352 VALIDATION AND LONG-TERM MONITORING OF THE OPERATIONAL SNPP NUCAPS SOUNDING PRODUCTS

Nicholas R. Nalli* [1 2], Q. Liu[2], T. Reale[2], C. Tan[1 2], B. Sun[1 2], C. D. Barnet[3], A. Gambacorta[3], F. Tilley[1 2], F. Iturbide-Sanchez[1 2], M. Wilson[1 2], A. K. Sharma[4], T. King[1 2], *et al.*

[1]IMSG, Inc., Rockville, Maryland, USA
[2]NOAA/NESDIS/STAR, College Park, Maryland, USA
[3]STC, Inc., Silver Spring, Maryland, USA
[4]NOAA/NESDIS/OSPO, College Park, Maryland, USA

1. INTRODUCTION

The Joint Polar Satellite System (JPSS) comprises the next-generation, low Earth orbit, operational environmental satellite observing system in support of the U.S. National Oceanic and Atmospheric Adminstration (NOAA) (Goldberg et al. 2013). The Suomi National Polar-orbiting Partnership (SNPP) satellite, launched in 2011, constitutes the first satellite in the JPSS series and serves as the risk-reduction mission between the previous NOAA-series and the future JPSS-1 and -2 satellites. Onboard the JPSS series (including SNPP) are the hyperspectral infrared (IR) Cross-track Infrared Sounder (CrIS) and the microwave (MW) Advanced Technology Microwave Sounder (ATMS). These two instruments are synergistically designed to retrieve atmospheric vertical temperature and moisture profiles (AVTP and AVMP) under non-precipitating conditions (cloudy, partly cloudy and clear) with optimal vertical resolution, similar to predecessor IR/MW sounding systems.

The current operational retrieval algorithm for CrIS/ATMS is the NOAA-Unique CrIS/ATMS Processing System (NUCAPS) developed at NOAA/NESDIS/STAR (Gambacorta et al. 2012, 2015). The NUCAPS system processes CrIS/ATMS data based upon the same methodology used by the heritage EOS-Aqua Atmospheric Infrared Sounder (AIRS) (Chahine et al. 2006) and MetOp Infrared Atmospheric Sounding Interferometer (IASI) (Cayla 1993) systems, with the environmental data record (EDR) retrieval algorithm being a modular implementation of the multi-step AIRS Science Team retrieval algorithm (Susskind et al. 2003). In addition to AVTP and AVMP, NUCAPS also retrieves ozone (O_3) and carbon trace gas (CO, CO_2 and CH_4) profile EDRs.

To support calibration/validation (cal/val) of the SNPP CrIS/ATMS sensor data records (SDRs) and retrieved EDRs, JPSS has directly and indirectly funded a dedicated radiosonde observation (RAOB) program leveraging several collaborating institutions. Within the general sounder validation methodology, conventional and dedicated/reference RAOBs form the backbone of truth datasets used for the SNPP satellite sounder validation (Nalli et al. 2013b). To this end we have accumulated *in situ* truth datasets collocated with CrIS/ATMS going back to 2012. The current status of the validation of NUCAPS AVTP, AVMP and IR ozone profile EDRs based on these datasets is overviewed in this work.

2. JPSS SOUNDER EDR CAL/VAL OVERVIEW

Validation is defined as "the process of ascribing uncertainties to…radiances and retrieved quantities through comparison with correlative observations" (Fetzer et al. 2003). EDR validation supports monitoring of SDRs and cloud-cleared radiances and is also what enables development/improvement of algorithms. The JPSS Cal/Val Program defines four phases for cal/val of sensors and algorithms throughout the satellite mission lifetime: Pre-Launch, Early Orbit Checkout (EOC), Intensive Cal/Val (ICV), and Long-Term Monitoring (LTM). 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 JPSS-1 CrIS/ATMS EDR Cal/Val Plan has since been drafted during Jul–Aug 2015 and v1.0 was submitted on 20 August 2015; the revised draft v1.1 was submitted on 31 December 2015. Figs. 1 and 2 show the JPSS Level 1 Performance Requirements for AVTP/AVMP and trace gas EDRs, respectively.

