Validation and Utility of Satellite Retrievals of Atmospheric Profiles in Detecting and Monitoring Significant Weather Events

S. Kalluri¹, C. Barner², M. Divakarla³, R. Esmaili², N. Nalli³, K. Pryor¹, T. Reale¹, N. Smith², C. Tan³, T. Wang³, J. Warner⁴, M. Wilson¹, L. Zhou¹, T. Zhu³

Corresponding Author: satya.kalluri@noaa.gov

Capsule: The National Oceanic and Atmospheric Administration (NOAA) Unique Combined Atmospheric Processing System (NUCAPS) uses data from infrared and microwave sounders on polar-orbiting satellites to retrieve atmospheric profiles of temperature, water vapor, and trace gases. Forecasters operationally use temperature and water vapor profiles for predicting severe weather, and trace gas measurements contribute to the study of atmospheric chemistry.

¹Corresponding author address: NOAA JPSS Program Office, Building L40/Rm S674, 7700 Hubble Drive, Lanham, MD 20706
²Science and Technology Corp. (STC), 10015 Old Columbia Road, Suite E-250, Columbia, MD 21046
³IM Systems Group, NOAA/NESDIS/STAR, (E/RA2), NCWCP, 5830 University Research Court, College Park, MD 20740, USA
⁴CISESS, 5825 University Research Court, Suite 4001, University of Maryland, College Park, MD20740-3823

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ABSTRACT

Infrared and microwave sounder measurements from polar-orbiting satellites are used to retrieve profiles of temperature, water vapor, and trace gases utilizing a suite of algorithms called the National Oceanic and Atmospheric Administration (NOAA) Unique Combined Atmospheric Processing System (NUCAPS). Meteorologists operationally use the retrievals similar to radiosonde measurements to assess atmospheric stability and aid them in issuing forecasts and severe weather warnings. Measurements of trace gases by NUCAPS enable detection, tracking, and monitoring of greenhouse gases and emissions from fires that impact air quality. During the polar winters, when ultraviolet measurements of ozone are not possible, absorption features in the infrared spectrum of the sounders enable the assessment of ozone concentration in the stratosphere. These retrievals are used as inputs to monitor the ozone hole over Antarctica. This article illustrates the utility of NUCAPS atmospheric profile retrievals in assessing meteorological events using several examples of severe thunderstorms, tropical cyclones, fires, and ozone maps.

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Radiances from infrared and microwave sounders from polar-orbiting satellites provide critical inputs to Numerical Weather Prediction (NWP) models and significantly impact forecast skill (Joo et al. 2013). There have been substantial technical improvements in these satellite sounders’ capabilities over time. Each new generation of satellites is providing better spatial and spectral resolution that allows for resolving the atmosphere’s vertical structure and determines the composition with greater detail (Menzel et al. 2018). Earlier approaches using satellite sounding data in NWP primarily relied on retrievals of atmospheric profiles as a proxy for radiosondes. However, in the 1990s direct radiance assimilation became the dominant method, especially in the NWP centers with advanced fast radiative transfer models and high-performance computing (Eyre et al. 2020).

Nevertheless, techniques to improve retrievals as well as assimilation of radiances from satellite sounding instruments into NWP have progressed in parallel. Both these approaches have advantages and disadvantages, as well as different use cases. The underlying physical principles for assimilation and retrieval are similar (see Rodgers 2000, for theoretical background). NWP models use variational, ensemble, and hybrid methods for data assimilation from multiple sources, including satellite sounders to initialize conditions for forecasts (Benjamin et al. 2016), which require significant high-performance computing resources to execute (Bauer et al. 2015; Schulthess et al. 2019). In contrast, near real-time retrievals of atmospheric profiles from satellite observations can provide forecasters with the capability to examine and determine conditions such as atmospheric instability for nowcasting (Iturbide-Sanchez et al. 2018; Esmaili et al. 2020; Berndt et al. 2020). Satellite retrievals can exploit the full information content of a...
single satellite suite of instruments and provide much denser and frequent global coverage compared to radiosondes when multiple satellites are used (Esmaili et al. 2020). It has been shown that improvements in NWP model forecasts of hazardous weather can be achieved by assimilating profile retrievals obtained in real time from combined direct broadcast system (DBS) polar satellite hyperspectral and geostationary satellite multispectral radiance data (Smith et al. 2020). In addition to temperature and water vapor profiles, hyperspectral infrared sounders are also capable of retrieving profiles of thermodynamically active trace gases such as ozone (O₃), carbon monoxide (CO), methane (CH₄), and carbon dioxide (CO₂) which have strong absorption bands in the infrared channels. Unlike weather forecast models that predominantly use radiance assimilation, chemical transport models primarily use retrievals of trace gases in their assimilation schemes, and the use of satellite-derived profiles is growing for both forecasting (Hollingsworth et al. 2008) as well as for reanalysis (Inness et al. 2013; Miyazaki et al. 2015) of greenhouse gases. While direct assimilation of radiances at 9.6 μm wavelength provides some information regarding ozone, the assimilation of UV retrievals is still widely used by National Oceanic and Atmospheric Administration (NOAA), National Aeronautics and Space Administration (NASA), the US Navy, European Centre for Medium-Range Weather Forecasts (ECMWF) as well as most NWP centers in their models.

The NOAA Unique Combined Atmospheric Processing System (NUCAPS) operationally retrieves vertical profiles of temperature, water vapor, ozone, and trace gas Level 2 products (also called as Environmental Data Record (EDR)) from several infrared and microwave sounders on polar-orbiting satellites (NUCAPS, 2021). These include Interféromètre Atmosphérique de Sondage Infrarouge (IASI) and Advanced Microwave Sounding Unit on the...
Metop series (2006–present); and Cross track Infrared Sounder (CrIS) and Advanced Technology Microwave Sounder (ATMS) first on Suomi-NPP (S-NPP) (2011–present) and now on the Joint Polar Satellite System (JPSS) series of satellites (2017–present). The purpose of this article is to describe the retrieval approach briefly, and to demonstrate the utility of NUCAPS in detecting and forecasting significant weather events through various examples.

