Validated Maturity Science Review for NOAA-20 OMPS Ozone Profile EDR – V8Pro

Presented by Lawrence E. Flynn
with contributions from NOAA & NASA
OMPS SDR and EDR Teams
Date:2021/05/27

Disclaimer

"The contents of this presentation are mine personally and do not necessarily reflect any position of the US Government or the National Oceanic and Atmospheric Administration.“

Philosophy / Content

Some key material from the earlier Reviews is repeated here. A GREEN font is used to call out these earlier results. A BLUE font is used to call out current/newer results. And a PURPLE font is used to call out planned work with known paths forward for improvements. An ORANGE font is used to call out future work with open or unresolved issues. A RED font would used to call out unsolved problems that must be resolved prior to validated maturity. There are no RED issues at this time.

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

Outline

- Validated Maturity Definitions and Entry and Exit Criteria
- Algorithm Cal/Val Team Members
- EDR Product Overview/Requirements (What is our goal?)
- Evaluation and status of OMPS SDRs (What is the impact on EDRs?)
- S-NPP Validation (Why do we trust S-NPP V8Pro at the 5% level?)
  - Chasing Orbit Comparisons to NOAA-19
  - Comparisons to Ground-based and other satellite ozone records
- High level overview of algorithm refinement history
- Evaluation of algorithm performance to specification requirements
  - Quality flag analysis/validation
  - Algorithm improvements
  - Precision analysis / validation
  - Soft calibration results for forced agreement at the 5% level.
  - Where will we do better?
  - Algorithm version, processing environment
  - Required algorithm inputs
- User Feedback
- Downstream Product Feedback
- Risks, Actions, and Mitigations
- Documentation (Science Maturity Check List)
- Path Forward & Recommendation
- Summary & Conclusion
- Backup and details

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

JPSS Data Products Maturity Definition

1. **Beta**
   - Product is minimally validated, and may still contain significant identified and unidentified errors.
   - Information/data from validation efforts can be used to make initial qualitative or very limited quantitative assessments regarding product fitness-for-purpose.
   - Documentation of product performance and identified product performance anomalies, including recommended remediation strategies, exists.

2. **Provisional**
   - Product performance has been demonstrated through analysis of a large, but still limited (i.e., not necessarily globally or seasonally representative) number of independent measurements obtained from selected locations, time periods, or field campaign efforts.
   - Product analyses are sufficient for qualitative, and limited quantitative, determination of product fitness-for-purpose.
   - Documentation of product performance, testing involving product fixes, identified product performance anomalies, including recommended remediation strategies, exists.
   - Product is recommended for potential operational use (user decision) and in scientific publications after consulting product status documents.

3. **Validated**
   - Product performance has been demonstrated over a large and wide range of representative conditions (i.e., global, seasonal).
   - Comprehensive documentation of product performance exists that includes all known product anomalies and their recommended remediation strategies for a full range of retrieval conditions and severity level.
   - Product analyses are sufficient for full qualitative and quantitative determination of product fitness-for-purpose.
   - Product is ready for operational use based on documented validation findings and user feedback.
   - Product validation, quality assurance, and algorithm stewardship continue through the lifetime of the instrument.

Validated Maturity Review Entry and Exit Criteria

Entry Criteria

- Product Requirements
- Maturity Performance Validation
- Users feedback
- Risks, Actions, Mitigations
  - Potential issues, concerns
- Path forward to improved consistency
- Summary

Exit Criteria

- Maturity Performance is well characterized and meets/exceeds the requirements:
- Updated Maturity Slide Package addressing review committee’s comments for:
  - Cal/Val Plan and Schedules
  - Product Requirements
  - Maturity Performance
  - Risks, Actions, Mitigations
  - Path forward to improved consistency