We note that the requirements for the AVTP, AVMP and IR ozone profile EDRs (Figs. 1 and 2) are for

*Corresponding author address: N. R. Nalli, NOAA/NESDIS/STAR, NOAA Center for Weather and Climate Prediction #2841, 5830 University Research Court, College Park, MD 20740-3818 USA; e-mail: Nick.Nalli@noaa.gov

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

Figure 1: JPSS Level 1 specification performance requirements for CrIS/ATMS EDR uncertainty: (top) AVTP and (bottom) AVMP (source: L1RD 2014, pp. 41, 43).

CrIS Infrared Trace Gases
Specification Performance Requirements

PARAMETER	THRESHOLD
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%
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)

Figure 2: As Fig. 1 except for trace gas EDRs (source: L1RD 2014, pp. 45–49).

global, non-precipitating cases and defined for broad atmospheric layers that are to be computed as the average of coarse statistical layers ranging from 1 km to 5 km, whereas the carbon trace gas profile EDRs (Fig. 2, bottom) are defined for the total integrated columns. "Cloud fraction $< 50\%$" refers to "clear to partly cloudy" conditions whereby cloud-clearing was successful and IR retrieval algorithm converged to a solution. "Cloud fraction $\geq 50\%$" refers to "cloudy" conditions where cloud-clearing was not successful and the IR algorithm was thus unable to converge to a solution, thereby using the MW-only algorithm solution as the final product (thus providing retrievals for global, non-precipitating conditions).

The EDR validation methodology draws upon previous work with AIRS and IASI and classifies various approaches as part of a "validation methodology hierarchy" that includes (1) global numerical model comparisons, (2) satellite EDR intercomparisons, (3) conventional RAOB assessments, (4) dedicated/reference RAOB assessments, and (5) intensive campaign dissections (Nalli et al. 2013b). 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. In this paper we thus present results for the ICV to LTM phase sounder EDR validation using conventional and dedicated/reference RAOB collocations (Hierarchy Methods #3 and #4). Conventional RAOB collocations from synoptic WMO sites are routinely obtained via the NOAA Products Validation System (NPROVS) (Reale et al. 2012), as well as reference RAOB collocations from GRUAN sites; we note that NPROVS also readily allows for satellite EDR intercomparisons (Hierarchy Method #2). Dedicated radiosondes, on the other hand, are launched timed for SNPP overpasses and thus are optimally collocated at various selected sites. Using this base RAOB-satellite collocation system, an EDR validation archive (VALAR) has been created whereby SDR/TDR granules in the vicinity of RAOB "anchor points" are acquired for running offline retrievals, thus allowing validation flexibility (e.g., enables ozone and trace gas validation) and future algorithm development.

3. SNPP NUCAPS EDR VALIDATION RESULTS

3.1 Conventional RAOB

In this work we attempt to minimize mismatch error by employing tight space-time collocation criteria. For NPROVS-collocated conventional RAOBs we use the NPROVS PDISP graphical utility to sub-select only high quality RAOBs (Vaisala RS92 and RS41) and keep only single-closest FORs within $\delta x \leq 75$ km radius and $-120 < \delta t < 0$ minutes of launches ($\delta t \equiv t_{\mathrm{raob}} - t_{\mathrm{sat}}$); the spatial distribution of these collocations for the month of June 2015 is shown in Fig. 3. The NPROVS PDISP-computed statistics on 30 coarse-layers (based on the methodology described in Nalli et al. 2013b) for AVTP and AVMP are shown in Figs. 4 and 5 respectively. Blue lines show the results of the NUCAPS IR+MW retrievals (clear to partly cloudy) and orange lines show the collocated AIRS retrievals for comparison. The solid lines show the BIAS statistics given by the coarse-layer means and the dotted lines show the RMS statistics. The primary take-away from these figures is that the NUCAPS EDRs (both AVTP and