OVERVIEW OF NUCAPS

While NUCAPS can produce retrievals from several satellite missions, the description here is limited to retrievals from CrIS and ATMS instruments onboard JPSS satellites. CrIS is a Fourier transform spectrometer interferometer with 2211 spectral channels in the 3.92 µm to 15.38 µm spectral range whose Field of Views (FOV) have a nadir resolution of 14km (Han et al. 2013). A CrIS Field of Regard (FOR) is the observation footprint where a FOR has a matrix of 3x3 FOVs within it (Figure 1). ATMS covers 22 bands from 23 GHz to 183 GHz at variable spatial resolution, with the highest nadir spatial resolution ranging from 15.8 - 74.8km depending upon the band (Kim et al. 2014). Figure 1 illustrates the CrIS and ATMS footprints at satellite nadir, and how they are collocated for NUCAPS retrieval.

The NUCAPS design is based on the Advanced Infrared Sounder (AIRS) retrieval system described in (Susskind et al. 2003, 2006; NUCAPS 2021; Gambacorta and Barnet 2013). AIRS was the first hyperspectral infrared sounder on NASA’s Aqua satellite, and retrieval techniques from this sensor served as a pathfinder for future missions. The method has evolved over the years and has been optimized to run in NOAA’s operational satellite data production.
Combined microwave and infrared retrievals are generated in near real-time for National Weather Service (NWS) forecasters through the Satellite Broadcast Network (SBN). For stakeholders with antennas to receive JPSS data, NUCAPS is available in real-time using the Community Satellite Processing Package (CSPP) (Gumley et al. 2018) within a Direct Broadcast System (DBS). From the start, NOAA implemented NUCAPS to be instrument independent, which means that the retrieval method is not customized for a specific instrument, but instead can retrieve atmospheric state variables from any of the modern-era microwave and hyperspectral infrared suites.

NUCAPS employs statistical as well as physical methods to retrieve temperature and water vapor profiles and a host of trace gas species, namely O\(_3\), CO, CH\(_4\), and CO\(_2\). These atmospheric state variables are retrieved one at a time in the order listed here. NUCAPS uses a subset of microwave and infrared channels for temperature and moisture, selected for their information content and spectral purity concerning the target variable (Gambacorta and Barnet 2013). In contrast, NUCAPS retrieves the trace gases from only subsets of infrared channels since microwave spectra are insensitive to their emission signals. NUCAPS aggregates the measured infrared radiance spectra before sub-setting and retrieval according to the method described in (Chahine 1974, 1977, 1982; Susskind et al. 2003). It employs a cloud clearing method that linearly combines infrared spectra of every 3 x 3 cluster of the instrument FOVs to remove the radiative effect of clouds on the spectral measurements (Susskind et al. 2003). NUCAPS then selects its spectral channels from these aggregated, cloud-cleared radiances for use in the retrieval to represent the cloud-free atmospheric state. While aggregation during cloud clearing reduces the spatial footprint of NUCAPS soundings (~50 km compared to ~13 km of a CrIS...
measurement), it offers a significant advantage: robust, accurate soundings, with a global yield of ~75%, that are available in clear and partly cloudy scenes without requiring any prior knowledge about scene-specific cloud properties. Thus, most of the globe is characterized multiple times a day for most atmospheric conditions, excluding only those areas with optically thick, uniform cloud decks.

Figure 2 shows a high level flow chart of the NUCAPS retrieval system. Some salient features include:

1) A microwave-only retrieval module which derives profiles of cloud liquid water, temperature and water vapor, surface type, and microwave emissivity (Rosenkranz 2001). This approach employs the Rodgers (2000) optimal estimation method.

2) A first guess, derived from a fast eigenvector regression retrieval for temperature and moisture using ATMS channels and eigenvectors of CrIS channels as predictors, which provides the initial guess of profile state. The regression coefficients are generated beforehand by training ATMS and CrIS all-sky radiances against collocated ECMWF forecast-analysis (Goldberg et al. 2003).

3) A cloud-clearing module uses the atmospheric state derived in Step 2 and a set of infrared channels to produce cloud-cleared radiances for all infrared channels (Susskind et al. 2003). This step acts to remove the radiative effects of clouds from the retrieval. Thus, the profiles represent the atmospheric state around clouds, and not through them.

4) A second eigenvector regression retrieval trained with the collocated forecast-analysis-interpolated ECMWF, ATMS, and cloud-cleared radiances provides the first guess state for the final IR physical retrieval. This step also repeats the cloud-clearing using the state...
derived from the second eigenvector regression and optimizes cloud-cleared radiances for all IR channels.

5) The final infrared physical retrieval employs cloud-cleared CrIS radiances. The temperature and water vapor retrieval from Step 4 and a-priori profiles of trace gases are used as the first guess (Susskind et al. 2003). The microwave retrievals performed earlier (Step 1) are used as part of quality control.

