Validation of Atmospheric Profile Retrievals From the SNPP NOAA-Unique Combined Atmospheric Processing System. Part 1: Temperature and Moisture

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Validation of Atmospheric Profile Retrievals From the SNPP NOAA-Unique Combined Atmospheric Processing System. Part 1: Temperature and Moisture

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***Abstract*— This paper provides an overview of the validation of the operational atmospheric vertical temperature profile (AVTP) and atmospheric vertical moisture profile (AVMP) environmental data record (EDR) products retrieved from the Cross-track Infrared Sounder (CrIS) and the Advanced Technology Microwave Sounder (ATMS), two passive sounding systems onboard the Suomi National Polar-Orbiting Partnership (SNPP) satellite. The CrIS/ATMS suite serves as the U.S. low earth orbit (LEO) satellite sounding system and will span the future Joint Polar Satellite System (JPSS) LEO satellites. The operational sounding algorithm is the National Oceanic and Atmospheric Administration-Unique Combined Atmospheric Processing System (NUCAPS), a legacy sounder science team algorithm capable of retrieving atmospheric profile EDR products with optimal vertical resolution under nonprecipitating (clear to partly cloudy) conditions. The SNPP NUCAPS AVTP and AVMP EDR products are validated using extensive global *in situ* baseline data sets, namely, radiosonde observations launched from ground-based networks and ocean-based intensive field campaigns, along with numerical weather prediction model output. Based upon statistical analyses using these data sets, the SNPP AVTP and AVMP EDRs are determined to meet the JPSS Level 1 global performance requirements.**

***Index Terms*— Atmospheric profiles, calibration/validation (cal/val), environmental satellite, Joint Polar Satellite System (JPSS), National Oceanic and Atmospheric Administration (NOAA)-Unique Combined Atmospheric Processing System (NUCAPS), retrieval, soundings, Suomi National Polar-Orbiting Partnership (SNPP).**

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I. Introduction

The U.S. Suomi National Polar-Orbiting Partnership (SNPP) satellite was launched in 2011 and is the first operational U.S. satellite to feature the high spectral-resolution ("hyperspectral") Cross-track Infrared Sounder (CrIS) and Advanced Technology Microwave Sounder (ATMS) sounding system (previously referred to collectively as the Cross-track Infrared Microwave Sounder Suite (CrIMSS) [1]). The follow-on Joint Polar Satellite System (JPSS) is a U.S. National Oceanic and Atmospheric Administration (NOAA) operational satellite mission, in collaboration with joint international partnerships and the U.S. National Aeronautics and Space Administration [2], that will support NOAA's weather, climate, and environmental monitoring missions by providing operational timely global data to users. JPSS series will feature CrIS/ATMS onboard four satellites launched in the same orbit over the next two decades beginning in 2017. The CrIS/ATMS sounding system is designed to measure well-calibrated infrared (IR) and microwave (MW) radiances or sensor data records (SDRs) for synergistically retrieving atmospheric vertical profile environmental data records (EDRs) under nonprecipitating conditions (clear, partly cloudy, and cloudy) with relatively high vertical resolution (≈2–5 km) in much the same manner as predecessor sounding systems, namely, the MetOp-A and -B IR Atmospheric Sounding Interferometer (IASI) [3], [4] and the EOS-Aqua Atmospheric IR Sounder (AIRS) [5], [6]. The CrIS instrument is an advanced Fourier transform spectrometer that measures high-resolution IR spectra in 1305 channels over three bands spanning $\nu = [650, 2550]$ cm^{-1} (high spectral resolution is hereafter simply referred to as "hyperspectral"). The ATMS is an MW sounder with 22 channels ranging from 23 to 183 GHz [7]. These two instruments operate in an overlapping field-of-view (FOV) formation analogous to AIRS, with ATMS FOVs resampled to match the location and size of the 3×3 CrIS FOVs for retrievals under clear to partly cloudy conditions.

While hyperspectral sounder SDRs (radiances) have generally come to be directly assimilated into global numerical weather prediction models via variational analysis schemes, they also continue to be directly inverted operationally to retrieve orbital atmospheric profile EDRs in near-real time as originally envisioned by satellite sounding pioneers [8]–[13]. The operational EDR retrieval algorithm for CrIS/ATMS is currently the NOAA-Unique Combined Atmospheric Processing System (NUCAPS) developed at NOAA/National Environmental Satellite Data and Information Service (NESDIS)/Satellite Applications and Research (STAR) [14], [15], which superseded the original Interface Data Processing Segment (IDPS) CrIMSS algorithm in September 2013. The NUCAPS algorithm processes CrIS/ATMS data based on the heritage methodology developed for the EOS-Aqua AIRS and MetOp IASI systems, with the retrieval algorithm being a modular implementation of the multistep AIRS Science Team retrieval algorithm version 5 [16], [17]. For more details on the NUCAPS algorithm, the reader is referred to [15] and [16], or the algorithm theoretical basis document [18] available online. The primary EDR parameters retrieved by NUCAPS are the atmospheric vertical temperature profile (AVTP) and atmospheric vertical moisture profile (AVMP), which are output on the University of Maryland Baltimore County (UMBC) radiative transfer algorithm (RTA) [19] 100 levels (i.e., layer boundaries) and layers, respectively. In addition to AVTP and AVMP, NUCAPS retrieves ozone (O_3) and carbon trace gases, including carbon monoxide (CO), carbon dioxide (CO_2), and methane (CH_4) profile EDRs on 100 RTA layers. Current users of the NUCAPS EDRs include NOAA National Weather Service weather forecast offices via the Advanced Weather Interactive Processing System. Sounder EDRs are also invaluable for numerous global environmental research studies [20], [21].

