Validation of Atmospheric Profile Retrievals from the SNPP NOAA-Unique Combined Atmospheric Processing System. Part 2: Ozone

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***Abstract*—This paper continues an overview of the validation of operational profile retrievals from the Suomi National Polar-orbiting Partnership (*SNPP*), with focus here given to the infrared (IR) ozone profile environmental data record (EDR) product. The *SNPP* IR ozone profile EDR is retrieved using the Cross-track Infrared Sounder (CrIS), a Fourier transform spectrometer that measures high resolution IR Earth radiance spectra containing atmospheric state information, namely vertical profiles of temperature, moisture and trace gas constituents. The *SNPP* CrIS serves as the U.S. low earth orbit (LEO) satellite IR sounding system and will be featured on future Joint Polar Satellite System LEO satellites. The operational sounding algorithm is the NOAA-Unique Combined Atmospheric Processing System (NUCAPS), a legacy sounder science team algorithm that retrieves atmospheric profile EDR products, including ozone and carbon trace-gases, with optimal vertical resolution under non-precipitating (clear to partly cloudy) conditions. The NUCAPS ozone profile product is assessed in this paper using extensive global *in situ* truth datasets, namely ozonesonde observations launched from ground-based networks and from ocean-based intensive field campaigns, along with numerical weather prediction model output. Based upon rigorous statistical analyses using these datasets, the NUCAPS ozone profile EDRs are determined to meet the JPSS Level 1 global performance requirements.**

***Index Terms*—atmospheric measurements, algorithms, geophysical measurements, infrared measurements, measurement errors, ozone, radiosondes, remote sensing, satellite applications**

I. Introduction

The operational U.S. Suomi National Polar-orbiting Partnership (*SNPP*) satellite features the hyperspectral infrared (IR) Cross-track Infrared Sounder (CrIS) and Advanced Technology Microwave Sounder (ATMS) sounding system. The follow-on Joint Polar Satellite System (JPSS) is a U.S. National Oceanic and Atmospheric Administration (NOAA) operational satellite mission will feature CrIS/ATMS sounders onboard four satellites launched in the same orbit over the next two decades beginning in late 2017. The CrIS instrument is an advanced Fourier transform spectrometer (FTS) that measures well-calibrated sensor data records (SDRs) consisting of high-resolution IR spectra in 1305 channels over three bands spanning $\nu \approx [650, 2550]$ cm^{-1}. The CrIS spectra allow for retrieval of atmospheric vertical profile environmental data records (EDRs) with the highest possible vertical resolution ($\approx$ 2–5 km) comparable to predecessor sounding systems, namely the *MetOp-A* and *-B* Infrared Atmospheric Sounding Interferometer (IASI) [1], [2] and the *EOS-Aqua* Atmospheric Infrared Sounder (AIRS) [3], [4].

Although sounder SDRs (radiances) have come to be directly assimilated into global numerical weather prediction (NWP) models via variational analysis schemes, they continue to be directly inverted operationally to retrieve orbital atmospheric profile EDRs in near-realtime, as originally envisioned by satellite sounding pioneers [5]–[7] and [8]–[10]. One advantage of direct inversion is the ready capability of inverting for numerous state parameters beyond atmospheric vertical temperature and moisture profiles (AVTP and AVMP), namely trace gases, clouds, aerosols, surface emissivity, among others.

The operational EDR retrieval algorithm for CrIS/ATMS is the NOAA-Unique Combined Atmospheric Processing System (NUCAPS) [11], [12]. The NUCAPS algorithm is based upon the heritage methodology developed for the *EOS-Aqua* AIRS and is a modular implementation of the multi-step AIRS Science Team retrieval algorithm Version 5 [13], [14]. For more details on the NUCAPS algorithm, the reader may refer to [12], [13] or the Algorithm Theoretical Basis Document (ATBD) available online. The multi-step NUCAPS physical retrieval module retrieves individual parameters in a step-by-step fashion, using only channels rigorously determined to be sensitive to that parameter [15], beginning with temperature and water vapor profiles, followed by ozone (O_3) and trace gases, with the result output on the radiative transfer algorithm (RTA) 100 layers (AVTP is output on layer boundaries). The NUCAPS IR ozone profile EDR is currently used by the NOAA Total Ozone Analysis using SBUV/2 and TOVS (TOAST), as well as in basic science applications.

Because of the multistep retrieval method, the quality of the ozone profile retrieval (and the other trace gases) will depend to some extent on the quality of the AVTP and AVMP retrievals. Thus the performances of the temperature and moisture EDRs were first overviewed in the Part 1

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companion paper [16], where it was demonstrated that the operational *SNPP* NUCAPS AVTP and AVMP EDRs comply with JPSS Level 1 requirements (and declared validated as of September 2014). In this paper the profile EDR validation is extended to the *SNPP* NUCAPS IR ozone profile EDR using ozonesonde collocations from land-based networks and ocean-based dedicated launches, along with numerical model comparisons.

II. NUCAPS IR Ozone Profile EDR Overview

As mentioned above, users of the NUCAPS IR ozone profile EDR include the NOAA Total Ozone Analysis using SBUV/2 and TOVS (TOAST), in addition to science users interested in atmospheric chemistry and air quality [17], [18]. Satellite sounder EDR datasets are generally invaluable for numerous global environmental research studies [19]. To illustrate, Figure 1 shows NUCAPS ozone retrievals for the 30 hPa RTA layer for 22 June and 22 September 2016, these being roughly the southern hemisphere (SH) winter solstice and spring equinox, respectively. As will be seen in Section III, the CrIS sensor has very good sensitivity to this layer, and as a result, the seasonal depletion of ozone from SH winter to spring, commonly referred to as the Antarctic "ozone hole" [20], is clearly observed by the NUCAPS ozone soundings.

