SNPP NUCAPS Full Spectral Resolution Trace Gas Validation Status

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Acknowledgments

- **SNPP Sounder Trace Gas EDR Validation Truth Dataset collection**
  - **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**

- **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 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

Oct 2017

Nalli et al. – Fall 2017 NSSTM
## JPSS Specification Performance Requirements

### CrIS Trace Gas EDR Uncertainty ($O_3$, CO, $CO_2$, CH$_4$)

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>THRESHOLD</th>
<th>OBJECTIVE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_3$ (Ozone) Profile Precision, 4–260 hPa (6 statistic layers)</td>
<td>20%</td>
<td>10%</td>
</tr>
<tr>
<td>$O_3$ (Ozone) Profile Precision, 260 hPa to sfc (1 statistic layer)</td>
<td>20%</td>
<td>10%</td>
</tr>
<tr>
<td>$O_3$ (Ozone) Profile Accuracy, 4–260 hPa (6 statistic layers)</td>
<td>±10%</td>
<td>±5%</td>
</tr>
<tr>
<td>$O_3$ (Ozone) Profile Accuracy, 260 hPa to sfc (1 statistic layer)</td>
<td>±10%</td>
<td>±5%</td>
</tr>
<tr>
<td>$O_3$ (Ozone) Profile Uncertainty, 4–260 hPa (6 statistic layers)</td>
<td>25%</td>
<td>15%</td>
</tr>
<tr>
<td>$O_3$ (Ozone) Profile Uncertainty, 260 hPa to sfc (1 statistic layer)</td>
<td>25%</td>
<td>15%</td>
</tr>
<tr>
<td>CO (Carbon Monoxide) Total Column Precision</td>
<td>35%, or full res mode 15%</td>
<td>3%</td>
</tr>
<tr>
<td>CO (Carbon Monoxide) Total Column Accuracy</td>
<td>±25%, or full res mode ±5%</td>
<td>±5%</td>
</tr>
<tr>
<td>$CO_2$ (Carbon Dioxide) Total Column Precision</td>
<td>0.5% (2 ppmv)</td>
<td>1.05 to 1.4 ppmv</td>
</tr>
<tr>
<td>$CO_2$ (Carbon Dioxide) Total Column Accuracy</td>
<td>±1% (4 ppmv)</td>
<td>NS</td>
</tr>
<tr>
<td>CH$_4$ (Methane) Total Column Precision</td>
<td>1% (=20 ppbv)</td>
<td>NS</td>
</tr>
<tr>
<td>CH$_4$ (Methane) Total Column Accuracy</td>
<td>±4% (=80 ppmv)</td>
<td>NS</td>
</tr>
</tbody>
</table>

*Source: (L1RD, 2014, pp. 45-49)*
## Validation Methodology Hierarchies

### $T$/H$_2$O/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 Network Matchup Assessments**
   - Total Carbon Column Observing Network (TCCON) spectrometers (Wunch et al. 2010, 2011)
   - AirCore balloon-borne in situ profile measurements (Membrive et al. 2017)
   - Provide routine independent measurements representing global zones akin to RAOBs
   - Limitations: Small sample sizes, uncertainties in unit conversions, different sensitivities to atmospheric layers

4. **Intensive Field Campaign In Situ Data Assessments**
   - Include ancillary datasets, ideally funded aircraft campaign(s)
   - E.g., ATom, ACT-America, 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 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
Observed 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 CH₄, offline v6 runs for CO₂ 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 CO₂, CO, CH₄, N₂O 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 CO₂, stats are performed simply for atmospheric column averages (in PPMV)

- For NUCAPS CO, CH₄ profile EDRs on 100 RTA layers are integrated to obtain total column abundances (molecules/cm²) (e.g., Nalli et al. 2013)

  \[
  \sum_i(x) \approx \int_{z_i}^{z} N_i(z') \, dz' \\
  \sum_i(x_s) \approx F_{BL} N_{i,L_b} \delta z_{L_b} + \sum_{L=1}^{L_b-1} N_{i,L} \delta z_L
  \]

- TCCON CO, CH₄ (in dry mole fractions, ppm) are converted to total column abundance \( \Sigma_i \) (molecules/cm²) using the following formula

  \[
  \sum_i(x) = \frac{N_A p_s}{g M_{dry}} - \varepsilon \Sigma_{w_i}(x_s)
  \]

  where \( x_i \) is the TCCON-measured dry mole fraction for species \( i \), and \( \Sigma_{w_i} \) is the H₂O column abundance (provided by NUCAPS retrieval).

- A more rigorous methodology employing the TCCON averaging kernels is currently being researched and implemented, and will be the subject of near-future work
Status of NUCAPS FSR Trace Gas EDR Validation

SNPP NUCAPS VERSUS AIRS
Total Column Carbon Monoxide (CO) EDRs
17 Feb 2015 Focus Day, All Cases

AIRS v6
AIRS CO (17-Feb-15, ASC)

NUCAPS v2.0.5.4
NUCAPS v2.0.5.4 acc CO (17-Feb-15, ASC)

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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

AIRS v6
AIRS CH$_4$ (17–Feb–15, ASC)

NUCAPS v2.0.5.4
NUCAPS v2.0.5.4 acc CH$_4$ (17–Feb–15, ASC)

AIRS CH$_4$ (17–Feb–15, DES)

NUCAPS v2.0.5.4 acc CH$_4$ (17–Feb–15, DES)
NUCAPS v2.0.5.4 CH\textsubscript{4} – AIRS v6 CH\textsubscript{4}

17 Feb 2015 Focus Day, Accepted Cases

NUCAPS v2.0.5.4 acc – AIRS CH\textsubscript{4} (17–Feb–15, ASC)