The NUCAPS algorithm operates under clear to partially cloudy conditions by first cloud-clearing [16] the 3×3 CrIS FOV arrays, which are referred to as the "field of regard" (FOR). Fig. 1 shows a schematic of the CrIS/ATMS FOV sampling for an example NUCAPS FOR. The current method selects a 3×3 array of ATMS footprints[1] based on a center footprint matched with CrIS, and then simply averages the antenna temperature data records (TDRs) for each channel to obtain the value for a single MW footprint (thereby emulating the earlier AIRS/AMSU configuration illustrated in [5]). Although there are more sophisticated ways of doing this (e.g., matching individual footprints instead of simply the center), they have been found to have very small impact and may even lead to scene-dependent biases. Then, by assuming that radiance differences in the FOV are only due to clouds, a "clear-column" IR radiance spectrum is extrapolated for each FOR. More details and discussion on the cloud-clearing methodology and cloud-cleared radiance product can be found in numerous previously published papers [14], [16], [22]. The multistep NUCAPS physical retrieval module then retrieves individual parameters sequentially (as opposed to simultaneously), using only channels rigorously determined to be sensitive to each parameter [23], beginning with temperature, then water vapor, followed by ozone and other trace gases. Fig. 2 shows the selected CrIS IR channels in

[1]The term "footprint" refers to the sensor FOV projected onto the earth's surface.

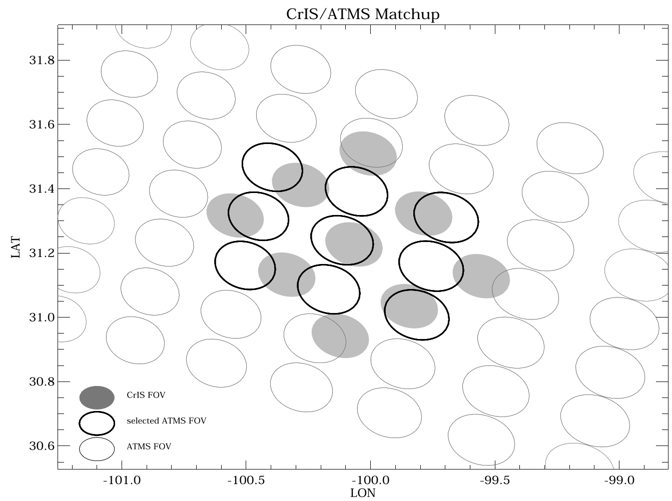

Fig. 1. Example CrIS/ATMS FOV configuration for a single NUCAPS FOR used for cloud clearing. The cross-track scanning direction is roughly top left/bottom right and the gray unfilled ellipses show approximate ATMS FOV footprints for a beam width of 1.1° (channels 17–22) [7]. The gray ellipses show the 3×3 CrIS FOV footprints comprising a NUCAPS FOR, and the black unfilled ellipses show the selected ATMS footprints (based on the center footprint matched to a CrIS footprint) comprising an effective MW FOV analogous to the AIRS/AMSU configuration [5]. The ellipses depicted are approximations for illustration purposes only and do not represent the exact spatial footprints of those instruments.

the longwave, midwave, and shortwave IR bands used for the AVTP and AVMP retrievals. The operational NUCAPS algorithm (version 1.5) has run on nominal CrIS resolution spectra at $\Delta\nu \approx 0.625$, 1.25, and 2.5 cm^{-1} for the longwave, midwave, and shortwave IR bands, respectively [1], [2].

To ensure that the SNPP NUCAPS-retrieved EDR products meet their mission specification objectives, in this paper, we have conducted a formal validation of the AVTP and AVMP EDRs (v1.5 nominal CrIS resolution) using radiosonde collocations from land-based networks and ocean-based dedicated launches. Section II provides an overview of the JPSS EDR calibration/validation (cal/val) program, Section III characterizes the operational algorithm performance (v1.5) based on rigorous statistical analyses, and finally Section V presents preliminary results (i.e., based on numerical model comparisons) of the NUCAPS algorithm for CrIS full-resolution data delivered in July–August 2017 (v2.0.5) in preparation for the launch of the JPSS-1 satellite. Validation of the operational NUCAPS IR ozone profile product will be the subject of the Part 2 companion paper.

II. JPSS Sounder EDR Cal/Val Overview

The direct goal of validating EDRs is to provide a general assessment and error characterization of the retrieved parameters relative to an assumed "truth" (or baseline) data set. Continued assessments in this manner in turn enable ongoing development and/or improvement of algorithms. Validation of EDRs can also facilitate the routine monitoring of SDRs from which they are derived (e.g., sea surface temperature EDRs [24]).

To support cal/val and long-term monitoring (LTM) of the SNPP satellite SDRs and retrieved EDRs, the JPSS cal/val program defines four phases for cal/val of sensors and algorithms throughout the satellite mission lifetime [25]: prelaunch, early