Ozone Cal/Val/Alg Team Membership

EDR	Name	Organization	Task
Lead	Lawrence Flynn	NOAA/NESDIS/STAR	Ozone EDR Team
Sub-Lead	Irina Petropavlovskikh	NOAA/ESRL/CIRES	Ground-based Validation
Sub-Lead	Laura Ciasto	NOAA/NWS/NCEP	Product Application
Sub-Lead	Trevor Beck	NOAA/NESDIS/STAR	Trace Gas Algorithm Development
Member	Jianguo Niu	STAR/IMSG	R&D, trouble shooting, TOAST, V8TOS
Member	Eric Beach	STAR/IMSG	Validation, ICVS/Monitoring, Data Management
Member	Zhihua Zhang	STAR/IMSG	V8 Algorithms implementation & modification
Member	Robert Lindsay	STAR/IMSG	Limb Algorithms implementation
Member	Koji Miyagawa	CIRES	Ground-based validation
Member	Jeannette Wild	UMD	Applications, CDRs, validation
JAM	Laura Dunlap	JPSS/Aerospace	Coordination
Adjunct	Bigyani Das	STAR/ASSISTT	Deliveries to NDE
PAL	Vaishali Kapoor	OSDPD	Atmospheric Chemistry Product Area Lead

3.4.4.1 Ozone Nadir Profile Product Requirements

The Ozone Nadir Profile is created from measurements made by the OMPS Nadir Profiler and the OMPS Nadir Mapper sensors. This product will continue the heritage ozone profile products made by the POES SBUV/2. These products have vertical resolution between 7 and 10 km in the middle and upper stratosphere.

DPS-635: The Ozone Nadir Profile product shall provide atmospheric vertical ozone profiles, in daytime, in clear conditions, at the refresh rates of the instrument. (Note: I have requested that this be changed to all conditions and that the performance be for SZA < 80°.)
DPS-811: The Ozone Nadir Profile BUFR product shall provide geolocated atmospheric vertical ozone profiles, converted from the Ozone Nadir Profile product, in BUFR format.
DPS-637: The Ozone Nadir Profile product shall provide atmospheric vertical ozone profiles with a measurement range of 0.1 to 15 parts per million by volume (ppmv) for 0-60 km.
DPS-638: The Ozone Nadir Profile product shall provide atmospheric vertical ozone profiles with a vertical cell size of 5 km. (Note: V8Pro reports with a vertical cell size of ~3 km.)
DPS-984: The Ozone Nadir Profile product shall provide atmospheric vertical ozone profiles with a vertical retrieval resolution of 7-10 kilometer at altitudes between 30 and 1 millibar; and 10-20 km at altitudes below 30 mb and above 1 mb.
DPS-639: The Ozone Nadir Profile product shall provide atmospheric vertical ozone profiles with a measurement precision of the greater of 20% or 0.1 ppmv at altitudes below 30 millibar (mb); 10% from 30 to 1 mb; and the greater of 10% or 0.1 ppmv at altitudes above 1 mb.
DPS-640: The Ozone Nadir Profile product shall provide atmospheric vertical ozone profiles with a measurement accuracy of the greater of 10% or 0.1 ppmv below 30 mb and above 1 mb; and 10% from 30 to 1 mb.

Accuracy and precisions requirements excluded in South Atlantic Anomaly.

Product Overview/Requirements: ±10% ≤ ±5% ±5%

Attribute	Threshold	Observed/validated
Geographic coverage	60% Global Earth 7 days	SZA < 86°, orbital track
Vertical Coverage	0-60 km	0-60 km
Vertical Cell Size	3-km reporting, 7-10 km	21 layers, averaging kernel
Horizontal Cell Size	250x250 km^2	250x50 km^2
Mapping Uncertainty	25 km	5 km
Measurement Range	0.1-15 ppmv	0.1-15 ppmv
Measurement Accuracy		
h < 25 km, p < 30 hPa	10% or 0.1 ppmv	±5% versus S-NPP
25 km < h < 50 km	10%	±5% versus S-NPP
h > 50 km, p > 1 hPa	10%	±5% versus S-NPP
Measurement Precision		Measurement noise and initial and final residuals have been evaluated. The values are consistent with the expected smaller FOV performance, the SDR improvements, and the v3r3 measurement fitting.
h < 25 km, p < 30 hPa	20% or 0.1 ppmv	
25 km < h < 50 km	10%	
h > 50 km, p > 1 hPa	10% or 0.1 ppmv	

https://www.jpss.noaa.gov/assets/pdfs/technical_documents/474-01543_JPSS-GSegDPS_A.pdf