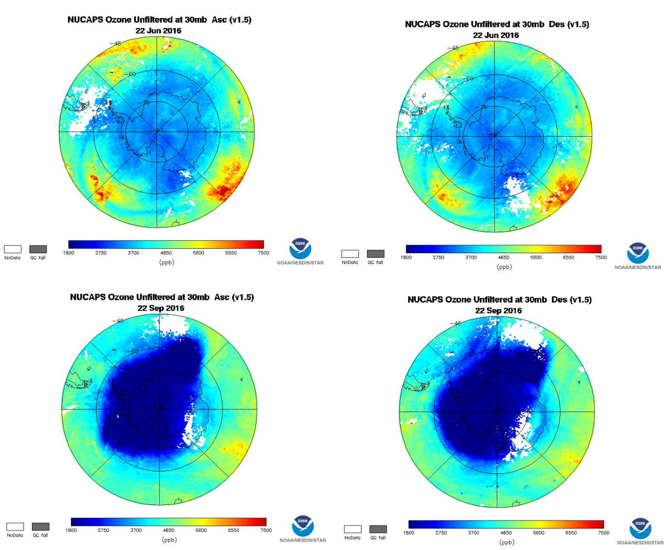


Fig. 1. NUCAPS retrieved 30 hPa layer ozone for ascending and descending orbits on 22 June 2016 (top plots) and 22 September 2016 (bottom plots) illustrating the seasonal depletion of ozone from SH winter to SH spring.

As also mentioned above, the NUCAPS physical retrieval algorithm utilizes information contained within the CrIS-measured IR Earth radiance spectra to retrieve ozone. The NUCAPS ozone retrieval step applies an optimal estimation (OE) method to retrieve ozone using sensitive channels [15] (see Figure 2, top) and an *a priori* background state consisting of a tropopause-based climatology [21].

Retrieval sensitivity to state parameters (e.g., ozone concentration) can be inferred from the averaging kernels (AKs) defined by [22]–[24]

$$\mathbf{A} \equiv \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}}, \quad (1)$$

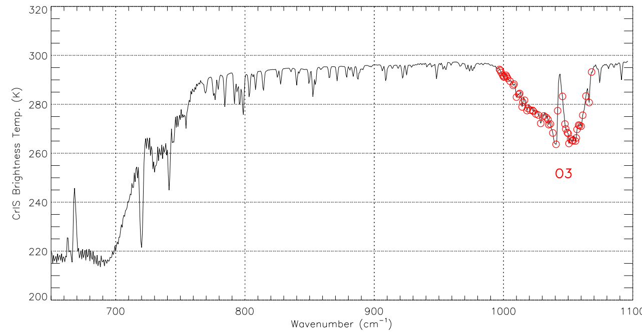


Fig. 2. Hamming apodized CrIS longwave IR brightness temperature spectrum (unapodized nominal spectral-resolution 0.625 cm^{-1}) for a marine nighttime case (10:22 UTC 9 June 2015, 6.5°N, 130.0°W) showing ozone channels (red circles) used in the NUCAPS multi-step physical retrieval.

where the AK matrix $\mathbf{A}$ is dimensioned $m \times m$ (m being the number of RTA layers), and $\hat{\mathbf{x}}$ and $\mathbf{x}$ denote the retrieved and true states, respectively. The NUCAPS algorithm computes "effective" AKs, $\mathbf{A_e}$, for each retrieval that account for the trapezoidal basis functions used in the physical retrieval, the details of which can be found in [25]. Figure 3 shows zonal-mean NUCAPS profiles taken from a global Focus Day 17 February 2015 for the tropics, northern and southern hemisphere (NH and SH) midlatitude, and polar zones. The left plot shows the RTA layer-averaged mean effective AKs for the ozone channels shown in Figure 2, where it can be seen that the layer and magnitude of peak sensitivity increases from the poles to the tropics. Polar sensitivity peaks at around 100 hPa, whereas midlatitude and tropical sensitivity peak higher in the upper troposphere to lower stratosphere (UT/LS), ≈50 hPa, with a sharper peak exhibited in the tropics along with a secondary peak below the tropopause (middle plot) at around 300 hPa, which when combined with the primary peak shows UT/LS sensitivity of the NUCAPS ozone product over the tropics [21]. The greater sensitivity seen in the NH polar cap (60–90°N) versus the SH is related to the relatively higher ambient LS ozone concentration found in the NH over the SH (right plot) during late boreal winter. The ability of the CrIS to provide information about the ozone profile is also demonstrated by considering the NUCAPS algorithm degrees-of-freedom (DoF) for the ozone retrieval, which are shown for the 17 February 2015 Focus Day in Figure 4. Generally speaking, DoF greater than unity is an indicator that more than one independent piece of information is contained within the measurements, thus enabling the retrieval to contribute vertical profile information to the *a priori*. In Figure 4 it can be seen that NUCAPS ozone DoF are generally $\gtrsim 1$ globally speaking, with larger values $\gtrsim 2$ found in midlatitude to polar zones, and smaller values ≈1 in regions of the tropics (possibly associated with deep convective clouds within the intertropical convergence zone, ITCZ) as well as over central Antarctica.