AVMP) are seen to perform comparably with those obtained from the AIRS sounder relative to RAOBs (AIRS representing a mature, validated system; e.g., Tobin et al. 2006; Divakarla et al. 2006; Nalli et al. 2006), with the primary exception being somewhat superior performance of AIRS AVTP relative to RAOBs (believed to be largely due to the neural network first guess). We note discrepancies of both NUCAPS and AIRS in the upper tropospheric layers for AVTP (30–5 hPa) and AVMP (300–100 hPa). The reason for these are believed to be associated with biases and precision limitations in the RAOBs. For AVTP it is due to radiation-induced biases (Sun et al. 2013), and for AVMP it is associated with extremely low water vapor conditions, a known problem at higher levels of the troposphere (e.g., Vömel et al. 2007). For AVMP this problem is additionally supported by a consistent pattern of discrepancies in BIAS with profiles from the European Centre for Medium-Range Weather Forecasts (ECMWF) model included in the plot (magenta lines).

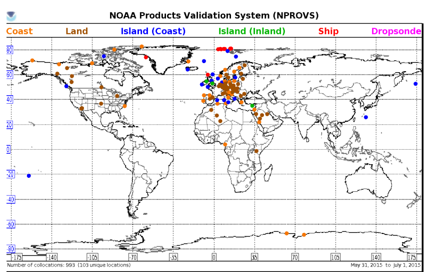

Figure 3: NPROVS (Reale et al. 2012) conventional synoptic RAOBs (Vaisala RS92 and RS41) collocated with NUCAPS accepted cases for June 2015 (single-closest FOR passing QA within 75 km radius of and 120–0 minutes prior to radiosonde launches).

3.2 Dedicated/Reference RAOB

Figs. 6 and 7 show JPSS-funded dedicated RAOB sites for Years 3 and 4 (2014–2015), respectively. The sites consist of U.S. DOE Atmospheric Radiation Measurement (ARM) sites (SGP, NSA and ENA), the Howard University BCCSO site in Beltsville, Maryland, the Pacific Missile Range Facility (PMRF) site on Kauai, Hawaii (operated by The Aerospace Corp.), and the Aerosols and Ocean Science Expedition (AEROSE) and CalWater/ACAPEX campaigns. As above, to minimize mismatch error we have assembled a NUCAPS-RAOB collocation dataset by employing stringent space-time collocation criteria, keeping all FORs within $\delta x \leq 50$ km radius and $-75 < \delta t < 0$ minutes of launches; the spatial distribution of these collocations is shown in Fig. 8. Using these datasets, we have computed coarse-layer statistics according the methodology described in Nalli et al. (2013b) for AVTP and AVMP from NUCAPS offline Version 1.5 (applying a new geographic surface area weighting scheme for tropics, midlatitude and polar regions), with results shown in Figs. 9 and 10, respectively. Blue lines show the results of the IR+MW retrievals (clear to partly cloudy) and magenta lines show MW-only results (cloudy). The righthand plots 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 the lefthand plots. The corresponding "coarse coarse-layer" results for AVTP and AVMP retrievals, shown with asterisks, are seen to fall within the JPSS requirements for both IR+MW and MW-only cases, with the only exception being IR+MW AVMP for the upper tropospheric layer (300–100 hPa), which falls somewhat outside of the requirements. As with the conventional RAOBs, the reason for this is believed to be associated with biases in the RAOBs,

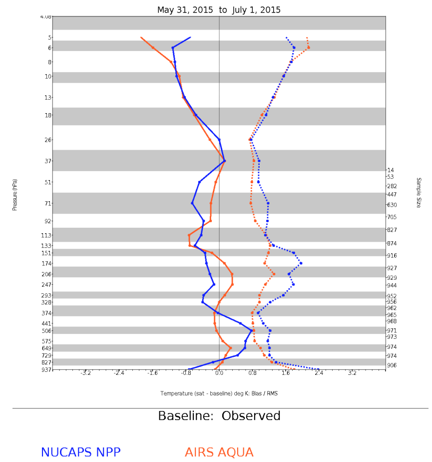

Figure 4: NPROVS PDISP coarse-layer statistical results for NUCAPS and AIRS AVTP EDR retrievals (operational) versus collocated conventional RAOBs. The solid and dotted lines show the BIAS and RMS results, with blue and dark orange lines indicating the NUCAPS IR+MW (clear to partly-cloudy) and AIRS retrievals, respectively. Collocation sample sizes for each coarse layer are indicated in the right margins of the plots.