The multistep NUCAPS physical retrieval module retrieves individual parameters sequentially (as opposed to simultaneously), using a subset of channels rigorously determined to be sensitive to each parameter (Gambacorta and Barnet 2013), beginning with temperature, then water vapor, followed by ozone and other trace gases. This multistep approach was first developed by the AIRS Science Team for the AIRS/AMSU retrieval algorithm (Susskind et al., 2003, 2014) and later adopted for CrIS/ATMS in NUCAPS as well as the Community Long-term Infrared Microwave Combined Atmospheric Product System (CLIMCAPS; Smith and Barnet 2019, 2020). NUCAPS employs a regression-based first guess to decrease latency and enable around-the-clock, real-time hazard monitoring, while CLIMCAPS employs the Modern-Era Retrospective analysis for Research and Applications, Version 2.0 (MERRA-2; Gelaro et al., 2017) as the retrieval first guess to enable a consistent, long term record of satellite soundings for studying the diurnal cycle and seasonal atmospheric processes.

The NUCAPS retrieval algorithm EDR products have been extensively validated according to a well-established validation methodology hierarchy (e.g., Nalli et al. 2013). The retrieved Atmospheric Vertical Temperature Profile (AVTP), Atmospheric Vertical Moisture Profile
(AVMP), infrared ozone profile, and carbon trace gases have been validated by comparison with model output, in situ measurements such as radiosondes and dropsondes, as well as with measurements made by other satellite sensors (e.g., Divakarla et al. 2006; Reale et al. 2012; Sun et al. 2017; Nalli et al. 2018a, 2018b). Based on correlative datasets, the empirically estimated global combined measurement uncertainties for AVTP and AVMP (accepted cases) versus dedicated radiosonde observations (expressed as RMSE for three broad atmospheric layers) under cloud-free to partly cloudy conditions have been determined to be approximately 0.8–1.2 K, and 0.02–1.2 g/kg, respectively (Nalli et al. 2018b). Likewise, the global combined measurement uncertainty for the infrared ozone retrievals (on two broad layers) are approximately 19–23% RMSE from the surface to 4 hPa (Nalli et al. 2018b).

NUCAPS carbon trace gas profiles of CO, CH$_4$, and CO$_2$ have been more recently validated according to a similar methodology hierarchy (Nalli et al. 2020) featuring model output (e.g., Copernicus Atmosphere Modeling Service, Peuch et al. 2018), data from satellites explicitly designed to measure atmospheric composition (e.g. TROPOspheric Monitoring Instrument (TROPOMI)), ground-based networks (e.g., Total Carbon Column Observing Network, Wunch et al. 2011), AirCore profiles (Membrive et al. 2017), and aircraft campaigns (viz., NASA’s Atmospheric Tomography (ATom) mission, Wofsy et al. 2018). The global measurement uncertainties (RMSE) for total integrated columns of retrieved CO, CH$_4$ and CO$_2$ (valid cases under clear-to-partly cloudy conditions) versus in situ aircraft measurements (from the ATom-1,-2 and -4 campaigns) are approximately 20%, 1.5% and 0.75%, respectively; when NUCAPS averaging kernels (AKs) are applied, these are reduced to approximately 9.2%, 1.5% and 0.3% (Nalli et al. 2020).
Conventional radiosondes are critical for initializing NWP models through data assimilation and evaluating forecasts. Like radiosondes, NUCAPS can provide real-time, model-independent information on atmospheric temperature and moisture. Because radiosondes are only launched twice-daily from 92 NWS sites in the United States, NUCAPS can supplement in-situ observations with dense satellite observations across a 2,200 km swath, at a rate of ~120 instantaneous soundings per 30 seconds. Furthermore, the existing Low Earth Orbit (LEO) satellites have mid-morning and early-afternoon overpasses, providing observations outside of regular 00 and 12 UTC radiosonde launch times. Radiosondes measure temperature and moisture at the point of contact as the balloon ascends, whereas NUCAPS measures atmospheric gradients from the top-down and are averaged over a large region. A NUCAPS sounding should be interpreted as a roughly cylindrical observation with ~50km diameter at instrument nadir view and ~150km at edge of scan that measures vertical layer averages with 1-3km resolution depending on altitude pressure (hPa and mb are used interchangeably as units of pressure throughout this paper). NUCAPS has a near real-time delivery (<30 minutes from an overpass) through the DBS network, making it suitable for rapid, pre-convective forecasting. NUCAPS EDR generation software is available to DBS users through the CSPP (Gumley et al. 2018). More than augmenting radiosondes, forecasters can visualize the high-density Gridded NUCAPS product to show horizontal spatial gradients of stability parameters, enabling situational awareness in 3D (Weaver et al. 2019; Esmaili et al. 2020; Berndt et al., 2020). Gridded NUCAPS allows forecasters to visualize incoming satellite swaths of NUCAPS soundings as...
horizontal or vertical cross-sections, instead of individual soundings one Skew-T diagram at a time.

