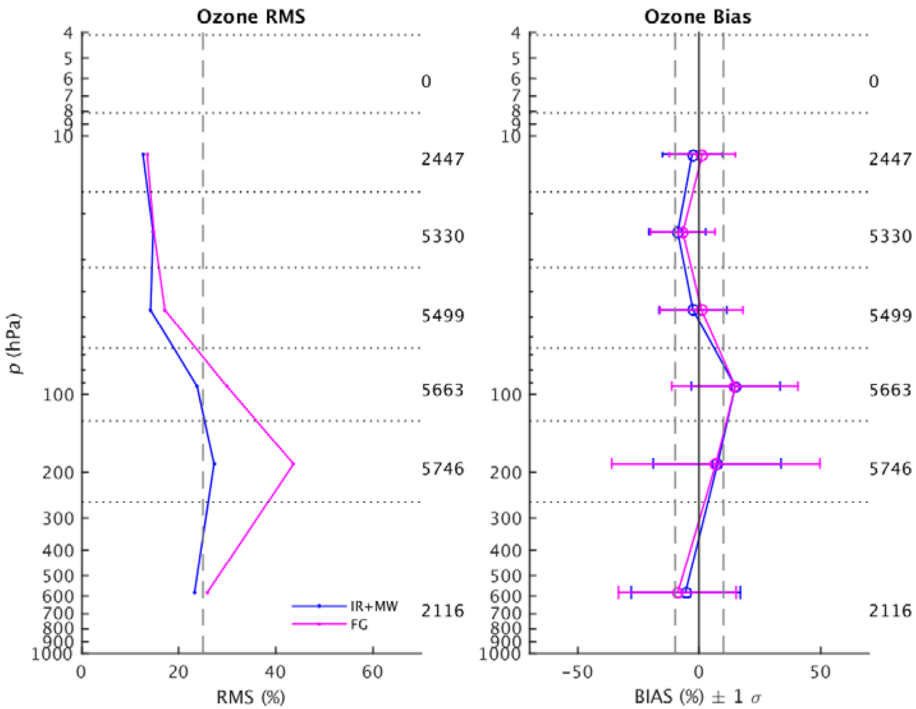
Stage-2 Ozone Profile Validation

NUCAPS Offline (v1.5) EDR versus Global Ozonesondes

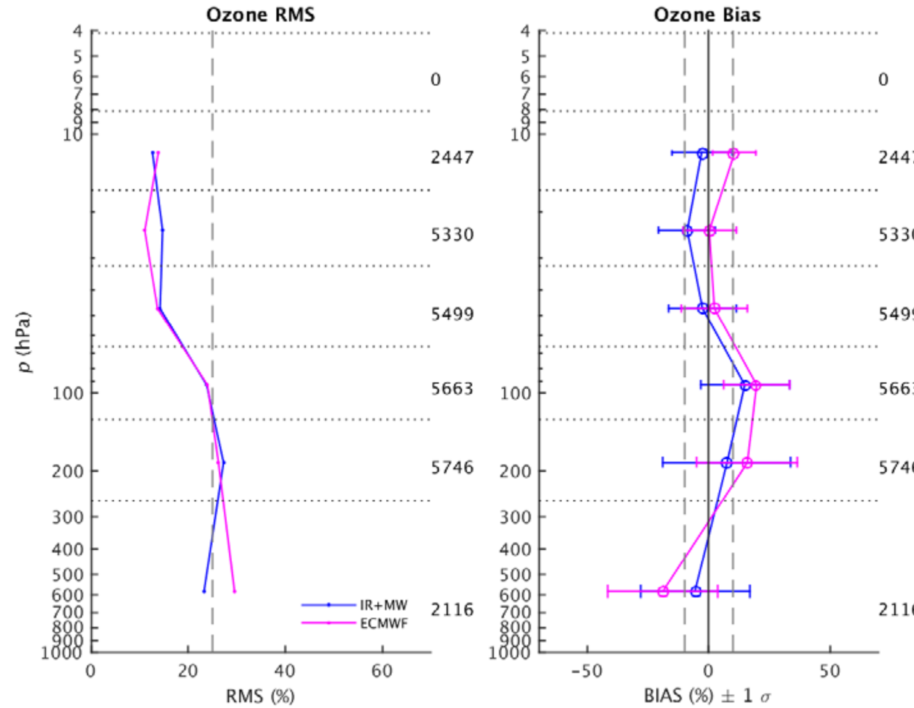
VALAR Dedicated, SHADOZ and WOUDC Ozonesonde Sample