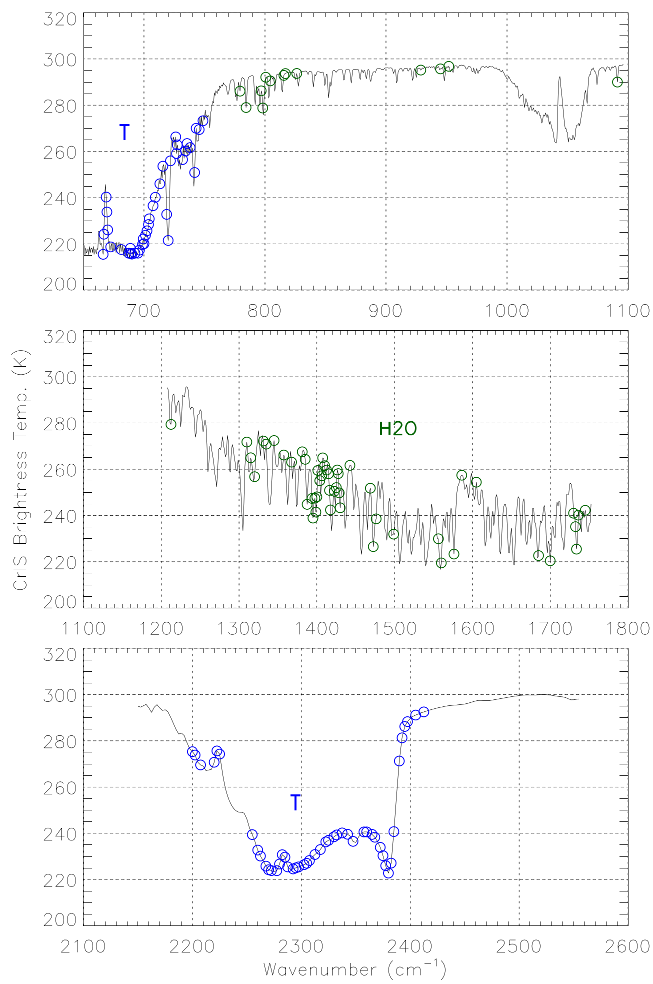

Fig. 2. Hamming apodized CrIS IR brightness temperature spectra for a marine nighttime case (10:22 UTC June 9, 2015, 6.5°N, 130.0°W) showing temperature and water vapor channels (blue and green circles, respectively) used in the NUCAPS multistep physical retrieval. (Top) Longwave IR (unapodized nominal resolution 0.625 cm^{-1}). (Middle) Midwave IR (unapodized nominal resolution 1.25 cm^{-1}). (Bottom) Shortwave IR (unapodized nominal resolution 2.5 cm^{-1}).

orbit checkout, intensive cal/val, and LTM. In accordance with the JPSS phased schedule, the SNPP CrIS/ATMS EDR cal/val plan was devised to ensure that the EDR would meet the mission Level 1 requirements [26]. The CrIS/ATMS EDR cal/val plan for the successor JPSS-1 satellite (or "J-1") was drafted during July–August 2015 and submitted on December 31, 2015.

The JPSS Level 1 performance requirements[2] for AVTP and AVMP are reproduced in Tables I and II, respectively. These serve as the metrics by which the system is considered to have reached validated maturity and met mission requirements. It is noted that the requirements are defined for global non-precipitating cases on three to five atmospheric "broad layers" that are computed as an average of "coarse layers" ranging from 1–5 km in thickness for AVTP and 2 km for AVMP. "Partly cloudy" conditions are defined by a successful cloud-clearing and IR retrieval converging to a solution. Conversely, "cloudy" conditions are defined by cases where cloud clearing is not successful and the IR algorithm is not able to converge to a solution, thereby resulting in an MW-only algorithm solution as the final product. It is in this manner that the NUCAPS system is capable of providing AVTP/AVMP

[2]In satellite product parlance, "Level 1" typically refers to the lowest level of the product chain (e.g., raw data records or SDRs) whereas "Level 2" refers to higher level EDRs or retrievals. However, in the current context of JPSS requirements, "Level 1" is a programmatic term that refers to the "highest level" program requirement.

TABLE I

JPSS Level 1 Requirements[a] for CrIS/ATMS AVTP Measurement Uncertainty

Global AVTP Measurement Uncertainty Requirement[b]		
Atmospheric Broad-Layer	Threshold	Objective
Cloud-Free to Partly Cloudy (IR+MW)[c]		
Surface to 300 hPa[d] (1 km layers)	1.6 K	0.5 K
300 hPa to 30 hPa (3 km layers)	1.5 K	0.5 K
30 hPa to 1 hPa (5 km layers)	1.5 K	0.5 K
1 hPa to 0.5 hPa (5 km layers)	3.5 K	0.5 K
Cloudy (MW-only)[e]		
Surface to 700 hPa (1 km layers)	2.5 K	0.5 K
700 hPa to 300 hPa (1 km layers)	1.5 K	0.5 K
300 hPa to 30 hPa (3 km layers)	1.5 K	0.5 K
30 hPa to 1 hPa (5 km layers)	1.5 K	0.5 K
1 hPa to 0.5 hPa (5 km layers)	3.5 K	0.5 K

[a] Source: Joint Polar Satellite System (JPSS) Program Level 1 Requirements Supplement – Final, Version 2.10, 25 June 2014, NOAA/NESDIS.
[b] Expressed as an error in layer average temperature.
[c] Partly cloudy conditions are those where both the IR and MW retrievals are used and are typically scenes with ≤ 50% cloudiness.
[d] The IR+MW surface to 300 hPa requirement is for over global ocean. Over land and ice mass, the Uncertainty is relaxed slightly to 1.7 K due to the state of the science of the land emissivity knowledge within the temperature sounding algorithm.
[e] Cloudy conditions are those where only the MW retrievals are used and are typically scenes with > 50% cloudiness.

TABLE II

JPSS Level 1 Requirements[a] for CrIS/ATMS AVMP Measurement Uncertainty

Global AVMP Measurement Uncertainty Requirement[b]		
Atmospheric Broad-Layer	Threshold	Objective
Cloud-Free to Partly Cloudy (IR+MW)[c]		
Surface to 600 hPa	greater of 20% or 0.2 g kg^{-1}	10%
600 hPa to 300 hPa	greater of 35% or 0.1 g kg^{-1}	10%
300 hPa to 100 hPa	greater of 35% or 0.1 g kg^{-1}	10%
Cloudy (MW-only)[d]		
Surface to 600 hPa	greater of 20% or 0.2 g kg^{-1}	10%
600 hPa to 300 hPa	greater of 40% or 0.1 g kg^{-1}	10%
300 hPa to 100 hPa	greater of 40% or 0.1 g kg^{-1}	NS

[a] Source: Joint Polar Satellite System (JPSS) Program Level 1 Requirements Supplement – Final, Version 2.10, 25 June 2014, NOAA/NESDIS.
[b] Expressed as a percent of average in 2 km layers.
[c] Partly cloudy conditions are those where both the IR and MW retrievals are used and are typically scenes with ≤ 50% cloudiness.
[d] Cloudy conditions are those where only the MW retrievals are used and are typically scenes with > 50% cloudiness.

retrievals for global nonprecipitating conditions. The original IDPS CrIMSS operational algorithm was validated through beta and provisional maturities [27], and the successor SNPP NUCAPS algorithm formally attained validated maturity in September 2014 [25] based on the analyses detailed below.

III. Temperature and Moisture Profile Assessment

Satellite sounder EDR validation methodology has been well established in previous validation work (i.e., with AIRS and IASI), with the various approaches being roughly classified as part of a hierarchy that includes [28]: 1) global numerical model comparisons; 2) satellite EDR intercomparisons; 3) conventional radiosonde assessments; 4) dedicated/reference radiosonde assessments; and 5) intensive campaign dissections. Those at the beginning of the hierarchy are typically employed in the early cal/val stages of a satellite's lifetime, whereas those near the top are employed during later stages.