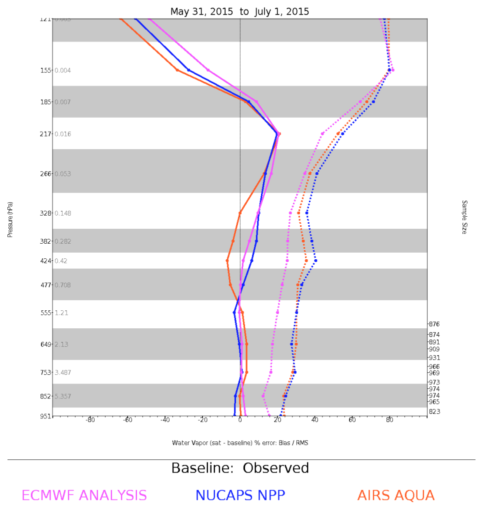

Figure 5: As Fig. 4 except for AVMP, with ECMWF results shown for comparison in magenta.

a known problem at higher levels of the troposphere. This is again supported by a completely consistent pattern of discrepancies in BIAS with profiles from the ECMWF model. We have therefore concluded that the NUCAPS AVTP and AVMP EDRs meet the JPSS Level 1 requirements.

3.3 Ozonesondes

For the IR ozone profile EDR, we have compiled a global truth dataset based upon ozonesondes launched from SHADOZ (Thompson et al. 2004) and WOUDC[1] "sites-of-opportunity" along with dedicated ozonesondes launched during NOAA AEROSE and the CalWater/ACAPEX campaign. These "sites-of-opportunity" were identified by launches occurring in close temporal proximity of overpasses, with preference given to launches occurring prior to overpasses. The locations of the truth ozonesondes used for our analysis are shown in Fig. 11, where it can be see that there is excellent global coverage.

As above, we have imposed relatively tight space-time collocation criteria on the NUCAPS-ozonesonde collocation dataset (albeit slightly more relaxed given the reduced variability of ozone and the need to maximize sample size) keeping FORs within $\delta x \leq 125$ km radius and $-240 < \delta t < +120$ min of launches (note that the actual collocations favored the ozonesondes launched prior to overpasses). Again we have computed the coarse-layer IR ozone profile EDR statistics (NUCAPS offline v1.5) with results shown in Fig. 12. The lefthand plots show the RMS uncertainties and the righthand plots show the BIAS statistics with $\pm 1\sigma$ error bars. The corresponding "coarse coarse-layer" results are again shown with asterisks, are seen to fall within the JPSS requirements both in terms of total uncertainty (RMS) and accuracy (BIAS). We have therefore concluded that the NUCAPS ozone profile EDR meets the JPSS Level 1 requirements.

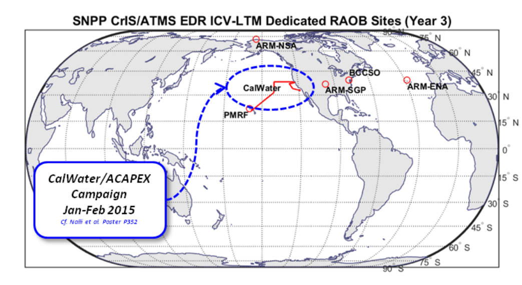

Figure 6: Dedicated RAOB truth sites for Year-3 JPSS funded dedicated RAOBs.

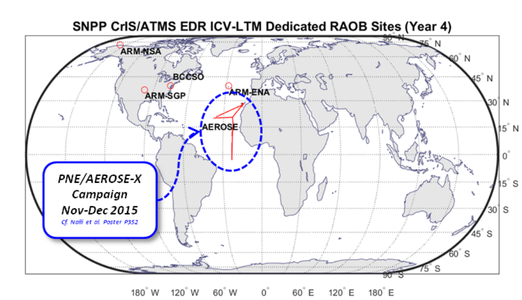

Figure 7: As Fig. 6 except for JPSS Year-4.