Retrieval and *A Priori* First Guess

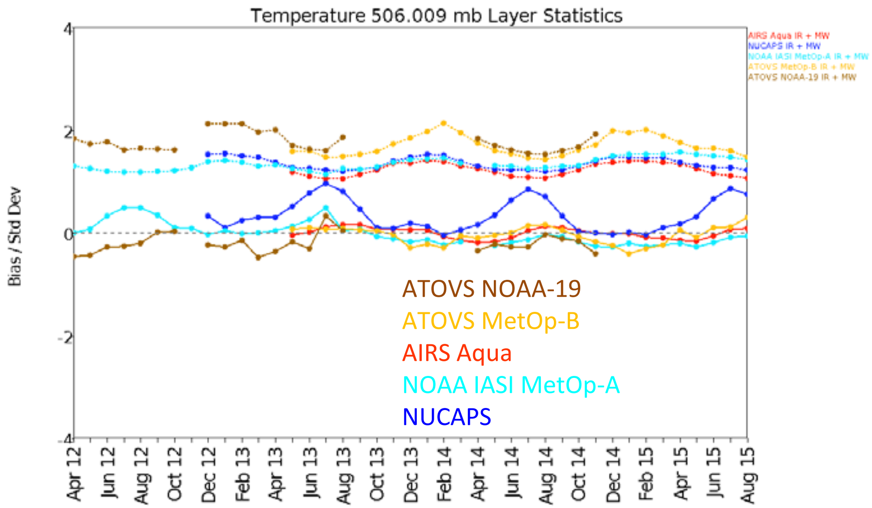


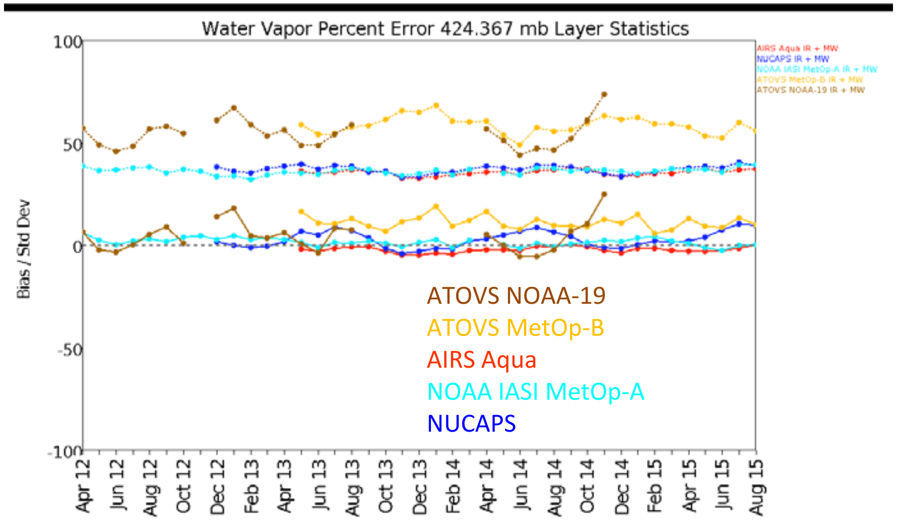
Retrieval and ECMWF



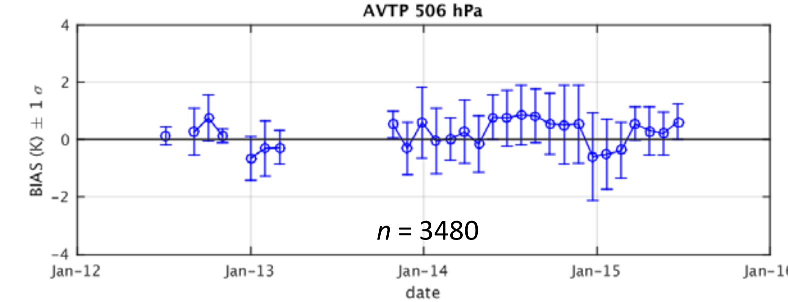
Long-Term Monitoring (LTM)

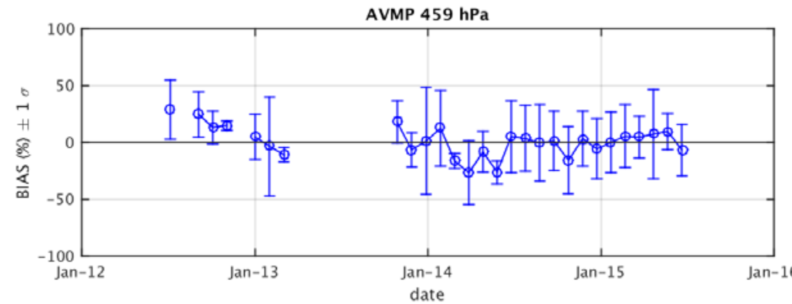
NPROVS NARCS Conventional RAOB Collocation (OPS-EDR)



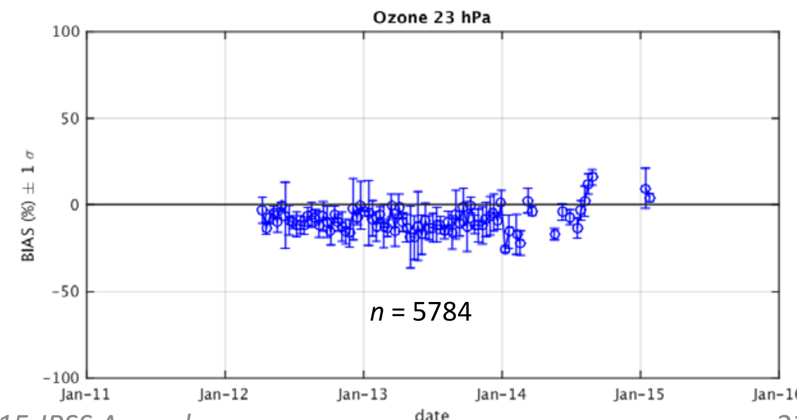


VALAR Dedicated/GRUAN Collocation (OPS-EDR)





VALAR Ozonesonde Collocation (Offline v1.5)



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 expansion, development and enhancements**
    - Support **AEROSE-X campaign (Atlantic Ocean, Nov-Dec 2015)**
    - Continue support of ARM dedicated RAOBs (including dual-launches, "best estimates")
    - Continue leveraging GRUAN reference RAOBs
    - Acquire carbon trace gas (CO, CO_2) truth 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 (CRTM, LBLRTM, SARTA, etc.)
  - Support skin SST EDR validation
  - Support EDR applications (AWIPS, AR/SAL, atmospheric chemistry users)

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 Offline (v1.5) EDR
VALAR Merged Dedicated/Reference RAOB + ECMWF

AVTP **AVMP**