III. IR Ozone Profile EDR Performance Assessment

The JPSS Level 1 requirements for the CrIS IR ozone profile EDR are given in Table I, which are defined for

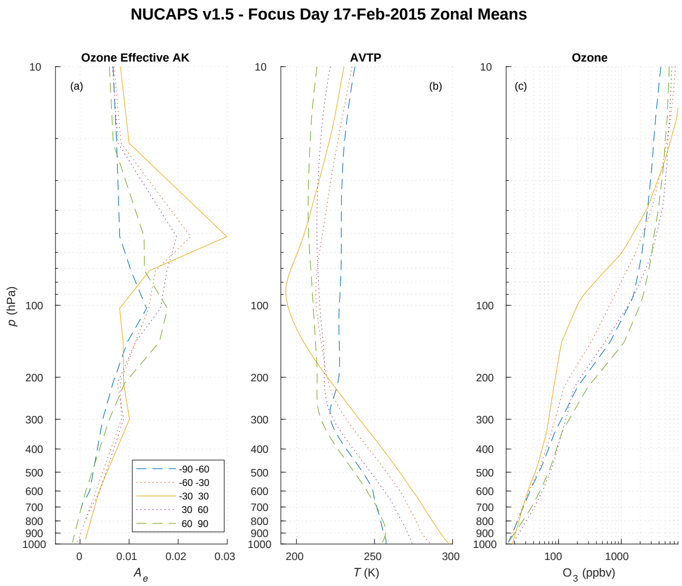
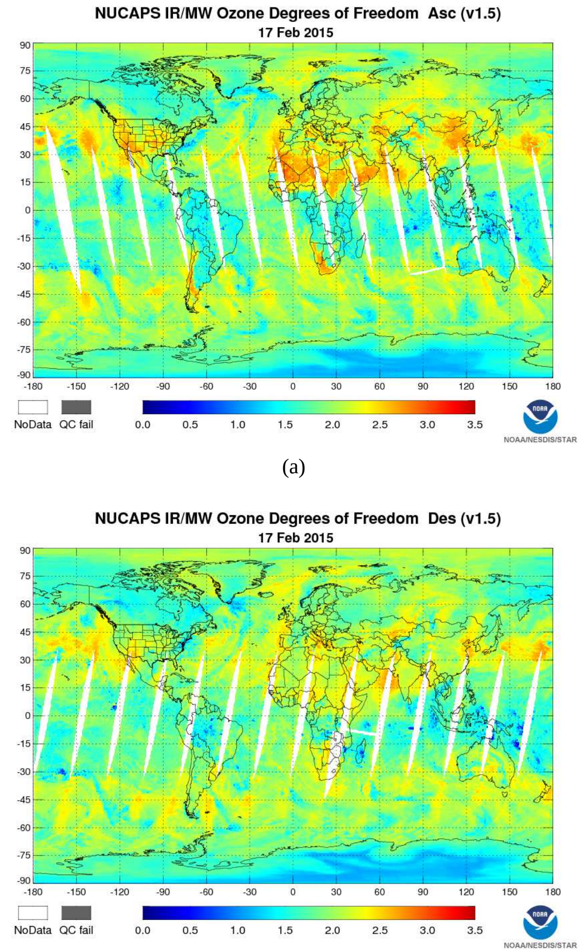


Fig. 3. Zonal-mean NUCAPS profiles calculated from a global Focus Day, 17 February 2015 ($n = 2686$ granules): (a) RTA layer-averaged effective averaging kernels A_e for nominal spectral-resolution CrIS ozone channels shown in Figure 2, (b) atmospheric vertical temperature profile retrievals, and (c) IR ozone profile retrievals (log-log plot). The solid lines are tropics (30°S to 30°N), dotted lines are midlatitudes (30–60°S and °N) and dashed lines are polar (60–90°S and °N).



(a)

(b)

Fig. 4. NUCAPS ozone degrees-of-freedom (DoF) for the global Focus Day, 17 February 2015: (a) ascending orbit, (b) descending orbit.

global, non-precipitating cases on broad atmospheric layers made up of coarse layers. In the case of ozone, there is only 1 tropospheric layer (a consequence of the CrIS ozone sensitivity as evidenced in the AKs) and 6 spanning from the upper troposphere to the stratosphere) that are to be computed as the average of coarse statistical layers. As described in [26], to avoid undesirable skewing of the sample distribution we weight each deviation by the ozone layer mass abundance squared (i.e., W^2 weighting) in the computation of coarse-layer root mean-square error (RMSE), bias (mean) and standard deviation (σ).

A. CrIS Nominal Spectral Resolution (NSR)

The operational NUCAPS algorithm (Version 1.5) has run on nominal spectral-resolution (NSR) CrIS SDRs at $\Delta\nu \approx$ 0.625 cm^{-1}, 1.25 cm^{-1} and 2.5 cm^{-1} for the longwave, midwave and shortwave IR bands, respectively [27], [28]. This subsection presents the validation of the operational ozone profile EDR based upon an offline v1.5 emulation.

1) Data: Validation of the operational ozone profile EDR is primarily based upon collocations of truth datasets consisting of *in situ* ozone soundings obtained from electrochemical concentration cell (ECC) ozonesondes along with global output from the European Centre for Medium-Range Weather Forecasts (ECMWF) NWP model. Ozonesondes used in the analyses were acquired from land-based World Ozone and Ultraviolet Radiation Data Centre (WOUDC) and Southern Hemisphere Additional Ozonesonde (SHADOZ) [29] network sites, along with unique *SNPP*-dedicated ECC ozonesondes launched during ship-based intensive cal/val campaigns [16], namely NOAA Aerosols and Ocean Science Expeditions (AEROSE) [17], [30] and the 2015 CalWater ARM Cloud Aerosol Precipitation Experiment (ACAPEX) [31]–[33]. We have accumulated ozonesonde truth datasets collocated with *SNPP* CrIS spanning the period of early-2012 through 2015; the locations of these sites are shown in Figure 5.

ECC ozonesondes typically measure ozone partial pressure in mPa with high vertical resolution (e.g., 1 second). These must be converted to fine layer abundances (molecules/cm^2) and then reduced to 100 RTA layer abundances to yield correlative data for the NUCAPS ozone retrieval [26]. Ozonesonde partial pressures are first converted to number densities N_x (molecules/cm^3) using the formula (in centimeter-gram-second units)

$$N_x(p_{x,\ell}, T_\ell) = 10^{-2}\left(\frac{p_{x,\ell}}{k\,T_\ell}\right), \qquad (2)$$

where $p_{x,\ell}$ is the partial pressure (in mPa) for constituent $x \equiv O_3$ at ozonesonde level ℓ, T_ℓ is the radiosonde temperature at level ℓ, k is the Boltzmann constant (ergs), and the factor 10^{-2} converts partial pressure from mPa to dPa. Equation (2) is then integrated from the balloon burst level down and interpolated to RTA layer boundaries (i.e., "levels") to enable calculation of RTA layer abundances [26].