NUCAPS meets the forecasters’ latency requirements for fast decision-making (Smith et al., 2019). However, in practice, it is equally essential for researchers to actively engage with NWS forecasters to ensure NUCAPS is an effective tool for pre-convective forecasting on 1-2 hour timescales (Esmaili et al. 2020). Through the JPSS Proving Ground and Risk Reduction (PGRR) program, researchers successfully transitioned NUCAPS from an experimental dataset for real-time forecasting to one that forecasters rely on operationally. This transition was facilitated through direct collaboration with NWS forecasters. NUCAPS is demonstrated in relevant field campaigns to first determine the value for applications, such as the recent collaboration with NOAA’s Hurricane Field Program (HFP), the joint NASA-NOAA FIREX-AQ field campaign, and the El Nino Rapid Response Field Campaign (Dole et al. 2018). The most rigorous evaluation of NUCAPS for severe weather forecasting occurs in the Hazardous Weather Testbed (HWT; Ralph et al. 2013). Facilitated by the PGRR program, NUCAPS has been evaluated annually by forecasters in the HWT since 2015 (Esmaili et al., 2020; Berndt et al., 2020). Some goals for evaluating NUCAPS in the HWT are (1) to provide tailored NUCAPS training to a group of forecasters, who can then transfer knowledge back to the regional offices and (2) to evaluate the NUCAPS delivery in the Advanced Weather Interactive Processing System (AWIPS II; Figure 3). AWIPS II is the primary data visualization and decision support platform for forecasters, so NUCAPS must be easily accessible, timely, and relevant. Participation in the HWT has fostered a two-way communication channel, which maximizes NUCAPS benefits to the NWS.
During the HWT, forecasters documented examples of scenarios where NUCAPS captured atmospheric phenomena well. For example, Figure 4a shows a NUCAPS sounding with an 800 mb temperature inversion (red arrow) in the Houston/Galveston, TX County Warning Area (Hazardous Weather Testbed 2019A). Temperature inversions can stratify a stable mid-troposphere from an unstable boundary layer and thus can suppress the development of thunderstorms. On this day, models predicted significant convection, so NUCAPS helped the forecaster diagnose the reason for the delayed onset of thunderstorms. In Figure 4b, a forecaster used Gridded NUCAPS 850-500 mb lapse rate to observe advancing dry air moving eastward (Hazardous Weather Testbed 2019B). Meteorological data are sparse over this region of West Texas, so satellite observations help evaluate NWP models. Figure 4c shows a NUCAPS sounding that was part of a larger mesoanalysis of instability building in the Tallahassee, FL CWA (Hazardous Weather Testbed 2019C). The weak temperature protrusion at 700 mb (red arrow) lowers the Convective Available Potential Energy (CAPE) and potentially reduces updraft intensity. The forecaster who identified this case also verified this vertical feature in a special sounding, which increased their confidence in NUCAPS.

Outside of the annual HWT, the PGRR program encourages ongoing collaboration between forecasters, product developers, validation teams, and scientists through the sounding applications initiative. These researcher-forecaster partnerships have increased stakeholders’ integration of NUCAPS in the NWS and beyond, including the US Navy and NOAA field campaigns. For example, collaboration in the PGRR has led to NUCAPS integration into a visualization tool called “Sounding and Hodograph Analysis and Research Program in Python.”
to increase data access (Blumberg et al., 2017) and for Cold Air Aloft monitoring for aviation weather (Weaver et al., 2019). These partnerships have also led to researchers using NUCAPS to study the thermodynamic structure of the Saharan air layer (Kuciauskas et al., 2020) and tropical cyclones (Barnet et al., 2019). A complete list of projects and training resources are available on: https://weather.msfc.nasa.gov/nucaps. While the examples in this section are a direct result of NWS forecaster feedback and interaction, the examples in the remainder of this article highlight analysis by scientists, researchers, and validation teams for the purpose of illustrating NUCAPS’ utility and building stakeholder confidence in using the products.

UTILITY OF NUCAPS SOUNDINGS IN STUDYING SEVERE STORMS

27 April 2020 South Texas Severe Thunderstorm Downbursts

A cluster of thunderstorms developed west of the dryline over the Davis Mountains of southwestern Texas during the afternoon of 27 April 2020, while a dryline extended from east of Midland, Texas to the Big Bend area as shown in the 2100 UTC surface analysis in Figure 5. The thunderstorm cluster then merged to form an intense mesoscale convective system (MCS) with a leading bow echo (not shown) near the westward bulge in the dryline. As noted by Schaefer (1986) and Ziegler et al. (1997), the dryline is often a focus of differential heating, boundary layer convergence, and solenoidal circulation with an attendant release of instability and convective storm intensification. After dryline interaction, the MCS tracked rapidly southeastward toward the Gulf Coastal Plain. By mid-afternoon, a NOAA-20 NUCAPS sounding profile captured the high potential of severe thunderstorm-generated straight-line winds nearly six hours before the onset of
the severe windstorm in the international border area of southern Texas. **Figure 6** shows a
NUCAPS physical retrieval sounding profile over Del Rio, Texas. The Skew-T diagram shows
considerable convective available potential energy (CAPE, > 4000 J/kg), a large lower
tropospheric temperature lapse rate (> 9°C/km), and a prominent mid-tropospheric unsaturated
layer that indicated a high probability of severe thunderstorm downburst occurrence. A microburst
windspeed potential index (MWPI) (Pryor 2015) value of 6.9 indicated thunderstorm wind gust
potential of 60 knots. MWPI values greater than 5 indicate a high probability of severe winds
greater than 50 knots in magnitude. In addition, the corresponding equivalent potential temperature
(theta-e) profile signified potential instability with a decreasing value from the surface upward to
a minimum in the middle troposphere. The calculated surface to 500 mb theta-e difference (∆θ_e)
of 29 K significantly exceeds the 20 K threshold for downburst occurrence as documented by
Atkins and Wakimoto (1991). Comparing the NUCAPS sounding profile to the 0000 UTC 28
April radiosonde observation (RAOB) from Del Rio shows that NUCAPS indicated a stronger
signal for severe thunderstorm and downburst occurrence over four hours prior to the RAOB
sounding. As the storm passed over the Del Rio, Texas area, severe downbursts were generated,
resulting in wind gusts of 67 and 65 knots, recorded at Del Rio International Airport at 0135 UTC
and at Laughlin Air Force Base at 0150 UTC 28 April, respectively.