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

NOAA-20 OMPS NP & NM SDR Status

- The V8Pro algorithm uses eight channels from 253 nm to 306 nm from the OMPS NP and four channels from 313 nm to 372 nm from the OMPS NM.
- Timeline of SDR Improvements
  - See SDR Readme's for details beyond those on the next three slides.
- Three RFAs from EDR at SDR Validated Maturity Review
  - Request for links to bandpass data at the ICVS → Received.
  - Need for Solar IBSL Investigation and Correction Plan → at IDPS for B2.3 Mx3.
  - Need for CCR on OMPS NP Wavelength Scale, Solar and calibration coefficients → TTO 8/21/2020.

https://drive.google.com/drive/folders/13F5S517ntc_aouZodQgYr8djkuiHSPOc

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

Key SDR changes

- DR8615 CCR18-3829: Bad NP macropixel calculations for five Cross-track FOV measurements. Fixed 7/2/2018.
- DR8616 PCR65318: 16-scan granule problem. Fixed 9/24/2018.
- DR8617 CCR18-4137: NP/NM FOV mismatch. New sample tables to correct mismatch. Fixed 11/9/2019.
- DR8730 CCR18-4133: Counts not uniformly distributed – Nonlinearity discretization. Fixed 12/4/2018.
- DR8816 CCR19-4303: Update tables. Fixed 4/11/2019.
- DR8617: FOV mismatch between TC and NP sample tables. Fixed April 19, 2019.
- DR8709 CCR18-4138: Smear transients and negative radiances. Fixed July 25, 2019.
- DR9093 CCR19-4638: New Stray Light, Calibration Coefficients and Day 1 Solar and Wavelength Scale tables are in testing for NOAA-20 OMPS NM and NP. Fixed 11/6/2019

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

EDR Team Summary at OMPS NP SDR Validated Maturity Review (with updates)

- The OMPS SDR Team has responded to the Request for Action on the wavelength scale. They performed new analysis leading to significant changes in the wavelength scale.
- The OMPS SDR Team has implemented a correction for the solar intrusion stray light in the northern hemisphere.
- There are remaining features in the S-NPP / NOAA-20 differences in the V8Pro channel radiance/irradiance ratios:
  - Differences in the longer wavelength channels (302 nm and 306 nm from the NP and 313 nm, 318 nm and 331 nm from the NM). These are under investigation. It is not known which instruments have better values.
  - Most of the differences with latitude for the features in the mid-ranges wavelengths were due to a code error in the NOAA-20 wavelength scale calculation for V8Pro.
- The EDR team recommended that the NOAA-20 OMPS NP SDR move forward to validated maturity.

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

Key SDR CCRs and DRs

- ADR9172 CCR-20-5018: Code Change to Fix Error in OMPS NM Dark Count Correction offset passed review August 2020. TTO 3/30/2021, B2.3 Mx1.
- ADR9066 CCR 20-5026: NOAA-20 OMPS NP SDR Wavelength Scale Accuracy. Updates to Wavelengths, Solar and Radiance and Irradiance Calibration Constant Tables moved to IDPS 8/21/2020.
- ADR9309 CCR 21-5364: NOAA-20 OMPS NP In-Band Solar Stray Light. Correction developed by NASA/GSFC 8/26/2020. Delivered to IDPS 4/9/2021 for B2.3 Mx3.
- ADR9308: Inconsistencies between S-NPP and NOAA-20 OMPS SDRs. Open – In analysis. Polarization sensitivity studies are envisioned as one potential area for work.
- Shift in NPP Wavelength Scale Table 2/2021. (Jump / Overcorrection, Doppler, Biweekly Extrapolation)