A. Data

To allow for adequate validation of the SNPP operational sounder EDRs, JPSS has directly and indirectly funded a dedicated radiosonde program leveraging several collaborating institutions. Dedicated radiosonde observations (RAOBs) are optimally collocated and synchronous with SNPP overpasses at various selected sites. In addition, we have leveraged Global Climate Observing System Reference Upper Air Network (GRUAN) RAOB sites (discussed in detail below). Collocations of NUCAPS CrIS/ATMS FORs with RAOBs are facilitated via the NOAA Products Validation System (NPROVS) [29]. NPROVS routinely collocates single-closest EDR profile retrievals from multiple platforms (including SNPP) with RAOB launch "anchor points." Using this base RAOB-satellite collocation system, an EDR validation archive has been created whereby CrIS SDR and ATMS TDR granules in the vicinity of RAOB "anchor points" are acquired for running offline retrievals, thus allowing flexibility and ongoing algorithm optimization and development.

Fig. 3 shows JPSS-funded dedicated RAOB sites for the SNPP sounder validation effort through 2016. These include U.S. DOE Atmospheric Radiation Measurement (ARM) sites [30], [31], namely, Southern Great Plains (SGP), North Slope of Alaska (NSA), Tropical Western Pacific (TWP) (Manus Island), and Eastern North Atlantic (ENA) sites. (The TWP site was discontinued in August 2014 and funded dedicated launches were subsequently transferred to the ENA site.) JPSS has also supported ship-based dedicated radiosondes during intensive campaigns of opportunity over open ocean during the 2013a,b/2015 NOAA Aerosols and Ocean Science Expeditions (AEROSE) [32], [33] and the January–February 2015 CalWater ARM Cloud Aerosol Precipitation Experiment (ACAPEX) [21], [34]. In addition to these, two collaborative land-based sites of opportunity (with data acquisition objectives spanning satellite sounder validation) include the Howard University Beltsville Center for Climate System Observation (BCCSO) site in Beltsville, Maryland, and combined RAOB and lidar data collected by the Aerospace Corporation from the Pacific Missile Range Facility (PMRF) site in Kauai, Hawaii [35]. Finally, there are three GRUAN sites that fortuitously happen to collocate well with SNPP overpasses; these are Lindenberg (LIN), Germany, Cabauw (CAB), the Netherlands, and Sodankyla (SOD), Finland [36]. These sites "automatically" collocate because of the local time zone, which is approximately UTC +1 h. Given that synoptic launch times are at 00 and 12 UTC, the local times of launches from these sites are ≈01:00 and 13:00 LT. The sun-synchronous SNPP orbit has local equator crossing times of 01:30 and 13:30 LT; thus, the satellite happens to overpass these locales just following the launches, thereby fortuitously "mimicking" dedicated launches.

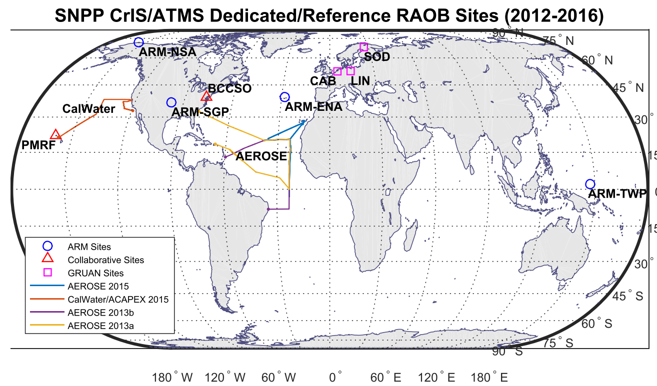

Fig. 3. SNPP-dedicated and GRUAN reference RAOB truth sites used for JPSS CrIS/ATMS EDR cal/val over the period 2012–2016. Blue circles denote ARM sites (NSA, SGP, TWP, and ENA), red triangles denote collaborative partner sites (BCCSO and PMRF), magenta squares denote collocated GRUAN reference sites (LIN, CAB, and SOD), and different colored lines denote ocean-based intensive campaign ship tracks (AEROSE and CalWater/ACAPEX). Map projection is equal area.

B. Error Analysis

Using these *in situ* data as the baseline, we compute coarse-layer and broad-layer uncertainties (defined in Section II) for AVTP and AVMP EDRs derived from an offline emulation[3] of the operational NUCAPS algorithm running on nominal CrIS resolution data (version 1.5). Details on the methodology for calculating coarse-layer statistics, namely, bias, standard deviation (σ), and root-mean-square uncertainty (RMSE) are described in [28]; for AVMP, we consistently apply W^2 moisture weighting to both the bias and RMSE calculations [28]. To minimize mismatch error in our statistical analyses, stringent space–time collocation criteria are applied, namely, quality-accepted retrievals within $\delta x \leq 75$ km radius and $-60 < \delta t < 0$ min of launches (the time criterion ensures that the radiosonde is airborne coincident with the satellite overpass). These criteria strike a good balance between sample size and mismatch error [37]. For the MW-only retrievals, it is noted again here that the JPSS requirements are specified for "cloudy" cases (i.e., >50% cloudiness, defined by failure of the IR algorithm to obtain an accepted solution; see Section II); thus,

[3]The offline code is an exact emulation of the operational code. However, the offline version generates additional diagnostic output files in Level 2 binary format, which facilitate validation on large samples. The offline code also enables algorithm development.