Defense Meteorological Satellite Program (DMSP) F-17 and Metop-A overpasses were optimal
for retrieving cloud microphysical properties before and shortly after the downburst in the Del Rio
area, as inferred from brightness temperature (TB) measurements shown in **Figure 7**. Imagery
from Special Sensor Microwave Imager Sounder (SSMIS) and Microwave Humidity Sounder
(MHS) displayed in **Figure 7** show remarkably cold cloud tops (white shading) and large graupel

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water path values (> 1 mm) that indicated significant storm severity. As shown in Figures 7a and 7b, the 91 GHz channel is an atmospheric “window” in the microwave spectrum. Scattering by ice-phase precipitation particles, especially graupel, hail, and snow above the freezing level causes the TB depression (Ferraro et al. 2015, Laviola et al. 2020) around the time of peak storm intensity. For this case, TB near the storm centroid was remarkably low (~120 K) and corresponded to a maximum in graupel water path (GWP) values (> 10 mm), indicating the presence of a dense core of graupel/hail. A large ice content and prominent dry-air notches on the lateral and downshear (forward) flanks of the storm indicated favorability for strong thunderstorm downdraft generation (Srivastava 1987, Knupp 1989). Metop-A MHS imagery shown in Figures 7c and 7d displayed remarkably cold cloud tops (white shading) and large graupel water path values (> 1 mm) that indicated significant storm severity.

This severe convective wind event’s intensive study demonstrates the science value added by the synergistic analysis of satellite and ground-based sensor data. This is illustrated by the afternoon NUCAPS vertical profile pointing to decreased stability and the potential for convection and verification by the appearance of severe convective storms in SSMIS and MHS imagery. Successive overpasses of DMSP F-17 and EPS Metop-A satellites shown in Figure 7 provided microwave imagery that effectively visualized the severe MCS evolution. This multicellular storm tracked east-southeastward with weak low-level shear that was nearly parallel to the MCS, which allowed for a short episode of severe downburst winds over the Del Rio area, followed by gradual weakening of the system and cessation of severe winds. Also apparent were inward-directed V-shaped TB gradients on the downwind (eastern) flank of the storm that suggests the occurrence of wake entrainment of sub-saturated air and subsequent downdraft acceleration by the process
detailed in Knupp (1989). The absence of an apparent rear-inflow jet was likely a factor in the episodic and short-lived occurrence of downburst winds at Del Rio with a duration only 15 minutes, from 0135 to 0150 UTC 28 April. However, these storms still produced significant structural damage and power outages on a local scale.

27 August 2020 Hurricane Laura Landfall, Louisiana Coast

Landfalling tropical cyclones (TC) can produce severe local-scale downburst winds generated by intense convective storms embedded within the principal and outer (distant) rain bands. An important component of forecasting hurricane landfall is an assessment of stability conditions and potential for damaging convective wind gusts. During the morning of 27 August 2020, Category 4 Hurricane Laura made landfall at Cameron, Louisiana, where a wind gust of 110 knots was recorded at Calcasieu Pass National Ocean Service (NOS) station, followed by a wind gust of 115 knots recorded at Lake Charles Regional Airport, 50 km inland from the point of landfall.

On the previous afternoon, an S-NPP NUCAPS sounding profile was retrieved in a partly cloudy region outside of the tropical cyclone cloud system over northwestern Louisiana at 1927 UTC 26 August, as shown in Figure 8a. This infrared + microwave physical sounding retrieval that passed QA and QC indicated favorable conditions for intense convective downdraft generation in the primary and outer (distant) rain bands that included a middle-tropospheric unsaturated layer with a surface-based layer of conditional instability. Favorable conditions for intense convective downdraft generation were also echoed in the corresponding theta-e profile (Figure 8b) that displayed a middle-tropospheric low theta-e layer and potential instability between the surface and...
the 700 mb level. During the afternoon of 26 August, an intense outer rain band, with embedded
deep convective storms, developed over the Louisiana coast and tracked northwestward, producing
strong surface outflow winds at Lake Charles Airport (46 knots recorded at 1723 UTC, not shown).
By the time of the NUCAPS sounding retrieval, two prominent bowing segments were apparent
in the outer rain band as shown in ATMS imagery and NEXRAD reflectivity (Figures 8c-d).

Metop-B MHS brightness temperature imagery in the 89 GHz window channel (Figure 9), one
hour prior to landfall on 27 August, 2020, shows the structure of the principal (“PRB”) and
secondary (“SRB”) rain bands with low brightness temperature (< 235 K) indicating the presence
of ice particles lofted into the upper levels of the embedded convective storm cells (Houze 2010).
In addition, Houze (2010) noted that the principal and outer (“distant”) rain bands of a tropical
cyclone are important structural features for the generation of intense convective downdrafts and
resultant downward transport of horizontal momentum and low theta-e air from the middle
troposphere. Closer to landfall, severe outflow wind gusts (53 knots) were recorded at Lake
Charles with the onset of the principal rain band near the time of the MHS 89 GHz brightness
temperature imagery displayed in Figure 9. The study of TC Laura also demonstrates the
importance of afternoon NUCAPS sounding retrievals over southern CONUS for anticipating
severe convective storm development well ahead of a landfalling tropical cyclone.

