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

Nicholas R. Nalli$^{1,2}$, A. Gambacorta$^{3}$, C. Barnet$^{3}$, Q. Liu$^{2}$, T. Reale$^{2}$, C. Tan$^{1,2}$, F. Iturbide-Sanchez$^{1,2}$, B. Sun$^{1,2}$, L. Borg$^{4}$, D. Tobin$^{4}$, E. Joseph$^{5}$, V. R. Morris$^{5}$, A. K. Mollner$^{6}$, T. King$^{1,2}$, W. W. Wolf$^{2}$, J. W. Smith$^{7}$, F. Tilley$^{1,2}$, D. Wolfe$^{8}$, et al.

$^{1}$IMSG, Rockville, Maryland, USA
$^{2}$NOAA/NESDIS/STAR, College Park, Maryland, USA
$^{3}$STC, Columbia, Maryland, USA
$^{4}$University of Wisconsin-Madison, Madison, Wisconsin, USA
$^{5}$Howard University, Washington, D.C., USA
$^{6}$The Aerospace Corp., El Segundo, California, USA
$^{7}$National Research Council, College Park, Maryland, USA
$^{8}$NOAA/ESRL/PSD, Boulder, Colorado, USA

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Outline

• JPSS Sounder EDR Cal/Val Overview
  – JPSS EDR validation
  – CrIS/ATMS (CrIMSS) Sounder Operational EDR
    ▪ NOAA-Unique CrIS/ATMS Processing System (NUCAPS)
  – JPSS Level 1 Requirements
  – Validation Methodology
    ▪ Validation “Hierarchy”
    ▪ Statistical Metrics
  – JPSS S-NPP 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
• **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 (O₃, CO, CO₂, CH₄)

[Images of NUCAPS AVTP, AVMP, O₃, CO]

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http://www.ospo.noaa.gov/Products/atmosphere/soundings/nucaps/index.html
**AVTP and AVMP EDR**

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>THRESHOLD</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVTP, Cloud fraction &lt; 50%, surface to 300 hPa</td>
<td>1.6 K / 1-km layer</td>
</tr>
<tr>
<td>AVTP, Cloud fraction &lt; 50%, 300–30 hPa</td>
<td>1.5 K / 3-km layer</td>
</tr>
<tr>
<td>AVTP, Cloud fraction &lt; 50%, 30–1 hPa</td>
<td>1.5 K / 5-km layer</td>
</tr>
<tr>
<td>AVTP, Cloud fraction &lt; 50%, 1–0.5 hPa</td>
<td>3.5 K / 5-km layer</td>
</tr>
<tr>
<td>AVTP, Cloud fraction ≥ 50%, surface to 700 hPa</td>
<td>2.5 K / 1-km layer</td>
</tr>
<tr>
<td>AVTP, Cloud fraction ≥ 50%, 700–300 hPa</td>
<td>1.5 K / 1-km layer</td>
</tr>
<tr>
<td>AVTP, Cloud fraction ≥ 50%, 300–30 hPa</td>
<td>1.5 K / 3-km layer</td>
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</tr>
<tr>
<td>AVTP, Cloud fraction ≥ 50%, 1–0.5 hPa</td>
<td>3.5 K / 5-km layer</td>
</tr>
</tbody>
</table>

**Trace Gas EDR**

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>THRESHOLD</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO (Carbon Monoxide) Total Column Precision</td>
<td>35%, or full res mode 15%</td>
</tr>
<tr>
<td>CO (Carbon Monoxide) Total Column Accuracy</td>
<td>±25%, or full res mode ±5%</td>
</tr>
<tr>
<td>CO₂ (Carbon Dioxide) Total Column Precision</td>
<td>0.5% (2 ppmv)</td>
</tr>
<tr>
<td>CO₂ (Carbon Dioxide) Total Column Accuracy</td>
<td>±1% (4 ppmv)</td>
</tr>
<tr>
<td>CH₄ (Methane) Total Column Precision</td>
<td>1% (=20 ppbv)</td>
</tr>
<tr>
<td>CH₄ (Methane) Total Column Accuracy</td>
<td>±4% (=80 ppmv)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>THRESHOLD</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₃ (Ozone) Profile Precision, 4–260 hPa (6 statistic layers)</td>
<td>20%</td>
</tr>
<tr>
<td>O₃ (Ozone) Profile Accuracy, 4–260 hPa (6 statistic layers)</td>
<td>±10%</td>
</tr>
<tr>
<td>O₃ (Ozone) Profile Uncertainty, 4–260 hPa (6 statistic layers)</td>
<td>25%</td>
</tr>
<tr>
<td>O₃ (Ozone) Profile Uncertainty, 260 hPa to sfc (1 statistic layer)</td>
<td>25%</td>
</tr>
</tbody>
</table>