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

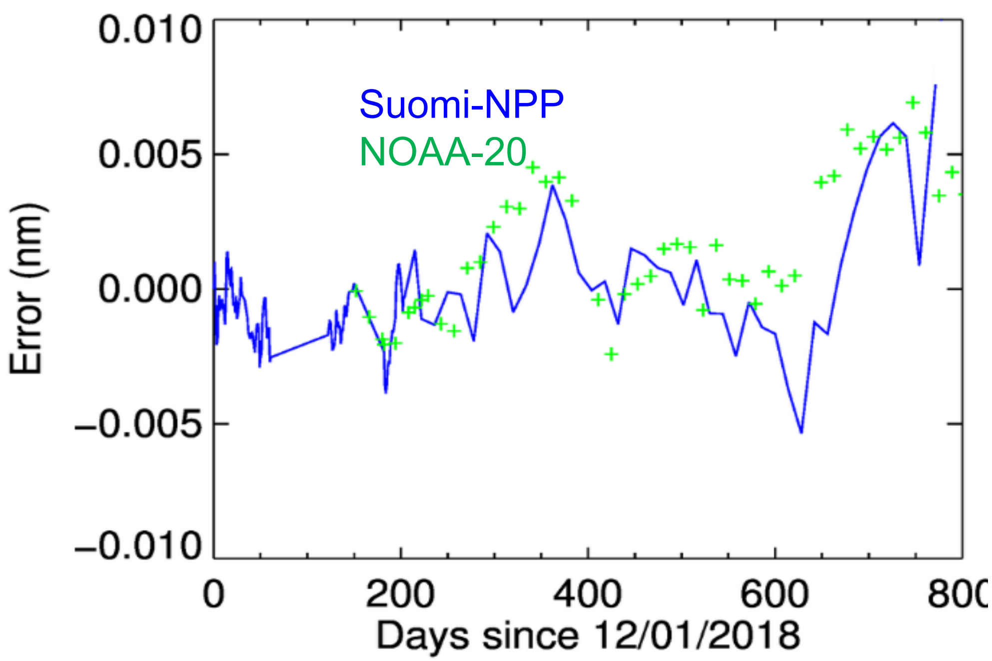
SDR Performance Translated to EDR Performance

- 3% Abs. Cal. R/I *1.5 (Soft calibration to ±1%)
  - Time dependent degradation
  - Why do we need soft calibration?
- 0.02 nm Wavelength Scale absolute knowledge uncertainty
- 0.01 nm intra-annual, intra-orbit and Doppler
  - Biweekly solar, also solar activity – Mg II Index
  - Earth view Mg II Core/Wing O3 gradient versus latitude
- 2% stray light (Check corrections with correlation of differences with smooth function of latitude)
- Noise differences for smaller FOVs
- Outlier and PMC filtering differences.
- Interpolation and bandpass model errors
- Polarization differences and modeling

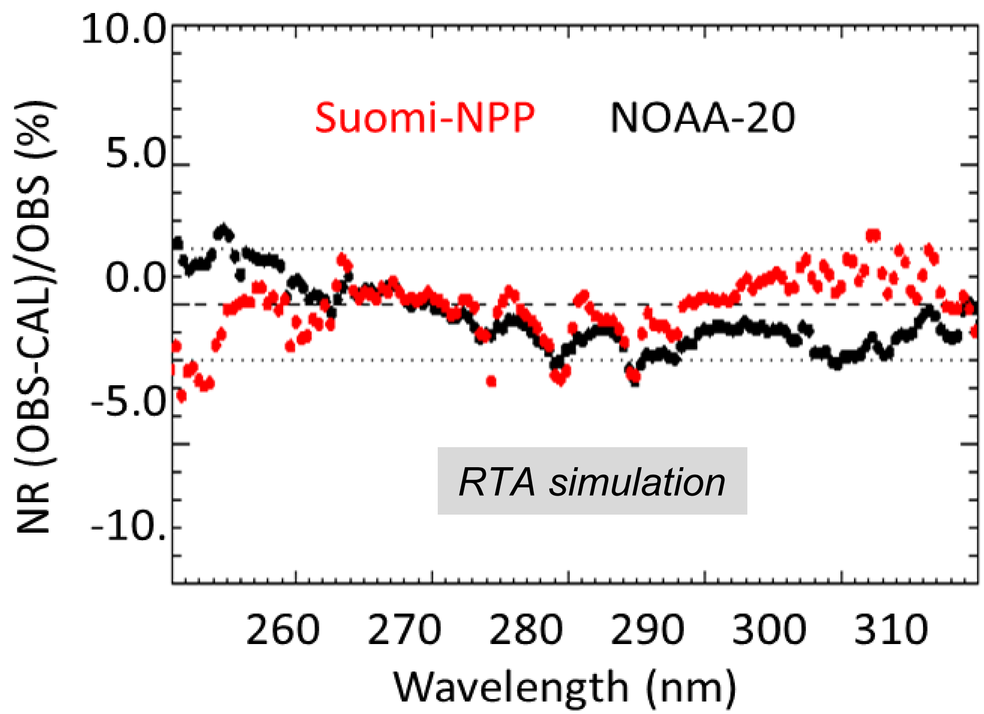
Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