MONITORING ATMOSPHERIC CHEMISTRY THROUGH NUCAPS PRODUCTS

Sudden Stratospheric Warming Over the South Pole, and Ozone Hole During 2019
A Sudden Stratospheric Warming (SSW) is caused by vertically propagating planetary waves (Matsuno 1971, Venkat Ratnam et al. 2004). Although such events are common in the northern hemisphere, this phenomenon is rare in the southern hemisphere (Dowdy et al. 2004). During an SSW, there is rapid warming of the stratosphere (>30 – 40 K) in just a few days (Butler et al. 2015). The events are categorized as significant if, at an atmospheric pressure level of 10 mb or below, the latitudinal mean temperature increases poleward from 60 degrees latitude, and an associated circulation reversal is observed (McInturff 1978). NUCAPS sounding EDRs are typically of value to operational meteorologists focused on severe weather applications in the troposphere (below an altitude of 5km). However, these soundings are produced up to 1 hPa (50km) and include reliable temperature profiles through the stratosphere. Beginning in late August 2019, meteorologists started noticing the onset of what would become a historic sudden stratospheric warming (SSW) event high above Antarctica with continued intensification through September (Lewis, 2019). Figure 10 shows the evolution of this warming trend at 11 hPa on 5, 15, and 19 September 2019, as observed by NUCAPS soundings. Using 26 August 2019 retrievals as a reference, the temperature departures on successive days were computed to track the SSW anomaly. Figure 11 shows the latitudinal mean temperature anomalies observed in the southern hemisphere from 5 September through 19 September, 2019. Each chart shows the temperature departure from the reference date of 26 August 2019 (dt = Temperature on a given day – Temperature observed on 26 August). These results indicate a maximum temperature difference (dt) at 11 hPa approaching 80 K on 19 September between 85°- 90° southern latitudes, with a rapid increase during the week from 5 September to 15 September 2019.
NUCAPS retrievals are routinely validated using radiosonde observations that are collocated in time and space as described by Reale et al., 2012. There are ten radiosonde sites over Antarctica including those from the Global Climate Observing System (GCOS) Reference Upper Air Network (GRUAN; www.GRUAN.org). Most radiosondes reach 20 hPa in this region with a sizable portion attaining 10 hPa or higher. Comparisons of collocated radiosonde and NUCAPS soundings, typically within a few hours and 50 km (defined at surface) show very close agreement in the stratosphere up to 10 hPa. Differences in atmospheric temperature between NUCAPS retrieval and those from collocated radiosondes at 10 hPa along the Antarctic coast during 2-6 September, 2019 were between 1-2 K.

The 2019 SSW event had significant impacts on zonal wind circulation and the Ozone hole size over Antarctica (Safieddine et al. 2020), similar to what was observed in 2002 (Kondragunta et al. 2005). During average years, the cold stratospheric temperatures during austral spring over the south pole convert halogen compounds over clouds to more reactive forms that catalyze ozone loss (Solomon 1999). The stratospheric warming disrupts this chemical process leading to a reduced loss of ozone. Ozone has a strong absorption band at 9.6 μm, and CrIS infrared channels are used together with the Ozone Mapping Profiler Suite (OMPS) on JPSS satellites to retrieve ozone operationally at NOAA. The CrIS infrared observations fill in the gaps in ultraviolet (UV) observations, especially at the poles when there is no sunlight to measure UV radiation during austral winter. **Figure 12** shows total ozone concentrations from CrIS retrieved by NUCAPS and OMPS data during September of 2018 and 2019. Significant reduction in the ozone hole is observed in 2019 that is attributed to the SSW event.
Tracking Carbon Monoxide from Australian Fires in 2019 and California Fires in 2020

NWP models predicted warmer than average weather patterns over Australia due to the SSW (Lewis 2019, Bureau of Meteorology 2019). While there is no direct evidence that the SSW event contributed to Australia’s massive fires during 2019, it was one of the factors that led to extremely hot and dry fire weather 2019 (MetOffice 2020). Over 3.8 million acres were burnt over Australia during this unprecedented fire season (Nolan et al. 2020). Fire emissions contribute to the carbon input to the atmosphere through emissions of carbon dioxide, methane, and CO. These fires injected massive amounts of smoke, aerosols, and trace gases such as CO and NO that traveled around the southern hemisphere (Kablick III et al. 2020). NUCAPS retrieves CO profiles from 24 CrIS channels in the 2155–2550 cm$^{-1}$ shortwave infrared region where the absorption features are very distinctive (Gambacorta et al. 2014), and the retrieval algorithms discussed here are most sensitive to CO concentrations in the mid-troposphere around 500 hPa (Smith and Barnet, 2020). Figure 13 shows total column CO mixing ratio (ppbv) at 500 hPa observed by NUCAPS from 17 December 2019 to 15 January 2020 over Australia and the South Pacific. The upper panel focuses on the relatively early stage of the large fires in December, where strong CO plumes were seen over regions of the state of New South Wales and in north-eastern Victoria. The CO concentrations near the fires were reduced during 1 and 15 January 2020. However, the NUCAPS CO shows extremely high values, several times the normal value in the transported plumes from the Tasman Sea to the South Pacific Ocean (see Figure 13 lower panel). Note that the typical background CO values at 500 hPa over the southern hemisphere ocean are approximately 40 ppbv (Warner et al. 2013).
In the United States, over 58,250 wildfires burned 10.3 million acres in 2020, with California accounting for nearly 40% of the impacted acres (Hoover and Hanson, 2021). Figure 14 shows multiple-day means of CO column averaged mixing ratios (xCO in ppbv) at 500 hPa (ppbv) using both S-NPP and NOAA-20 CrIS measurements taken 50 minutes apart. The earlier days of the fire emitted CO plumes were seen (see Figure 14 upper panel) from September 5 to 8, 2020, and the transported patterns are shown in the lower panel during September 11 through 17, 2020. The fire emissions were uplifted and transported eastward over the entire US and to the Atlantic. A smaller branch of the plumes was transported towards northwest and the Pacific. Based on the histogram of CO distributions (not shown), CO concentrations from these fires reached as high as 815 ppbv in this region, whereas the background CO concentrations at 500 hPa level are roughly 80 – 100 ppbv (Warner et al., 2013). Although the typical CO concentrations in the outside environment are not directly damaging to human health, it is a good tracer and can be used to determine the transport patterns of co-emitted species such as particulate matters from the smoke and ash that impact human health.