TABLE I
JPSS LEVEL 1 REQUIREMENTS* FOR IR OZONE PROFILE EDR

IR Ozone Profile (CrIS) Layer Average Proportional Error		
Atmospheric Broad-Layer	Threshold	Objective
Precision (random error, σ)		
Surface to 260 hPa (6 statistic layers)	20%	10%
260 hPa to 4 hPa (1 statistic layer)	20%	10%
Accuracy (systematic error, bias)		
Surface to 260 hPa (6 statistic layers)	±10%	±5%
260 hPa to 4 hPa (1 statistic layer)	±10%	±5%
Combined Uncertainty (RMSE)		
Surface to 260 hPa (6 statistic layers)	25%	15%
260 hPa to 4 hPa (1 statistic layer)	25%	15%

*Source: Joint Polar Satellite System (JPSS) Program Level 1 Requirements Supplement — Final, Version 2.9, 27 June 2013, NOAA/NESDIS, p. 49.

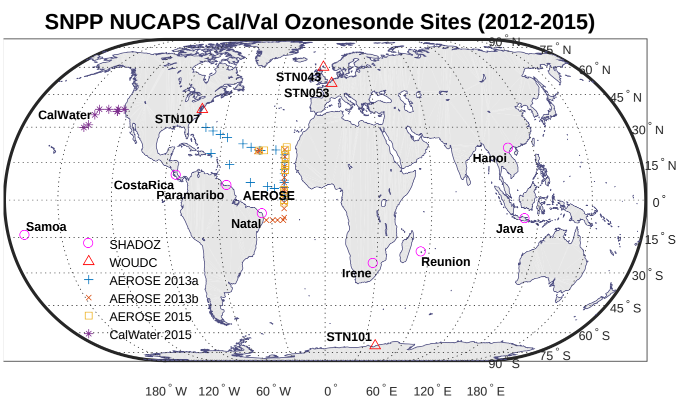


Fig. 5. Ozonesonde truth sites used for *SNPP* NUCAPS IR ozone profile EDR cal/val over the sampling period 2012–2015. Magenta circles denote SHADOZ sites, red triangles denote WOUDC sites, and blue +, red ×, gold □ and purple * denote SNPP-dedicated ozonesondes launched from ship-based intensive campaigns (AEROSE and CalWater/ACAPEX). Map projection is equal-area.

Although the NUCAPS effective-AKs (discussed in §II) can be applied to "smooth" the correlative truth data and remove null-space source error implicit to the retrieval algorithm (thus yielding improved statistics), the primary focus of the current paper is to evaluate the product's performance against the metrics defined by the JPSS Level 1 requirements summarized in Table I. The JPSS requirements are applicable to the total system error, which includes the null-space error, thus precluding the use of AKs in demonstrating the product meets requirements. Thus, a more detailed breakdown of algorithm error sources, including null-space error using AKs, falls outside the scope of the current effort and will be the subject of future work (e.g., the *JPSS-1* NUCAPS validation effort).

2) Error Analysis: As in the collocation methodology described in Part 1 [16], we have imposed space-time collocation criteria to the NUCAPS-ozonesonde collocation dataset, striking a balance between collocation mismatch uncertainty and sample size. In this case FORs are included within $\delta x \leq 125$ km radius and $-240 < \delta t < +120$ min of launches (note that the selected ozonesonde sites, including the dedicated ozonesonde launches, favored ozonesondes being launched prior to overpasses). Figure 6 shows the corresponding geographic histogram of the distribution of the ozonesonde collocation sample on an equal-area map projection, where it can be seen that the combination of the ozonesonde sites described above provide adequate representation of global climate zones (tropics, midlatitudes and polar) along with land and ocean surfaces.

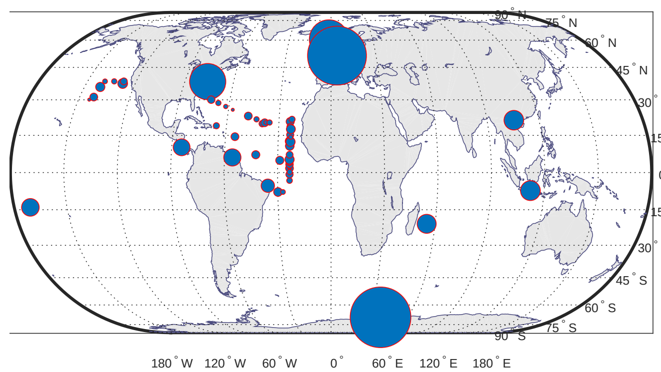


Fig. 6. Geographic histogram of *SNPP* NUCAPS FOR-ozonesonde collocation data used in the global land/sea statistical error analysis. Circle sizes depict the relative *SNPP*-ozonesonde collocation sample sizes for each ozonesonde launch location. Map projection is equal area.

The resulting global profile error statistics are given in Figure 7, along with those separated by polar, midlatitude and tropical zones given in Figures 8–10, respectively. In these figures, blue lines show the results of the NUCAPS retrievals (IR accepted cases, clear to partly cloudy) and magenta lines show the results of the *a priori* (climatological background) used in the physical retrieval. The left and right plots show the coarse-layer RMSE and bias $\pm 1\sigma$ statistics, respectively. The JPSS Level 1 global specification requirements (Table I) for RMSE and bias are shown with dashed gray lines the plots. The corresponding broad-layer averages for these statistics are depicted with asterisks in the plots, with the global results summarized in Table II. It should be noted that although we have included the JPSS global requirement lines and broad-layer averages in the zonal plots (Figures 8–10) for reference, JPSS requirements are specified for global ensembles only; thus, they do not have any direct bearing on results obtained for any type of subsample binning (e.g., latitude zones).