Overall Calibration Error

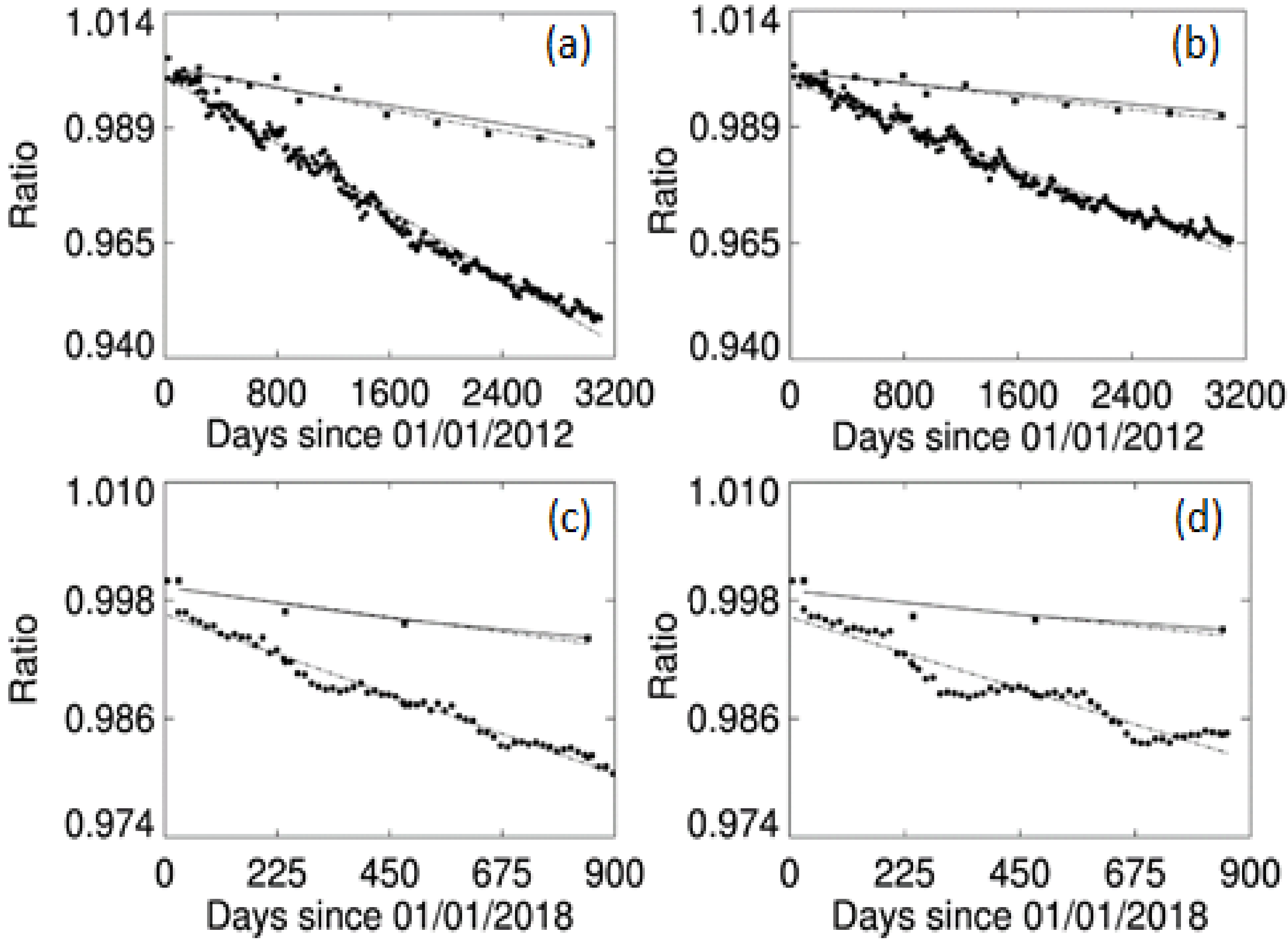
Error of Earth view wavelength calibration