[1]ABM, AEMET, AWI-NA, AWI-NM, CHMI-PR, DWD-MOL, FMI-SMNA, JMA, KNMI, ME, MeteoSwiss, NASA-WFF, PIMWM, RMIB, TSMS, UKMO. World Ozone and Ultraviolet Radiation Data Centre (WOUDC) [Data]. Retrieved 5, 10 November 2014, from http://www.woudc.org.

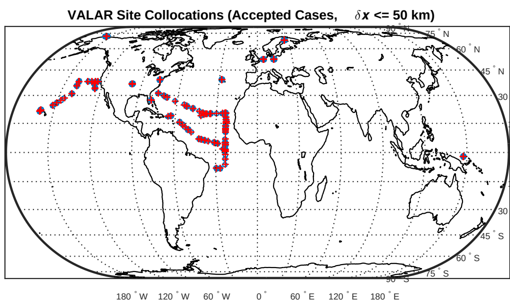

Figure 8: SNPP dedicated and reference RAOB sites (red +) collocated with NUCAPS accepted cases (all VALAR FOR passing QA within 50 km radius of and 75–0 minutes prior to radiosonde launches, blue circles).

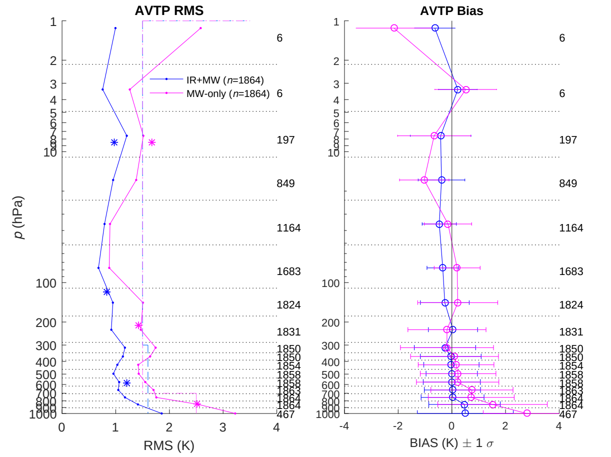

Figure 9: VALAR coarse-layer statistical results for NUCAPS AVTP EDR retrievals (offline v1.5) versus collocated dedicated/reference RAOBs. The left and right plots show the RMS and BIAS $\pm 1\sigma$ results, with blue and magenta lines indicating the IR+MW (clear to partly-cloudy) and MW-only (cloudy) retrievals, respectively. The JPSS Level 1 requirements for RMS in Fig. 1 are designated with dashed lines, with the corresponding "coarse coarse-layer" results indicated with asterisks in the left plot. Collocation sample sizes for each coarse layer are indicated in the right margins of the plots.

4. DISCUSSION AND FUTURE WORK

This work has presented CrIS/ATMS sounder NUCAPS EDR validation results based upon global truth datasets consisting of conventional and dedicated/reference RAOBs. These *in situ* datasets are considered to be optimal for validation purposes and are higher on the "validation hierarchy" as is appropriate to the ICV and LTM phases of the SNPP cal/val (e.g., Nalli et al. 2013b). For the ozone profile EDR, we relied on a combination of dedicated ozonesondes and "ozonesondes of opportunity" launched from SHADOZ and WOUDC sites. The SNPP NUCAPS AVTP, AVMP and IR ozone profile EDRs have been shown to meet JPSS global performance requirements and have thus been deemed validated. We note that the RAOB sites used in the analyses include those from three global zones (tropical, midlatitude and polar), as well as marine-based datasets 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. It should be borne in mind that while ocean cases are often considered "easy" within the satellite IR retrieval community, the data acquired during these campaigns include atmospheric conditions that pose difficulties for sounder retrievals. Furthermore, oceans cover $\simeq$70% of the Earth's surface area and this is where satellite data have the biggest impact on NWP (Le Marshall et al. 2006). Ocean-based truth data also carry unique value for cal/val given that the ocean surface is more straightforward to characterize radiatively, thus offering a greater degree of experimental control of variables.