A scatterplot of NUCAPS versus ozonesonde layer-averaged O_3 molecular abundances for the two broad atmospheric layers is shown in Figure 11. The majority of the data falls along the one-to-one line with the exception of a region between the two layers, where a small number of NUCAPS retrievals in the 260–4 hPa layer (red + symbols) are seen to significantly overestimate the ozone concentration relative to the ozonesondes. The region in question corresponds roughly to the tropopause region, where two potential sources of error would include *a priori* and null-space errors. Null-space errors

TABLE II
VALIDATED GLOBAL IR OZONE PROFILE EDR MEASUREMENT UNCERTAINTY

Atmospheric Broad-Layer	Observed Uncertainty				
	RMSE	bias	σ	r	p
Surface to 260 hPa	23.2%	-9.4%	21.2%	0.69	0
260 hPa to 4 hPa	18.9%	-1.8%	14.3%	0.77	0

result from the limitations in the CrIS instrument's vertical resolution and sensitivity (e.g., Figure 3); this issue will be explored using the NUCAPS effective AKs in a future paper. The correlation coefficients, r, along with corresponding p-values, are included in Table II, where it is seen that the broad-layer correlations between NUCAPS and ozonesondes is $\gtrapprox +0.7$.

In discussing further the results presented in Figures 7–10, it is first recalled that the NUCAPS ozone physical retrieval step uses an OE method that relies on a formal *a priori* derived based upon a climatological background state [21]. These figures demonstrate the ability of the retrieval (blue lines) to move the *a priori* state (magenta lines) toward the ozonesonde-observed state as evidenced by the significantly reduced σ and RMSE for layers where the CrIS channels have sensitivity (Figure 3a). Because the *a priori* (magenta) is based upon climatology, it is not surprising that it exhibits very little bias, making further improvement from the retrieval difficult to achieve (righthand plots). Thus, the value of the IR spectral information manifested in the NUCAPS OE ozone retrieval is the ability to measure deviations from the *a priori* (i.e., mean) state, resulting in the reduction of random errors (σ and RMSE), but not necessarily the systematic error.

We find that the global ozone profile EDR meets the JPSS requirements, with the only exception being the precision (σ) for the tropospheric broad-layer (surface to 260 hPa), which falls somewhat outside of the 20% requirement for this layer. However, referring back to the AKs shown in Figure 3, it is noted that the CrIS instrument possesses little sensitivity in the troposphere, thereby requiring the algorithm to relax to the *a priori*. The overall results for *SNPP* NUCAPS presented here are comparable to those reported previously for the *Aqua* AIRS Version 5 ozone product [34]. Therefore, based on our findings (Figure 7 and Table II), it is concluded that the NUCAPS ozone profile EDR generally meets the JPSS Level 1 requirements.

Similar performance patterns (both RMSE and bias) are observed in the three climate zones, with overall profile performances improving with latitude zone from the tropics to the poles. The diminished performance in the tropics (Figure 10) is associated with what may potentially be a suboptimal *a priori* (magenta lines) combined with reduced ozone DoF (Figure 4) and ozone AK sensitivity at higher altitudes (Figure 3). The physical retrieval significantly improves the *a priori* in UT/LS in both the polar and midlatitude zones (Figures 8 and 9, respectively), whereas the improvement is reduced, but

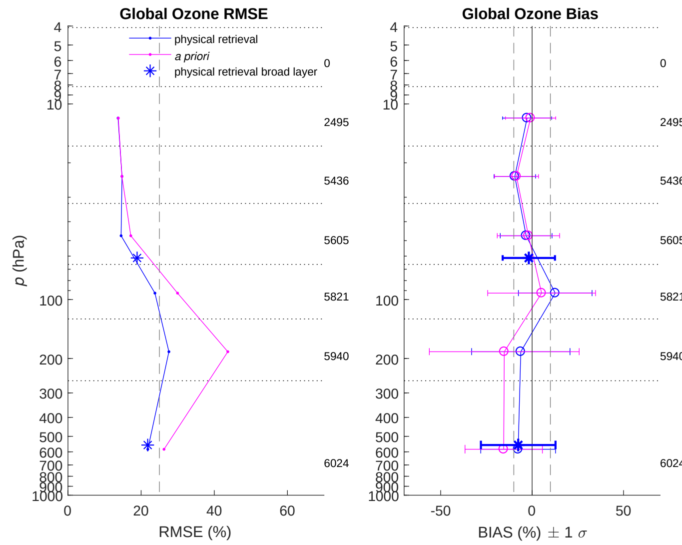


Fig. 7. Coarse-layer statistical assessment of the NUCAPS IR ozone profile EDR (offline v1.5 operational emulation, blue lines) versus collocated ozonesondes for retrievals accepted by the quality flag within space-time collocation criteria of $\delta x \leq 125$ km radius and $-240 \leq \delta t \leq +120$ minutes of launches over a sampling period of 4 April 2012 to 12 December 2015. The left and right plots show the RMSE and bias $\pm 1\sigma$ results, respectfully. NUCAPS IR physical retrieval (under clear to partly cloudy conditions) and *a priori* (climatological background) performances are given in blue and magenta respectively, with collocation sample size for each coarse-layer given in the right margins. The gray dashed lines designate the JPSS Level 1 global performance requirements for two broad atmospheric layers defined in Table I, with asterisks denoting the calculated broad-layer averages for the physical retrievals.