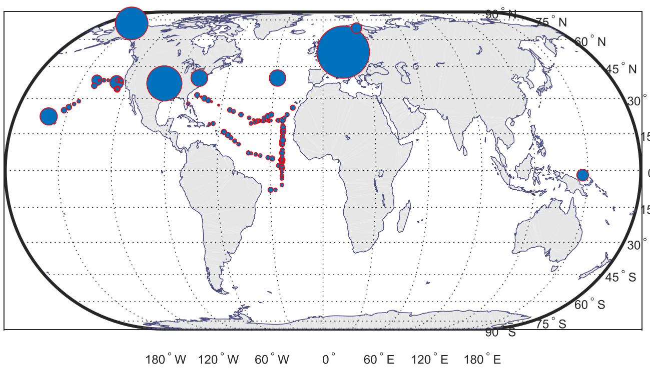

Fig. 4. Geographic histogram of SNPP CrIS/ATMS FOR-RAOB showing zonal representation of collocation data used in the global land/sea statistical error analysis. Circle areas depict the relative SNPP-RAOB collocation sample sizes for each RAOB launch location (prior to zonal and land/sea area weighting described in the text). Map projection is equal area.

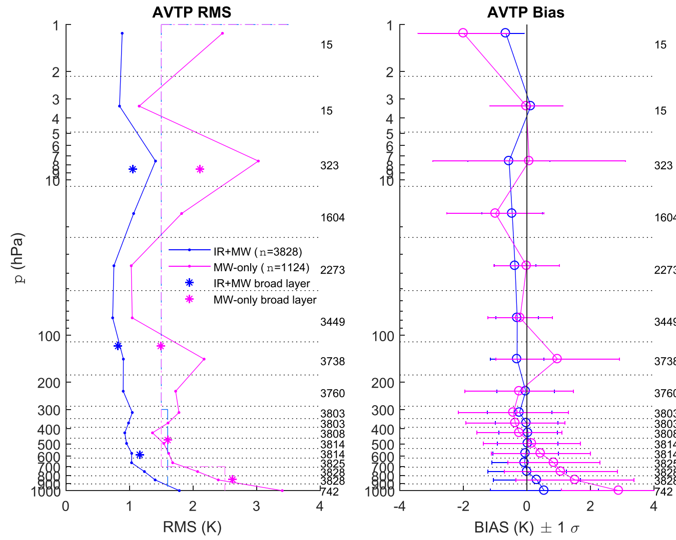

Fig. 5. Coarse-layer statistical uncertainty assessment of the NUCAPS AVTP EDR retrievals (offline v1.5 operational emulation) versus collocated dedicated/reference RAOBs for retrievals accepted by the quality flag within space–time collocation criteria of $\delta x \leq 75$ km radius and $-60 \leq \delta t \leq 0$ min of launches over a sampling period of January 9, 2013 to December 13, 2015. (Left) RMSE results. The light-blue dashed line in the RMS plots designate the JPSS Level 1 global performance requirements for "broad layers," and the asterisks show the calculated broad-layer RMSE. (Right) Bias $\pm 1\sigma$ results. NUCAPS IR+MW (clear to partly cloudy, defined by IR+MW accepted cases) and MW-only (cloudy, defined by the intersection of MW-only accepted cases and IR+MW rejected cases) performances are given in blue and magenta, respectively, with IR+MW collocation sample size for each coarse layer given in the right margins.

the MW-only samples are given by cases accepted by the MW-only quality flag but rejected by the IR+MW quality flag. Fig. 4 shows a geographic histogram (on an equal-area map projection) of the distribution of the RAOB collocation sample, where it can be seen that the combination of the RAOB sites described above provides an adequate coverage of global climate zones (tropics, midlatitudes, and polar) along with land and ocean surfaces. However, it is also noted that midlatitude land-based sites tend to dominate the sample, whereas the JPSS Level 1 requirements are derived based on global model calculations that cover the earth's ocean/land/zonal surface areas. Therefore, we subsequently apply a geographic zonal area weighting scheme over 15°latitude zones and land/sea surface areas in our statistical calculations. This scheme gives proportionately greater weight to tropical ocean RAOB collocations and lesser weight to high-latitude land-based collocations, which is in accordance with the JPSS requirements implicitly having such weighting built in.

The resulting global profile error statistics for AVTP and AVMP are given in Figs. 5 and 6, respectively. Figs. 5 (right) and 6 (right) show the bias statistics given by the coarse-layer means with $\pm 1\sigma$ given by the error bars. The JPSS Level 1 specification requirements are defined in terms of RMS statistics shown with dashed lines in Figs. 5 (left) and 6 (left). The corresponding broad-layer results for AVTP and AVMP retrievals are shown with asterisks and summarized in Tables III and IV, respectively. We find that both EDRs meet the JPSS requirements for both IR+MW and MW-only cases, with the only exception being MW-only AVTP for the upper tropospheric layer (30–1 hPa), which falls somewhat outside of the 1.5 K requirement for this layer. However, we see in Fig. 5 that the collocation samples fall off dramatically starting at about 14 hPa as radiosonde balloons tend to burst somewhere below this level. In fact, it should be noted that the available 15 data points in the top two layers above 5 hPa are due to merged lidar-RAOB data provided by the PMRF site [35]. In Fig. 5 (right), an elevated random error (magenta $\pm 1\sigma$ bars) occurs in the coarse layer between 10 and 5 hPa, and a significant negative bias (magenta line) occurs above 2 hPa, although this cannot be considered statistically significant. It should be noted that the MW-only samples correspond to cases rejected by the IR+MW quality flag; thus, sample sizes are ≈30% the IR+MW sizes and generally correspond to more difficult geophysical cases. A more detailed examination of the AVTP performance from 110 to 10 hPa versus radio occultation measurements showing comparable results can be found in [38].

The reader may also have noted that in Fig. 6, the AVMP results for the 300–100 hPa broad layer fall outside the requirement lines for both the IR+MW (blue asterisk) and MW-only retrievals, with an oscillation between significant positive and negative biases in the two coarse layers comprising the broad layer. Some of these discrepancies are believed to be associated with biases and precision limitations in the RAOBs. For RAOB temperature, it is due to radiation-induced biases [39], and for moisture, it is associated with extremely low water vapor conditions, a known problem at higher levels of the troposphere [40]. For moisture, this explanation is supported by a completely consistent pattern of discrepancies in bias with profiles from the European Centre for Medium-Range Weather Forecasts (ECMWF) model as seen in Fig. 7. Nevertheless, the JPSS threshold requirements for AVMP (Table II) allow for the greater of a fractional error (%) or an absolute error (g kg^{-1}). The AVMP results summarized in Table IV show in the last column absolute errors of 0.02 g kg^{-1}, which are well below the 0.1 g kg^{-1} threshold, and thus in spite of the fractional differences the moisture product nevertheless meets requirements in the upper layer. Based on the above results, we have concluded that the operational SNPP NUCAPS AVTP and AVMP EDRs meet the JPSS Level 1 requirements; similar statistical results versus RAOBs have been observed in [41].