NUCAPS v2.0.5.4 acc – AIRS CH\textsubscript{4} (17–Feb–15, DES)
Total Column Carbon Dioxide ($CH_2\) EDRs
17 Feb 2015 Focus Day, All Cases

AIRS v6 acc average CO$_2$ (17–Feb–15, ASC)

NUCAPS v2.0.5.4 acc average CO$_2$ (17–Feb–15, ASC)

AIRS v6 acc average CO$_2$ (17–Feb–15, DES)

NUCAPS v2.0.5.4 acc average CO$_2$ (17–Feb–15, DES)
NUCAPS v2.0.5.4 CO$_2$ – AIRS v6 CO$_2$
17 Feb 2015 Focus Day, Accepted Cases

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Status of NUCAPS FSR Trace Gas EDR Validation

SNPP NUCAPS VERSUS TCCON
TCCON (Wunch et al. 2011)
NUCAPS-AIRS vs TCCON Box Plots
17 Feb 2015 Focus Day

NUCAPS v2.0.5.4 acc (17-Feb-15)

All FOR within threshold radius (150 km)
Time window (±6 hours) versus mean TCCON
NUCAPS-AIRS vs TCCON Scatter Plots
17 Feb 2015 Focus Day

NUCAPS v2.0.5.4 acc (17-Feb-15)

All FOR within threshold radius (150 km)
Time window (±6 hours) versus mean TCCON

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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 Stations (17-Feb-15 17-Jul-15 Focus Days)

TCCON (Wunch et al. 2011)
NUCAPS vs TCCON Boxplots
17 Feb 2015 and 17 Jul 2015 Focus Days

NUCAPS v2.0.5.4 acc (17-Feb-15 17-Jul-15)

Carbon Monoxide

Methane

Carbon Dioxide

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

NUCAPS v2.0.5.4 acc (17-Feb-15 17-Jul-15)

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

NUCAPS v2.0.5.4 acc (17-Feb-15 17-Jul-15)

Carbon Monoxide

$n = 128$

Methane

$n = 128$

Carbon Dioxide

$n = 128$
### NUCAPS v2.0 FSR Trace Gas Summary Stats

<table>
<thead>
<tr>
<th></th>
<th>TCCON Baseline One Focus Day $N = 151$</th>
<th>TCCON Baseline Two Focus Days $N = 128$</th>
<th>AIRS Baseline One Focus Day $N = O(100,000)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trace Gas EDR</td>
<td>BIAS (%)</td>
<td>STD (%)</td>
<td>RMS (%)</td>
</tr>
<tr>
<td><strong>CO</strong></td>
<td>+2.1 (±5.0)</td>
<td>12.9 (15.0)</td>
<td>13.1</td>
</tr>
<tr>
<td><strong>CO$_2$</strong></td>
<td>−0.3 (±1.0)</td>
<td>0.6 (0.5)</td>
<td>0.7</td>
</tr>
<tr>
<td><strong>CH$_4$</strong></td>
<td>−3.0 (±4.0)</td>
<td>4.4 (1.0)</td>
<td>5.3</td>
</tr>
</tbody>
</table>

Yield = 83.4%  Yield = 83.7%  Yield = 83.4%
## NUCAPS EDR Maturity Status

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

<table>
<thead>
<tr>
<th>Sensor</th>
<th>Product</th>
<th>Priority</th>
<th>Validated Maturity Review Date &amp; Status</th>
<th>Review Panel Recommendations</th>
</tr>
</thead>
<tbody>
<tr>
<td>CrIS/ATMS</td>
<td>Atm. Vertical Moisture Profile (AVMP)</td>
<td>3</td>
<td>*</td>
<td>Validated Maturity</td>
</tr>
<tr>
<td>CrIS/ATMS</td>
<td>Atm. Vertical Temperature Profile (AVTP)</td>
<td>3</td>
<td>*</td>
<td>Validated Maturity</td>
</tr>
<tr>
<td>CrIS/ATMS</td>
<td>Ozone Profile EDR</td>
<td>3</td>
<td>Oct-2016</td>
<td>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</td>
</tr>
<tr>
<td>CrIS</td>
<td>Outgoing Longwave Radiation</td>
<td>3</td>
<td>Oct-2016</td>
<td>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</td>
</tr>
<tr>
<td>CrIS/ATMS</td>
<td>Carbon Monoxide</td>
<td>4</td>
<td>&amp;</td>
<td>Validated Maturity Review for Fall 2017</td>
</tr>
<tr>
<td>CrIS/ATMS</td>
<td>Carbon Dioxide</td>
<td>4</td>
<td>&amp;</td>
<td>Validated Maturity Review for Fall 2017</td>
</tr>
<tr>
<td>CrIS/ATMS</td>
<td>Methane</td>
<td>4</td>
<td>&amp;</td>
<td>Validated Maturity Review for Fall 2017</td>
</tr>
</tbody>
</table>

*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.
CO, CH₄, CO₂ Trace Gas Summary

- **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 in this presentation show the products are reasonably close to meeting JPSS Level 1 requirements.

- **Next Steps / Future Work**
  - **Process additional Focus Days** to increase the TCCON data sample
    - Including at least 2 additional days for Spring and Autumn seasons
  - **Apply TCCON AKs (currently underway, results forthcoming)**
  - Pending results of above, may need to 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**
  - **Utilize field campaign datasets** (e.g., ATom)
  - **Utilize AirCore datasets** where available
  - **Further optimization of NUCAPS trace gas a priori**
Status of NUCAPS FSR Trace Gas EDR Validation

THANK YOU! QUESTIONS?