SUMMARY

NUCAPS is an enterprise EDR product generation system at NOAA that operationally generates satellite soundings from infrared and microwave measurements made by instruments on polar-orbiting platforms in mid-morning and early afternoon orbits. NUCAPS enables mesoscale situational awareness of the 3-dimensional atmospheric state with consistent quality across 2,200 km wide swaths and multiple observation times throughout a 24-hour cycle. In 2014 NUCAPS
became available within the NWS AWIPS system, and through direct broadcast via CSPP. The examples discussed here have been selected from several significant meteorological and environmental events during 2019-2020 where NUCAPS data could be applied to provide additional information in detecting and monitoring the atmospheric conditions associated with them. The intent of this article is to demonstrate the value of new and additional capabilities to enable improved monitoring and modeling of these phenomena, particularly in severe weather and atmospheric composition that have significant societal impacts.

NUCAPS retrievals fill in the spatial gaps of conventional radiosondes, and gridded imagery of atmospheric variables at different heights in the atmosphere enables a synoptic view of the atmospheric state. This allows operational meteorologists to study the vertical and horizontal gradients in atmospheric fields of temperature and water vapor, which augments other data such as satellite imagery and NWP model outputs that forecasters use.

Satellite liaisons worked with forecasters in their NWS Weather Forecast Offices (WFO) for several weeks every year and gathered feedback on the strengths and weaknesses of NUCAPS soundings during various weather events. Algorithm developers collaborated with atmospheric chemistry modelers at various NOAA laboratories to determine which model parameters can be derived from NUCAPS and assimilated into models. Through close partnerships between algorithm and product developers, validation teams, scientists and operational forecasters, NUCAPS soundings have been assessed in various forecasting scenarios, including pre-convective environments, the evolution of hurricanes, and atmospheric chemistry studies. The strong collaboration among scientists, developers and users also led to continuous product

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improvement and tools such as SharpPy, gridded NUCAPS and averaging kernels that enable greater usage and impact of NUCAPS products.

NUCAPS soundings are not typically studied within hurricanes since the data are predominantly cloudy where the IR+MW retrievals are not possible. Nevertheless, as shown in the hurricane Laura example, there could be valid IR+MW retrievals outside of the hurricane core that provide additional information on rainband cellular convection and hurricane structure. This information could enable a forecaster to anticipate the onset of severe convective winds augmenting other data such as microwave imagery, NEXRAD and NWP model outputs in providing warnings and advisories.

NUCAPS products are model independent and provided additional inputs of trace gasses to NWP. Optical sensors such as VIIRS and MODIS provide column integrated measurements of atmospheric components such as aerosols, dust, CO and CO$_2$, but NUCAPS provides vertical profiles from soundings that provide measurements of trace gasses in different layers of the atmosphere. While NUCAPS was primarily designed for weather forecasters, the examples shown here demonstrate the utility of these soundings, especially trace gas retrievals for monitoring other significant environmental events as well. Although NWP models assimilate data from multiple satellites to monitor events such as the sudden stratospheric warming and ozone concentrations over the poles, individual retrievals derived without NWP model inputs provide additional confidence in the model outputs. Infrared soundings are particularly useful in ozone retrievals during polar night when UV measurements are not effective. Efforts are currently underway to assimilate NUCAPS trace gas measurements in to the NOAA Unified
Forecast System (UFS) Real-time Air Quality Modeling System (RAQMS) to improve the
ability to forecast poor air quality associated with wildfire events. When infrared and microwave
sounders from multiple missions are cross-calibrated, NUCAPS retrievals can also provide long-
term climate data records of temperature, water vapor, and trace gases at different layers of the
atmosphere.

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Severe Thunderstorm event. The views, opinions, and findings contained in this report are those
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Figure 1. A CrIS Field of Regard (FOR) has three Field of Views (FOVs), and each FOV has a 14km spatial resolution at nadir (A). ATMS FOVs have three spatial resolutions that are nested (B), and the FOV depends on the channel (C). The CrIS and ATMS measurements are co-registered (D and E). This colocation of MW and IR observations enables them to be used synergistically in NUCAPS.
<table>
<thead>
<tr>
<th>NUCAPS Retrieval Algorithm/Approach</th>
<th>Description</th>
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<tbody>
<tr>
<td><strong>MW Physical Retrieval</strong></td>
<td>Uses ECMWF based MW-apriori, calibrated MW radiances/brightness temperatures in the MW physical retrieval to derive temperature, water vapor, cloud liquid water, and MW surface emissivities (Rosenkranz, 2003).</td>
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<tr>
<td><strong>All-Sky regression</strong></td>
<td>The All-sky regression retrieval generates the first guess temperature, water vapor, and other surface parameters using IR and MW radiances/brightness temperatures using principal component regression (Goldberg et al., 2003). Instrument specific all-sky regression Look up Tables (LUT) are based on the focus day training data sets of IR/MW observations and time and space collocated ECMWF forecast/analysis of temperature and water vapor profiles. The retrieved atmospheric state is used to generate cloud cleared IR radiances.</td>
</tr>
<tr>
<td><strong>Cloud clearing of IR channels</strong></td>
<td>The approach assumes that the differences in the observed IR radiances are solely attributed to the differences in the fractional cloudiness in each field of view while everything else is uniform across the field of regard.</td>
</tr>
<tr>
<td><strong>Cloud-clear Regression</strong></td>
<td>The clear regression retrieval uses cloud-cleared radiances and principal component regression methodology to compute first guess retrieval. Methodology to derive instrument specific cloud-cleared regression LUTs are the same as in step 2. This step also repeats cloud-clearing to optimize cloud-cleared radiances for the final retrieval.</td>
</tr>
<tr>
<td><strong>IR Physical Retrieval</strong></td>
<td>The IR physical retrieval algorithm is an iterative physical retrieval algorithm minimizing observed and calculated radiances (Susskind et al. 2003). The algorithm uses the Stand-alone AIRS Radiative Transfer (SARTA) model (Strow 2003) for radiance calculations using sensor/channel specific fast forward model LUTs generated offline.</td>
</tr>
</tbody>
</table>