Future work related to SNPP NUCAPS ICV and LTM includes ongoing AVTP/AVMP, IR ozone profile validation and monitoring, including NUCAPS implementation of full spectral-resolution CrIS SDRs and applying the NUCAPS averaging kernels within error analyses. Carbon trace gas validation (CO, CO_2, CH_4) will commence pending successful implementation of NUCAPS on full spectral-resolution CrIS data. The trace gas validation will require acquisition of suitable truth data which can include satellite datasets (i.e., AIRS, MLS, OCO-2, etc.) for global coverage and *in situ* datasets (e.g., MOZAIC aircraft and NOAA ESRL flask CO data) for conducting spot checks on these global data. VALAR will continue to acquire data including the latest 2015 AEROSE-X campaign (Atlantic Ocean, Nov-Dec 2015), data from ARM dedicated RAOBs (including dual-launches), and continued leveraging of GRUAN reference RAOB (including GRUAN reprocessing of RS92 RAOB data). Other research will include collocation uncertainty estimates, calc − obs analyses (e.g., Nalli et al. 2013a), skin SST EDR validation, and continued support for NUCAPS EDR user applications (AWIPS users).

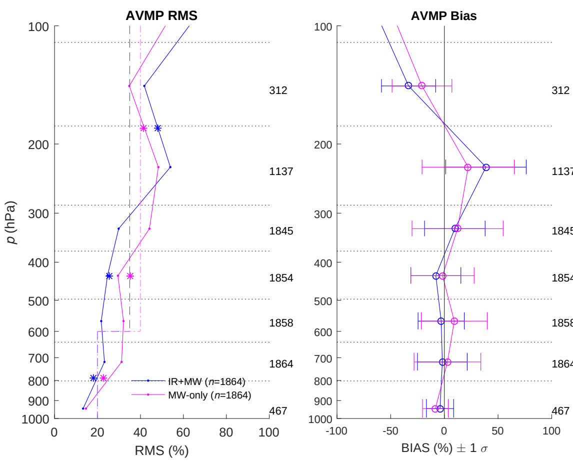

Figure 10: As Fig. 9 except for AVMP.

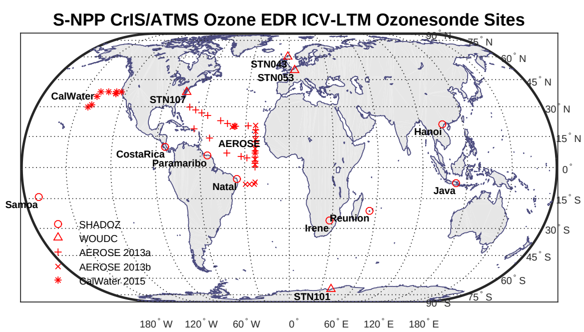

Figure 11: Ozonesonde truth sites compiled on VALAR for NUCAPS IR ozone profile EDR validation

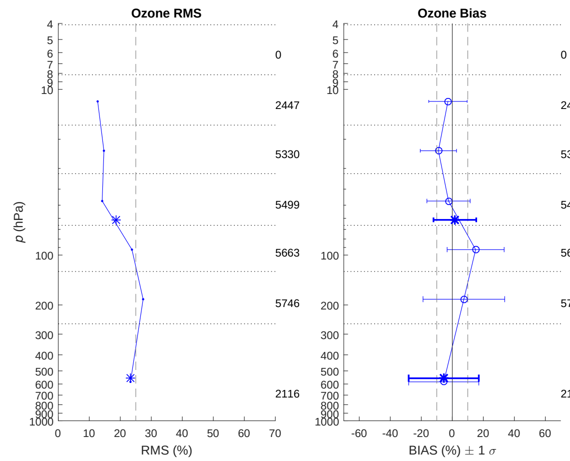

Figure 12: Coarse-layer statistical results for NUCAPS IR ozone EDR retrievals (offline v1.5) versus collocated ozonesondes. The left and right plots show the RMS and BIAS $\pm 1\sigma$ results. The JPSS Level 1 requirements for RMS (uncertainty), BIAS (accuracy) and STD (precision) in Fig. 1 are designated with dashed lines, with the corresponding "coarse coarse-layer" results indicated with asterisks. Collocation sample sizes for each coarse layer are indicated in the right margins of the plots.

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