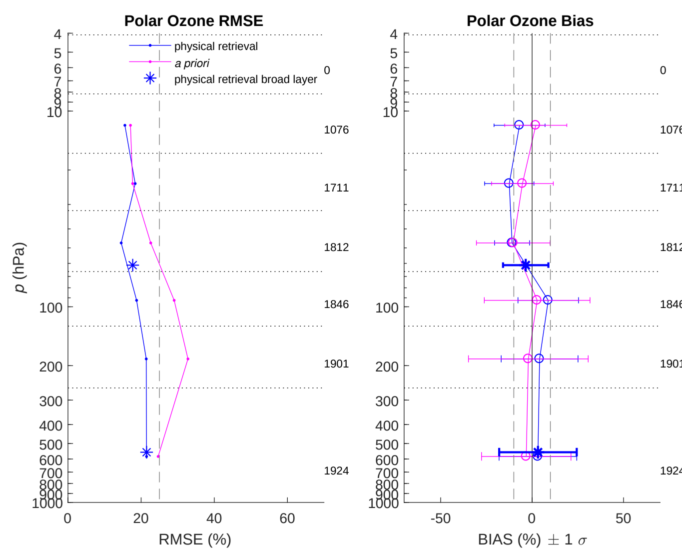


Fig. 8. As Figure 7 except for NUCAPS retrievals collocated with ozonesondes in the NH and SH polar caps.

nevertheless still evident, for the tropical cases (Figure 10). Global seasonal stability in the retrievals for three UT/LS coarse-layers (23 hPa, 47 hPa and 93 hPa) over the ozonesonde acquisition period is demonstrated in Figure 12. Weekly biases generally fall within -20 to 0% for the 23 hPa layer, $\pm 20\%$ for the 47 hPa layer and -10 to +40% at 93 hPa, with very little seasonal variability or long-term trends. Note that two short acquisition periods at the beginning and ending of 2015

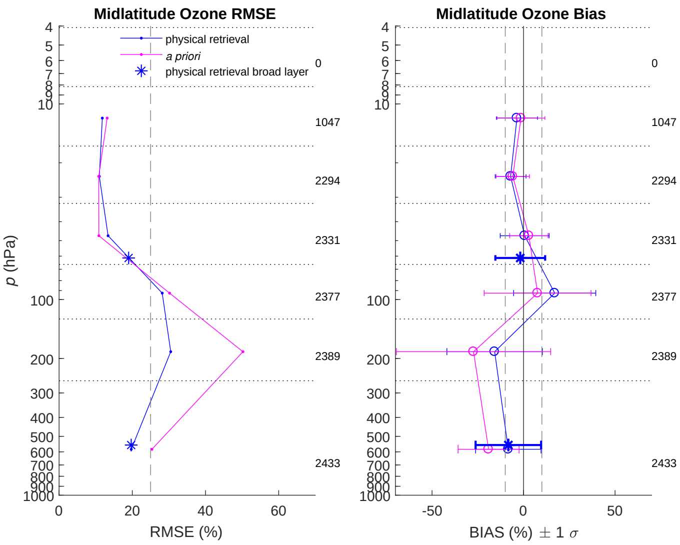


Fig. 9. As Figure 7 except for NUCAPS retrievals collocated with ozonesondes in the midlatitude zones.

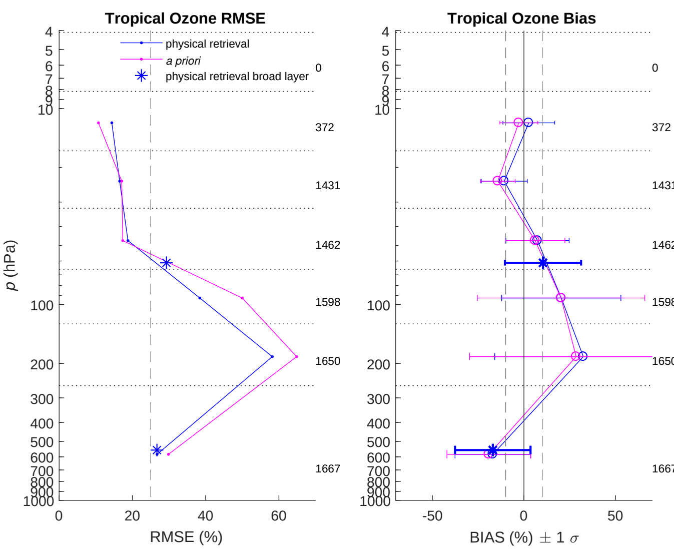


Fig. 10. As Figure 7 except for NUCAPS retrievals collocated with ozonesondes in the tropical zone.

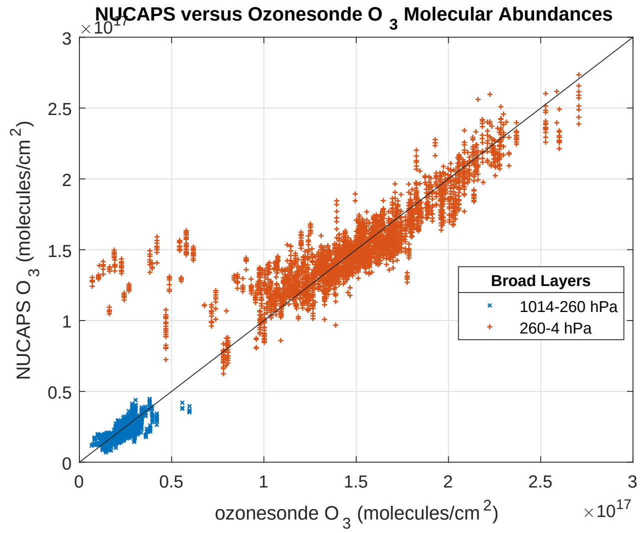


Fig. 11. Scatterplot of NUCAPS versus ozonesonde layer-averaged O_3 molecular abundances (molecules/cm^2) for the two broad atmospheric layers defined in the paper: 1014–260 hPa (blue $\times$) and 260–4 hPa (red +); correlation coefficients r and p-values are given in Table II.