Calibration error of normalized radiance

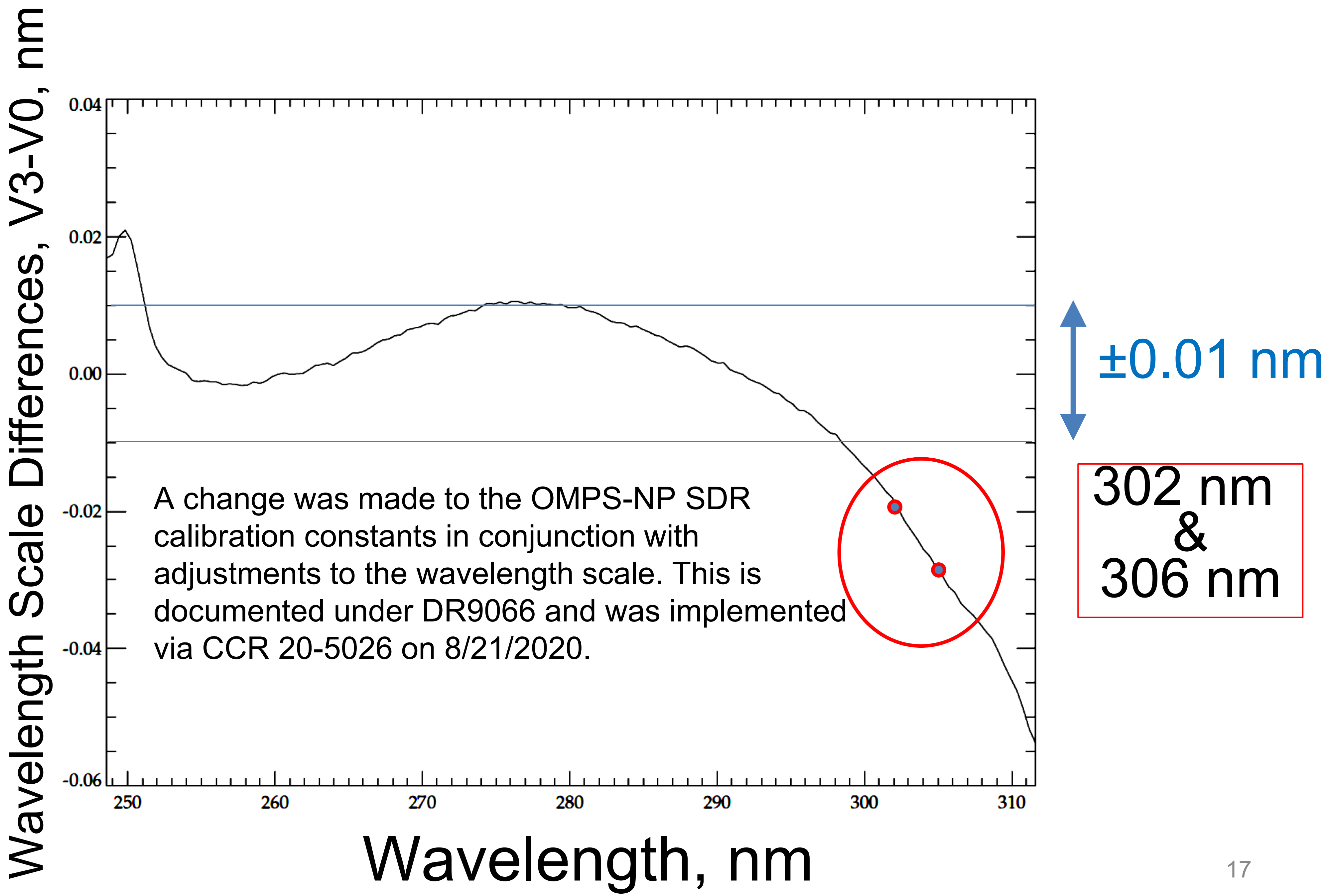


Degradation is small and well-characterized



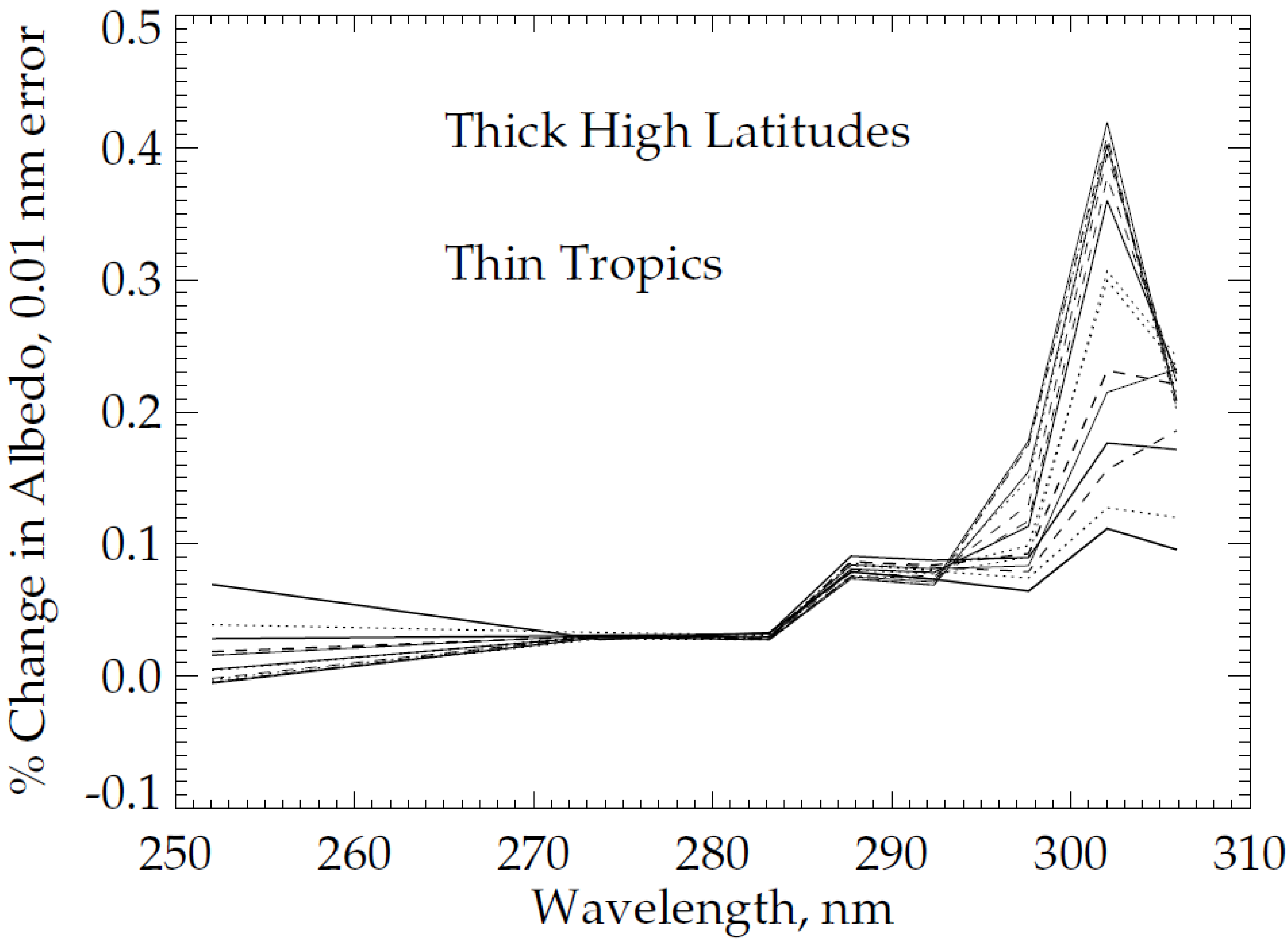
Degradation trending for 2 channels: 267.8 nm for the S-NPP NP (a) and NOAA-20 NP (c); 299.3 nm for the S-NPP NP (b) and NOAA-20 NP (d). Each subfigure illustrates the response change in the working diffuser (dot), reference diffuser (square), and sensor degradation (solid line), as well as dot-dashed line that fits the diffuser change in a time series. (From paper by C. Pan)