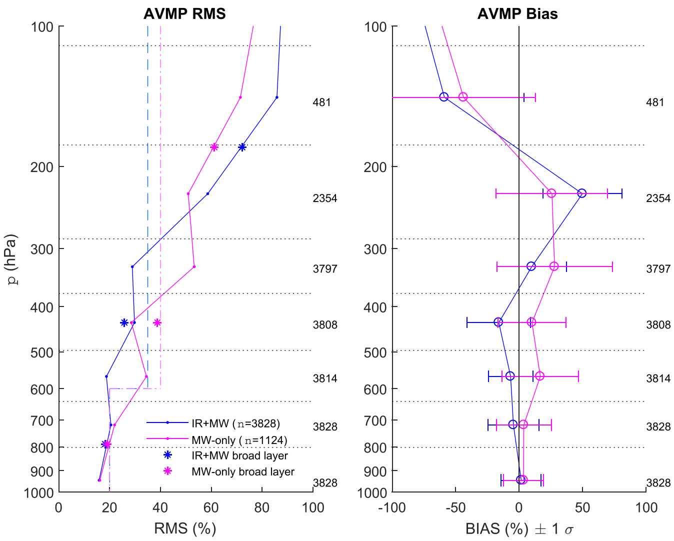

Fig. 6. Coarse-layer statistical uncertainty assessment of the NUCAPS AVMP EDR retrievals (offline v1.5 operational emulation) versus collocated dedicated/reference RAOBs for retrievals accepted by the quality flag within space–time collocation criteria of $\delta x \leq 75$ km radius and $-60 \leq \delta t \leq 0$ min of launches over a sampling period of January 9, 2013 to December 13, 2015. (Left) RMSE results. The light-blue dashed line in the RMS plots designate the JPSS Level 1 global performance requirements for "broad layers," and the asterisks show the calculated broad-layer RMSE. (Right) Bias $\pm 1\sigma$ results. NUCAPS IR+MW (clear to partly cloudy, defined by IR+MW accepted cases) and MW-only (cloudy, defined by the intersection of MW-only accepted cases and IR+MW rejected cases) performances are given in blue and magenta, respectively, with IR+MW collocation sample size for each coarse layer given in the right margins.

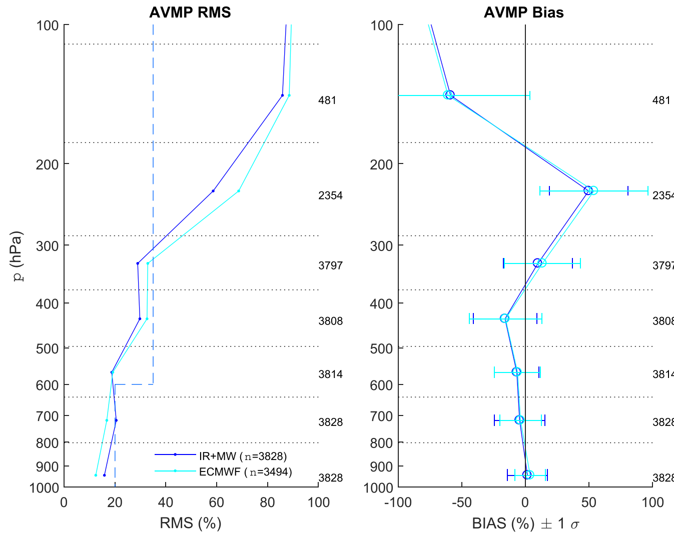

Fig. 7. Statistical uncertainty assessments versus RAOBs of NUCAPS IR+MW moisture profile retrievals (blue lines) alongside collocated ECMWF output (analysis or forecast nearest in time) for reference (cyan lines). (Left) RMSE results. (Right) Bias $\pm 1\sigma$ results.

TABLE III
VALIDATED GLOBAL AVTP EDR MEASUREMENT UNCERTAINTY

Atmospheric Broad-Layer	Land/Ocean	Ocean Only
Cloud-Free to Partly Cloudy (IR+MW)		
1014 to 300 hPa	1.16 K	1.08 K
300 hPa to 30 hPa	0.82 K	0.81 K
30 hPa to 1 hPa	1.05 K	1.08 K
Cloudy (MW-only)		
1014 to 700 hPa	2.62 K	2.46 K
700 hPa to 300 hPa	1.60 K	1.58 K
300 hPa to 30 hPa	1.49 K	1.42 K
30 hPa to 1 hPa	2.11 K	1.78 K

TABLE IV
VALIDATED GLOBAL AVMP EDR MEASUREMENT UNCERTAINTY

Atmospheric Broad-Layer	Fractional	Absolute
Cloud-Free to Partly Cloudy (IR+MW)		
1014 to 600 hPa	18.2%	1.23 g kg^{-1}
600 hPa to 300 hPa	25.8%	0.30 g kg^{-1}
300 hPa to 100 hPa	72.2%	0.02 g kg^{-1}
Cloudy (MW-only)		
1014 to 600 hPa	19.0%	1.36 g kg^{-1}
600 hPa to 300 hPa	38.8%	0.51 g kg^{-1}
300 hPa to 100 hPa	61.2%	0.02 g kg^{-1}

IV. LONG-TERM MONITORING

The LTM of sounder profile EDRs is facilitated using conventional RAOB launches from synoptic WMO sites due to their ongoing regular launch schedule. Conventional RAOB collocations are routinely obtained via NPROVS, which collocates single-closest EDR profile retrievals from multiple platforms (including SNPP) with RAOB launch "anchor points" [29] and provides graphical user interface Java applet tools to assist EDR algorithm developers, users, and validation scientists in the routine monitoring and diagnostic troubleshooting of sounding products. Profile statistics based on conventional RAOBs have been found to be similar to those obtained based on dedicated/reference RAOBs, as reported in [41].