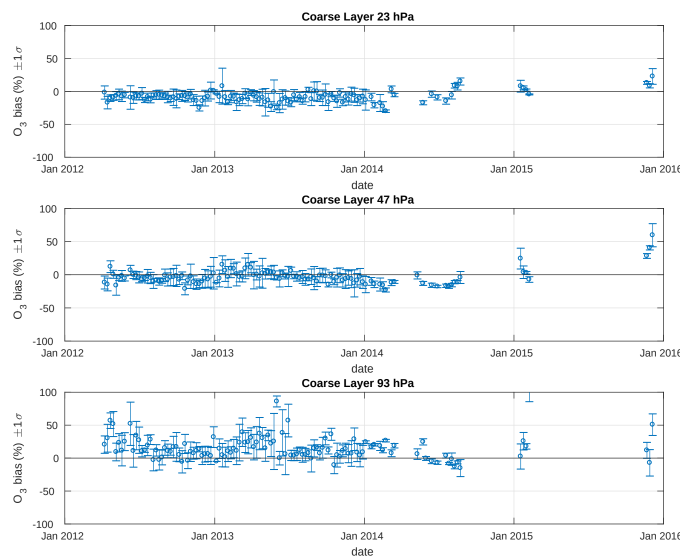


Fig. 12. Weekly statistical time-series (bias $\pm 1\sigma$) for NUCAPS v1.5 IR ozone profile EDR retrievals versus the collocated ozonesondes (Figure 6) acquired over the sampling period of 2012 through 2015 for three UT/LS coarse-layers: (top) $\approx$23 hPa, (middle) $\approx$47 hPa and (bottom) $\approx$93 hPa.

correspond to dedicated ozonesondes acquired over ocean during the 2015 CalWater/ACAPEX and AEROSE campaigns, the former obtained under inclement weather conditions in the Pacific [32], [33], the latter obtained over the tropical Atlantic (see Figure 5).

B. *CrIS Full Spectral Resolution (FSR)*

As discussed in the Part 1 companion paper [16], the operational *SNPP* NUCAPS v1.5 has previously run on on CrIS spectra with reduced resolution in the midwave and shortwave bands due to truncated interferograms in those bands during operational processing; these reduced-resolution spectra have been referred to as "nominal resolution" as this was the original (nominal) resolution of the operational SDRs. However, offline production of *SNPP* full spectral-resolution (FSR) CrIS SDRs ($\Delta\nu \approx 0.625$ cm^{-1} in all three bands) began in December 2014 [35], with operational Interface Data Processing Segment (IDPS) production starting in March 2017. Given that CrIS FSR SDRs will be produced operationally going forward (i.e., for the remainder of the *SNPP* lifetime as well as the follow-on JPSS satellite series, with the *JPSS-1* launch tentatively scheduled for Novemeber 2017), a preliminary experimental offline NUCAPS version was developed to run on CrIS FSR data for demonstration studies [36]. A completed version (v2.0.5), representing the operational delivery of the NUCAPS system in FSR mode, was demonstrated and delivered for operational implementation in July–August 2017.

Because CrIS FSR SDRs were not operationally available during the ozonesonde acquisition period, a preliminary assessment of the NUCAPS FSR algorithm has been performed versus numerical forecast model output (viz., ECMWF) for a global Focus Day (17 February 2015) [26] where the CrIS FSR SDRs were made available offline. As in Section III-A2, Figure 13 shows the global results, with Figures 14–16 show the breakdowns by latitude zones. In these figures the red lines show the FSR v2.0.5 NUCAPS results with blue lines showing the v1.5 NSR results for comparison. The patterns are similar (but not identical) to those obtained when using ozonesondes as the baseline (cf. Figures 7–10), with improved performance occurring with latitude zone from tropical (Figure 16) to midlatitude (Figure 15) to polar zones (Figure 14). Of particular note, the NUCAPS v2.0.5 FSR algorithm demonstrates a significant improvement over the v1.5 NSR algorithm in the IR+MW retrieval quality acceptance yield, from 63.5% to 83.4%, while demonstrating comparable performance. Rejected cases typically occur under environmental conditions that present challenges to passive IR retrievals but are otherwise of meteorological interest (e.g., cloudiness associated with convection). In spite of this, it is seen that the NUCAPS FSR (v2.0.5) algorithm otherwise performs comparably to the fully-validated NUCAPS NSR (v1.5), with the broad-layer averages (denoted with asterisks) generally meeting the JPSS Level 1 requirements relative to ECMWF.

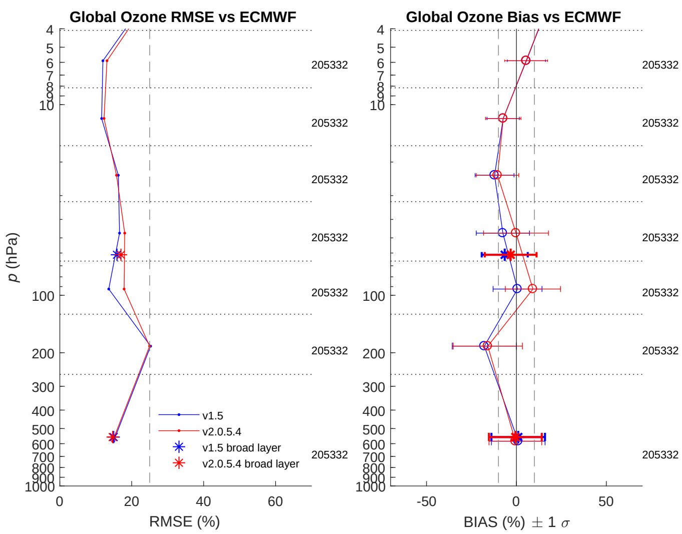


Fig. 13. As Figure 7 except statistical assessment of offline NUCAPS v2.0.5 (CrIS FSR, red lines) and v1.5 (CrIS nominal-resolution, blue lines) IR physical retrievals versus collocated ECMWF model output (analysis or forecast nearest in time, red lines) for retrievals accepted by the quality flag for a global Focus Day, 17 February 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 quality acceptance yield.