**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.

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

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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

\[
\text{RMS}(\Delta T_{\mathcal{L}}) = \sqrt{\frac{1}{n_j} \sum_{j=1}^{n_j} (\Delta T_{\mathcal{L},j})^2} \quad \text{BIAS}(\Delta T_{\mathcal{L}}) \equiv \overline{\Delta T_{\mathcal{L}}} = \frac{1}{n_j} \sum_{j=1}^{n_j} \Delta T_{\mathcal{L},j} \\
\text{STD}(\Delta T_{\mathcal{L}}) \equiv \sigma(\Delta T_{\mathcal{L}}) = \sqrt{[\text{RMS}(\Delta T_{\mathcal{L}})]^2 - [\text{BIAS}(\Delta T_{\mathcal{L}})]^2}
\]

### AVMP and O₃

- 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

\[
\Delta q_{\mathcal{L},j} = \frac{q_{\mathcal{L},j} - q_{\mathcal{L},j}}{q_{\mathcal{L},j}} \quad \text{RMS}(\Delta q_{\mathcal{L}}) = \sqrt{\frac{\sum_{j=1}^{n_j} W_{\mathcal{L},j} (\Delta q_{\mathcal{L},j})^2}{\sum_{j=1}^{n_j} W_{\mathcal{L},j}}}, \quad \text{water vapor weighting factor, } W_{\mathcal{L},j},
\]

\[
\text{BIAS}(\Delta q_{\mathcal{L}}) = \frac{\sum_{j=1}^{n_j} W_{\mathcal{L},j} \Delta q_{\mathcal{L},j}}{\sum_{j=1}^{n_j} W_{\mathcal{L},j}}, \quad W_{\mathcal{L},j} = \begin{cases} 
1, & W^0 \\
q_{\mathcal{L},j}, & W^1 \\
(q_{\mathcal{L},j})^2, & W^2
\end{cases}
\]

\[
\text{STD}(\Delta q_{\mathcal{L}}) = \sqrt{[\text{RMS}(\Delta q_{\mathcal{L}})]^2 - [\text{BIAS}(\Delta q_{\mathcal{L}})]^2}
\]
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
  - Online 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
  - HDFS-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)

ACAPEX/CalWater2 Campaign (Jan-Feb 2015)
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)
NOAA Products Validation System (NPROVS)

AVMP (BIAS and RMS)
NOAA Products Validation System (NPROVS)

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

AVTP (BIAS and RMS)

NOAA Products Validation System (NPROVS)

September 1, 2014 to September 11, 2014

Pressure (hPa)

Temperature (sat-baseline) deg K; Bias / Std Dev

Baseline: Radiosonde Radiosonde

AIRS AQUA  NUCAPS NPP

AVMP (BIAS and RMS)

NOAA Products Validation System (NPROVS)

September 1, 2014 to September 11, 2014

Pressure (hPa)

Water Vapor (sat-baseline) % error: Bias / Std Dev

Baseline: Radiosonde Radiosonde

AIRS AQUA  NUCAPS NPP
VALAR RAOB sample weighted by zonal surface areas

Large random error due to RAOB drift in high latitudes?

n = 1881
VALAR RAOB sample weighted by zonal surface areas

Extreme dry subsidence in tropical sites (AEROSE)?
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

VALAR Site Accepted Matchups ($\delta x \leq 125$ km)

Ozone RMS ($n_{qa}=902$)

Ozone Bias ($n_{qa}=902$)
Long-Term Monitoring (LTM)

NPROVS NARCS Conventional RAOB Collocation

- Temperature 506.00 mb Layer Statistics
- NPROVS
- NARCS
- Conventional RAOB
- VALAR
- Dedicated/GRUAN/Ozonesonde Collocation

ATOVS NOAA-19
AIRS Aqua
NOAA IASI MetOp-A
NUCAPS

VALAR Dedicated/GRUAN/Ozonesonde Collocation

- AVTP 506 hPa
  - $n = 1838$
- AVMP 459 hPa
- Ozone 12 hPa
  - $n = 893$

Water Vapor Percent Error 424.367 mb Layer Statistics

ATOVS NOAA-19
AIRS Aqua
NOAA IASI MetOp-A
NUCAPS
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 (O₃, CO, CO₂) 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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• Contributions to the S-NPP validation data collection effort: B. Demoz and M. Oyola (Howard University); J. E. Wessel (Aerospace).
The measurement equation (e.g., *Taylor and Kuyatt*, 1994) for retrieval includes forward and inverse operators (*Rodgers*, 1990) to estimate the measurand, \( x \), on forward model layers:

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

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 \( \rightarrow \) column abundances), interpolate to RTA (arbitrary) levels, then compute RTA layer quantities, e.g.,

\[
\sum_x(z) = \int_{z_f}^{z} N_x(z') \, dz'
\]
NUCAPS AVTP/AVMP (NDE-OPS) versus VALAR Dedicated RAOB
Ocean Only Day and Night

RAOB sample weighted by zonal surface areas

VALAR Site Accepted Matchups ($\delta x \leq 75$ km)

$n = 382$