While NPROVS will always provide a low earth orbit (LEO) satellite collocation with the RAOB using an inclusive ± 6 h time window with launch times (scanning instruments onboard sun-synchronous LEO satellites provide twice-daily near-global coverage), in this paper, we attempt to minimize mismatch error by employing tight space–time collocation criteria. For NPROVS-collocated conventional RAOBs, we keep only single-closest FORs within $\delta x \leq 25$ km radius and $-30 < \delta t < 0$ min of launches ($\delta t \equiv t_{\text{raob}} - t_{\text{sat}}$). A typical distribution of conventional RAOB collocations with SNPP acquired over a month's time period is shown in Fig. 8. NPROVS archive statistics (NARCS) for monthly mid-troposphere temperature and moisture versus conventional RAOB collocations over the course of the SNPP mission life are shown in Figs. 9 and 10, respectively. Blue lines show the results of the NUCAPS IR+MW retrievals (clear to partly cloudy), and cyan lines show the collocated AIRS retrievals for comparison. The solid lines show the bias statistics, and the dotted lines show the RMS statistics. These results show reasonable interannual stability in the NUCAPS EDRs, with comparable performance against those obtained from the AIRS relative to RAOBs with the primary exception being somewhat superior performance of AIRS AVTP relative to RAOBs;

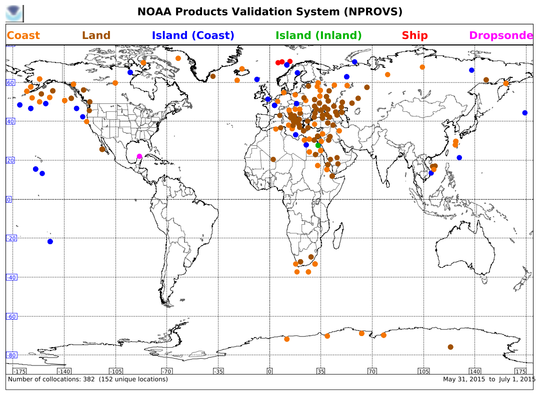

Fig. 8. NPROVS conventional synoptic RAOBs collocated with SNPP NUCAPS retrievals for June 2015 (single-closest FOR within 50-km radius of radiosonde launch sites and 0–30 min following launches).

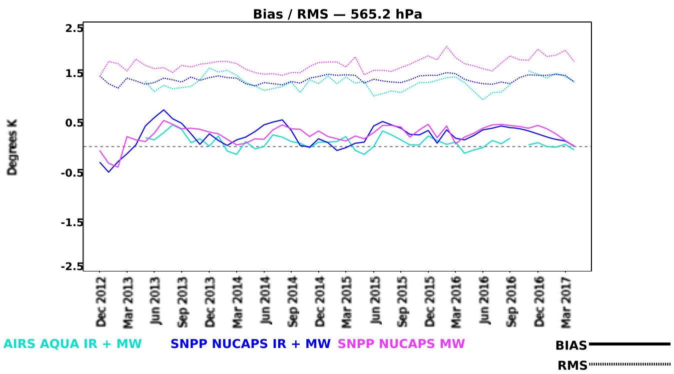

Fig. 9. NPROVS NARCS monthly statistical time series for NUCAPS (operational v1.5) and AIRS (v6) temperature EDR retrievals versus collocated conventional RAOBs at a nominal mid-tropospheric RTA level (565.2 hPa). The solid and dotted lines show the bias and RMSE results, with blue, magenta, and cyan lines indicating the NUCAPS IR+MW (clear to partly cloudy), MW-only (cloud), and AIRS retrievals, respectively.

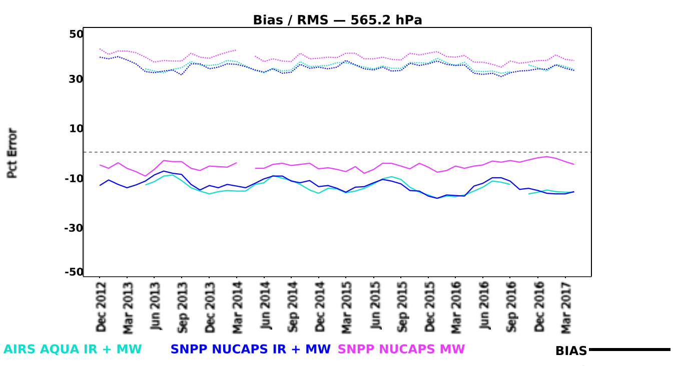

Fig. 10. NPROVS NARCS monthly statistical time series for NUCAPS (operational v1.5) and AIRS (v6) moisture EDR retrievals versus collocated conventional RAOBs at a nominal mid-tropospheric RTA level (565.2 hPa). The solid and dotted lines show the bias and RMSE results, with blue, magenta, and cyan lines indicating the NUCAPS IR+MW (clear to partly cloudy), MW-only (cloud), and AIRS retrievals, respectively.

AIRS represents a mature validated system [30], [42]–[45]. The improvement in accuracy of AIRS is believed to be at least in part due to the nonlinear neural network first guess employed in the AIRS v6 algorithm. NUCAPS continues to use a linear regression for its first guess (similar to AIRS v5), which simply cannot capture the same degree of variability in fine vertical structure for the physical retrieval to "pivot" off of, thereby yielding greater null-space errors with respect to high-resolution RAOBs.