IV. Summary and Future Work

This work has presented the formal validation of *SNPP* NUCAPS IR ozone profile EDR in continuation of the validation of atmospheric vertical temperature and moisture profile EDRs described in the Part 1 companion paper [16]. Based upon a globally representative sample of collocated ozonesondes and

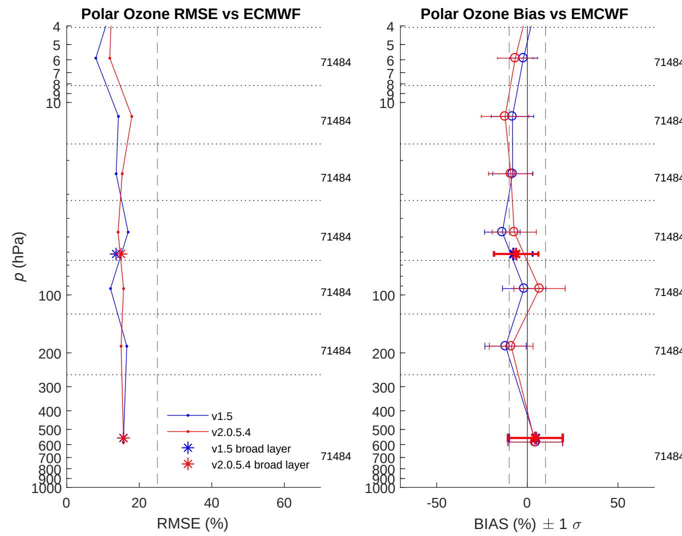


Fig. 14. As Figure 13 except for NUCAPS retrievals collocated with ECMWF within the NH and SH polar caps.

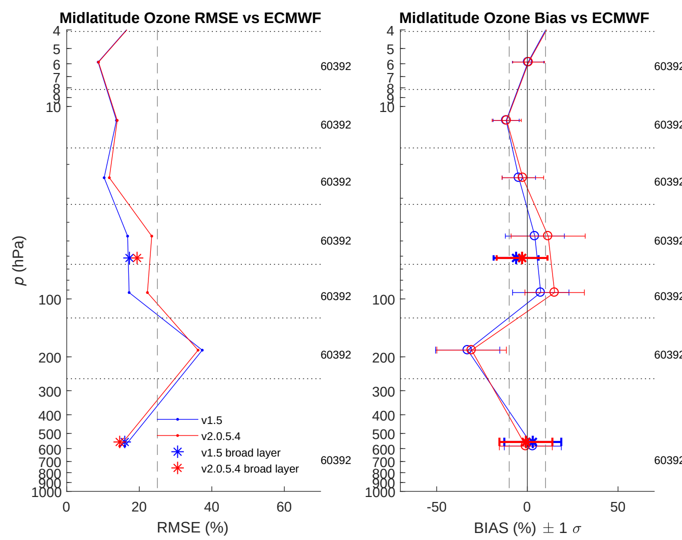


Fig. 15. As Figure 13 except for NUCAPS retrievals collocated with ECMWF within the midlatitude zones.

ECMWF model output, it has been shown that the NUCAPS v1.5 IR ozone profile EDR (CrIS-FSR) meets JPSS Level 1 broad-layer global performance requirements (Tables I and II) and has thus attained Validated Maturity. It is noted that the ozonesonde sites used in this analysis (Figure 5) include those from all global climate zones (tropical, midlatitude and polar), as well as unique marine-based datasets obtained from ship over both the Pacific and Atlantic Oceans (i.e., AEROSE and CalWater/ACAPEX campaigns). The NUCAPS OE physical retrieval was shown to improve upon the climatological *a priori* in UT/LS layers (Figures 7 and 13) where CrIS has sensitivity (Figure 3). Results vary somewhat depending on latitude zone (tropical, midlatitude and polar), with a general improvement seen at higher latitudes as would be expected given the variation in ozone DoF (Figure 4) and in vertical sensitivity (Figure 3). The algorithm has been successfully implemented for *SNPP* CrIS-FSR SDRs (v2.0.5), these being

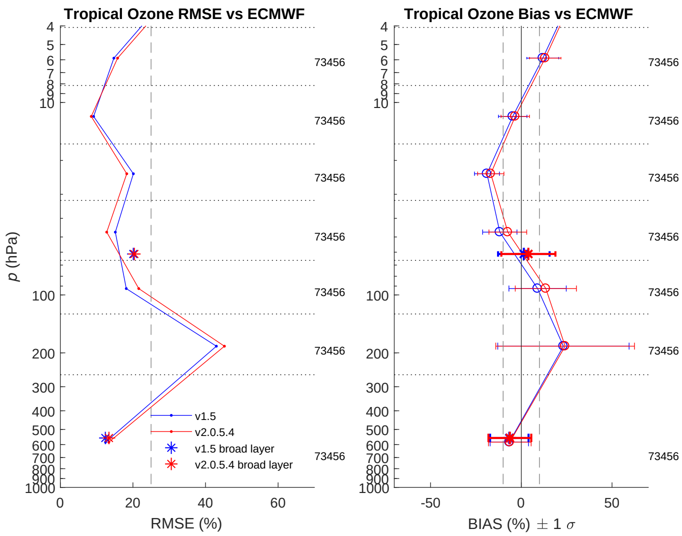


Fig. 16. As Figure 13 except for NUCAPS retrievals collocated with ECMWF within the tropical zone.

produced for future JPSS satellites and operationally from *SNPP* since March 2017, with increased yield and comparable performance versus the validated NUCAPS v1.5 algorithm (Figure 13). Full validation of the *JPSS-1* NUCAPS-FSR algorithm (including future upgrades) versus global ensembles of collocated ozonesondes (including dedicated ozonesondes) will be the subject of future work.

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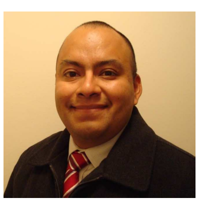

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