**Figure 2.** A sequential flow of MW and IR based retrievals in the NUCAPS system
Figure 3: Example of NUCAPS display in the AWIPS II system from 20 December, 2020 at 1900 UTC near Oklahoma City, OK county warning area (CWA). Forecasters can click a color-coded (a) footprint to display the (b) skew-T log-P sounding in the AWIPS National center Sounding and Hydrograph Analysis Research Program (NSHARP) display. NSHARP calculates several measures of CAPE and other severe weather parameters. The quality control flag footprint colors in (a) represent where retrievals passed all steps (green), where the MW-only passed, but the MW+IR failed (yellow, use with caution), or where the MW+IR failed (red, do not use).
Figure 4: Three cases identified by HWT forecasters, where NUCAPS profiles and Gridded NUCAPS provided additional value to pre-convective forecasting. These represent examples where NUCAPS was useful for identifying (a) temperature inversions, (b) gradients in lapse rates ($^\circ$C/km), and (c) vertical features that may reduce CAPE.
Figure 5. Surface analysis over much of Texas and southeastern New Mexico region at 2100 UTC 27 April 2020. The black circled region labeled “DRT” represents the location of the Del Rio, Texas and the location of the NOAA-20 sounding retrieval. “CI” represents the convective initiation region over the Davis Mountains of Texas. Courtesy of NOAA/National Weather Service/Weather Prediction Center.
Figure 6. (a) A NOAA-20 NUCAPS sounding profile retrieved during the afternoon of 27 April 2020 as compared to (b) a radiosonde observation (RAOB) at Del Rio, Texas (DRT) at 0000 UTC 28 April 2020; (c) A NOAA-20 NUCAPS theta-e profile retrieved during the afternoon of 27 April 2020 as compared to (b) a RAOB theta-e profile at Del Rio, Texas (DRT) at 0000 UTC 28 April 2020.
Figure 7. South Texas Regional F-17 SSMIS (a) 91 GHz brightness temperature (TB) image at 00:57 UTC 28 April 2020 with (b) overlying graupel water path (GWP) measurements; (c)
METOP-A Microwave Humidity Sounder (MHS) 89 GHz brightness temperature image at 0225 UTC 28 April 2020 with (d) overlying graupel water path measurements. Units of brightness temperature are Kelvin and graupel water path measurements are in millimeters (mm) with a contour interval of 2.5 mm for SSMIS and 0.25 mm for MHS. White circle marks the location of downburst occurrence at Del Rio. The diamond-shaped regions surrounding the storm centroid indicate the coldest brightness temperatures below 120 K in (a) and (b), and below 160 K in (c) and (d), respectively.
Figure 8. (a) An S-NPP NUCAPS sounding profile retrieved during the afternoon of 26 August 2020 over northwestern Louisiana and a corresponding (b) theta-e profile at 1927 UTC 26 August 2020; (c) S-NPP ATMS 88 GHz brightness temperature (Kelvin) image at 1933 UTC 26 August 2020 over the Hurricane Laura domain and (d) with Lake Charles (LCH) NEXRAD reflectivity overlaid. Black and blue right-pointing triangles mark the location of Calcasieu Pass, Louisiana,
and Lake Charles Regional Airport, respectively. “NPP” marks the location of the NUCAPS retrievals shown in (a-b) at latitude 32.4°N/longitude 93.8°W.
Figure 9. (a) Metop-B MHS 89 GHz brightness temperature (Kelvin) image at 0340 UTC 27 August 2020 over the Hurricane Laura domain (eastern Texas – Louisiana) and (b) a higher resolution view of the MHS brightness temperature (Kelvin) image with Lake Charles (LCH) NEXRAD reflectivity overlaid. White diamond-shaped region in the eye wall indicates the coldest brightness temperatures below 200 K. Black and blue right-pointing triangles mark the location of Calcasieu Pass, Louisiana, and Lake Charles Regional Airport, respectively. “NPP” marks the location of the NUCAPS retrievals shown in Figure 8 at latitude 32.4°N/longitude 93.8°W. “PRB” and “SRB” represent the principal and secondary rainbands of Hurricane Laura, respectively.
Figure 10: NUCAPS temperature (Kelvin) fields at 11 hPa displayed in southern hemisphere polar projection on 5 September 2019 (A), 15 September 2019 (B) and 19 September 2019 (C). These images show the progression of the southern stratospheric warming.
Figure 11. Zonal mean temperature (Kelvin) anomalies observed in the southern hemisphere on 5 September 2019 (A), 15 September 2019 (B) and 19 September 2019 (C). Each chart shows the temperature (Kelvin) departure from 28 August 2019.
Figure 12. The ozone hole over the south pole during September 2018 (top) and September 2019 (bottom) as observed by CrIS sensor on Suomi NPP (top) and NOAA 20 (below) satellites. Ozone concentration is in Dobson units. Source: https://www.ospo.noaa.gov/Products/atmosphere/ntoast/index.html
Figure 13. NUCAPS CO mixing ratios (ppbv) at 506 hPa equivalent pressure level from S-NPP CrIS measurements averaged during 17 to 31 December 2019 (top panel) and 1 to 15 January 2020 (bottom panel) periods.
Figure 14. Multiple-day means of CO mixing ratios (ppbv) from S-NPP and NOAA-20 CrIS measurements taken 50 minutes apart. Upper panel shows CO from September 5 to 8, 2020, and the lower panel is the average for September 11 through 17, 2020.