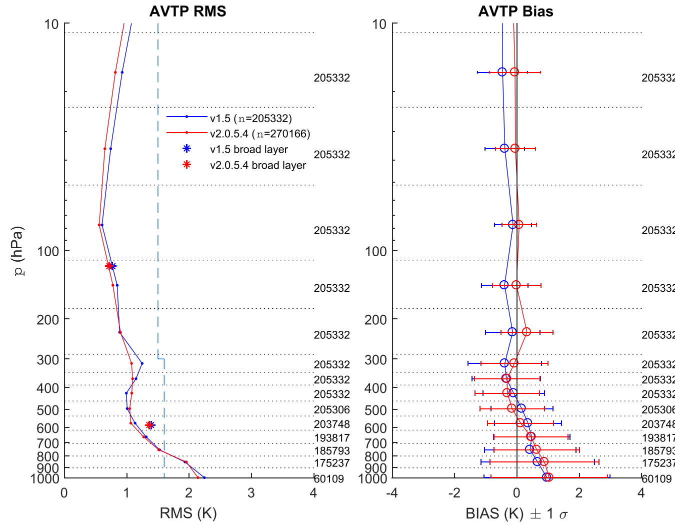

Fig. 11. Statistical assessment of offline NUCAPS AVTP v2.0.5 (CrIS full resolution, red lines) and v1.5 (CrIS nominal resolution, blue lines) versus collocated ECMWF model output (analysis or forecast nearest in time) for retrievals accepted by the quality flag for a global focus day, February 17, 2015. Global yields for v2.0.5 and v1.5 accepted cases are 83.4% and 63.5%, respectively, indicating a marked improvement in the v2.0.5 acceptance rate. (Left) RMSE results. (Right) Bias $\pm 1\sigma$ results.

V. Preparation for JPSS-1: CrIS Full Resolution

As mentioned in Section I, the operational SNPP NUCAPS v1.5 runs on CrIS spectra at the original nominal spectral resolution spectra of $\Delta\nu \approx 0.62$, 1.25, and 2.5 cm^{-1} for the longwave, midwave, and shortwave IR bands, respectively. The reduced resolution in the midwave and shortwave bands is the result of the interferograms being truncated in those bands during operational processing of the SDRs. The reduction in spectral resolution in these bands was not anticipated to have a negative impact upon the primary temperature and moisture profile EDRs, but it was known that there would be adverse impact upon trace gases, especially carbon monoxide, and this was later empirically demonstrated in [46]. Requests for access to full-resolution CrIS ($\Delta\nu \approx 0.625$ cm^{-1} in all three bands) from EDR science teams eventually led to offline production of full-spectral resolution (full-res) CrIS SDRs beginning in December 2014 [47]. In preparation for the ingest of operational full-res SDRs (including both SNPP and JPSS-1, to be launched tentatively in November 2017), a preliminary experimental offline NUCAPS version (v1.8.x) was developed to run on CrIS full-res data for demonstration studies [46]. The finalized version representing the operational delivery of the NUCAPS system in full-res mode (July–August 2017) using the UMBC full-res RTA has since been developed (v2.0.5) and has undergone testing for Provisional Maturity. CrIS full-res SDRs were not operationally available during the dedicated/reference RAOB acquisition period discussed in Section III, but the full-resolution SDRs were processed for a global focus day, February 17, 2015, for which global numerical ECMWF model comparisons have been performed (per the first method in the "validation hierarchy" referred to in Section III).

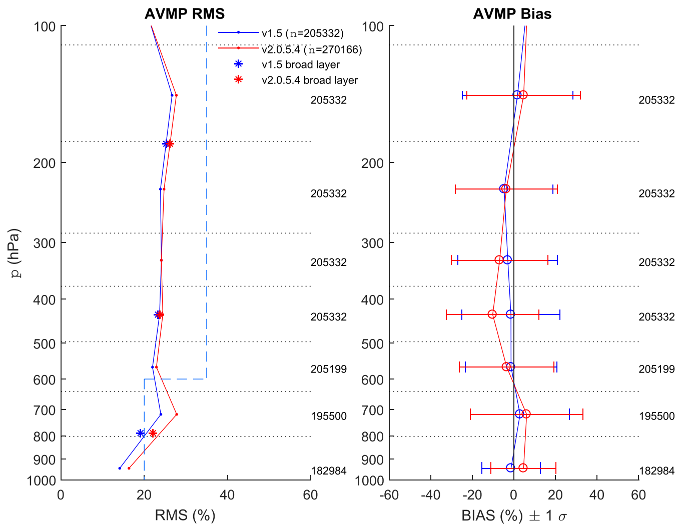

Fig. 12. Statistical assessment of offline NUCAPS AVMP v2.0.5 (CrIS full resolution, red lines) and v1.5 (CrIS nominal resolution, blue lines) versus collocated ECMWF model output (analysis or forecast nearest in time) for retrievals accepted by the quality flag for a global focus day, February 17, 2015. Global yields for v2.0.5 and v1.5 accepted cases are 83.4% and 63.5%, respectively, indicating a marked improvement in the v2.0.5 acceptance rate. (Left) RMSE results. (Right) Bias $\pm 1\sigma$ results.

Figs. 11 and 12 correspondingly show the statistical profile errors for AVTP and AVMP, respectively. These preliminary results show that the retrievals are comparable to that obtained using the operational v1.5 (nominal-resolution CrIS) and generally meet JPSS Level 1 requirements.

VI. Conclusion

This paper documents the formal validation of the SNPP NUCAPS temperature and moisture profile (AVTP and AVMP) EDRs based on a globally representative sample of dedicated/reference RAOBs, where it has been shown that the NUCAPS EDRs meet JPSS Level 1 global performance requirements and have thus reached validated maturity. We note that the RAOB sites used in the analyses include those from the three global zones (tropical, midlatitude, and polar), as well as marine-based data sets obtained from ship over both the Pacific and Atlantic Oceans (i.e., AEROSE and CalWater/ACAPEX campaigns) under a range of very different thermodynamic meteorological conditions germane to users of sounder EDR (and SDR) products. The NUCAPS mid-tropospheric temperature and moisture show reasonable stability (seasonal variability of AVTP and AVMP biases roughly within 0.5 K and 10%, respectively, with no discernible interannual trends) over the SNPP lifetime, and the algorithm has been successfully implemented for future operational full-resolution CrIS data. The NUCAPS version for CrIS full-res data (v2.0.5) has undergone preliminary testing for Provisional Maturity and operational delivery in July–August 2017. Validation of the operational SNPP NUCAPS IR ozone profile product will be the subject of a forthcoming companion paper.

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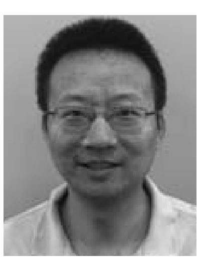

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