Response to Wavelength Scale RFA: NOAA-20 OMPS NP SDR (V3) versus Old Provisional

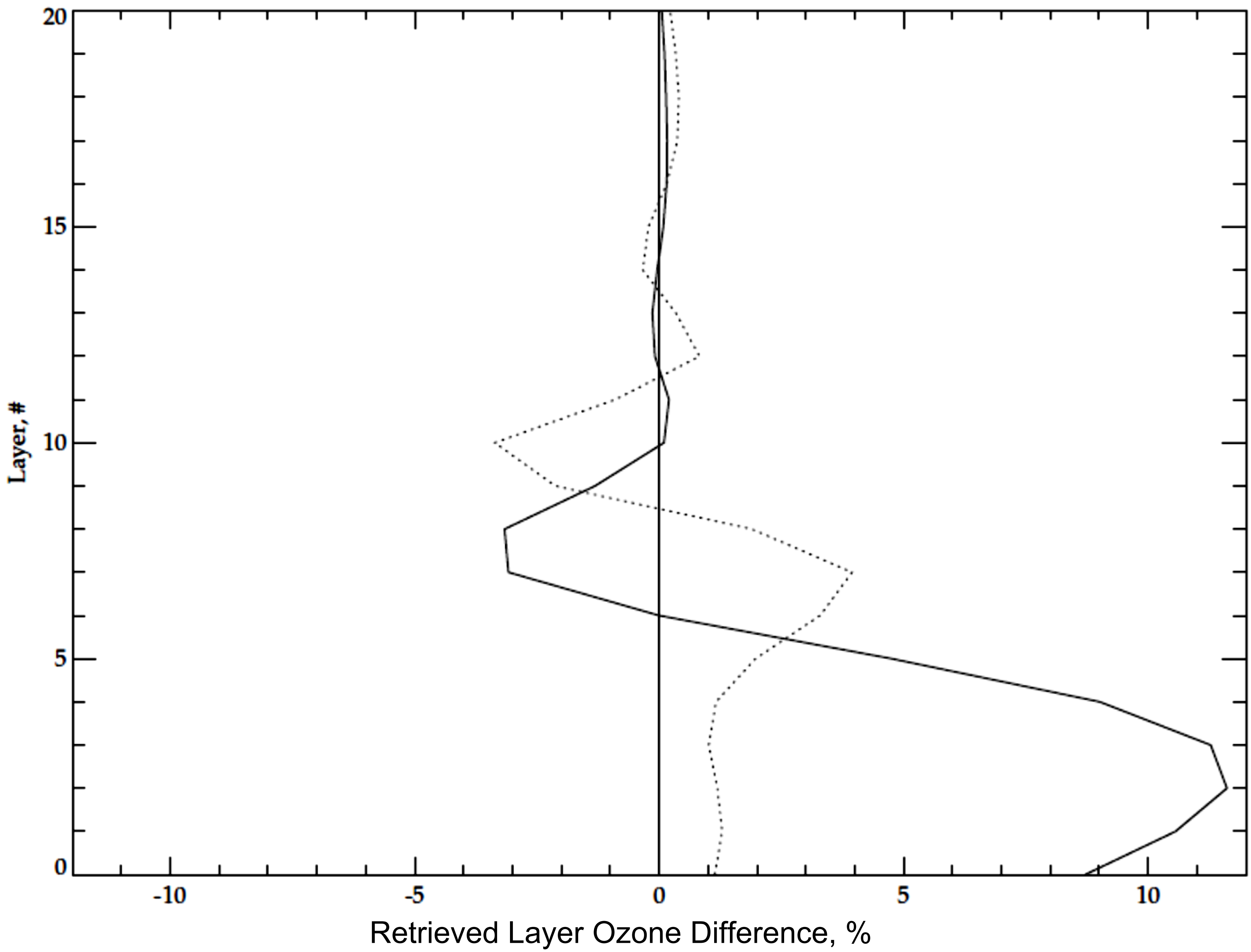


A change was made to the OMPS-NP SDR calibration constants in conjunction with adjustments to the wavelength scale. This is documented under DR9066 and was implemented via CCR 20-5026 on 8/21/2020.

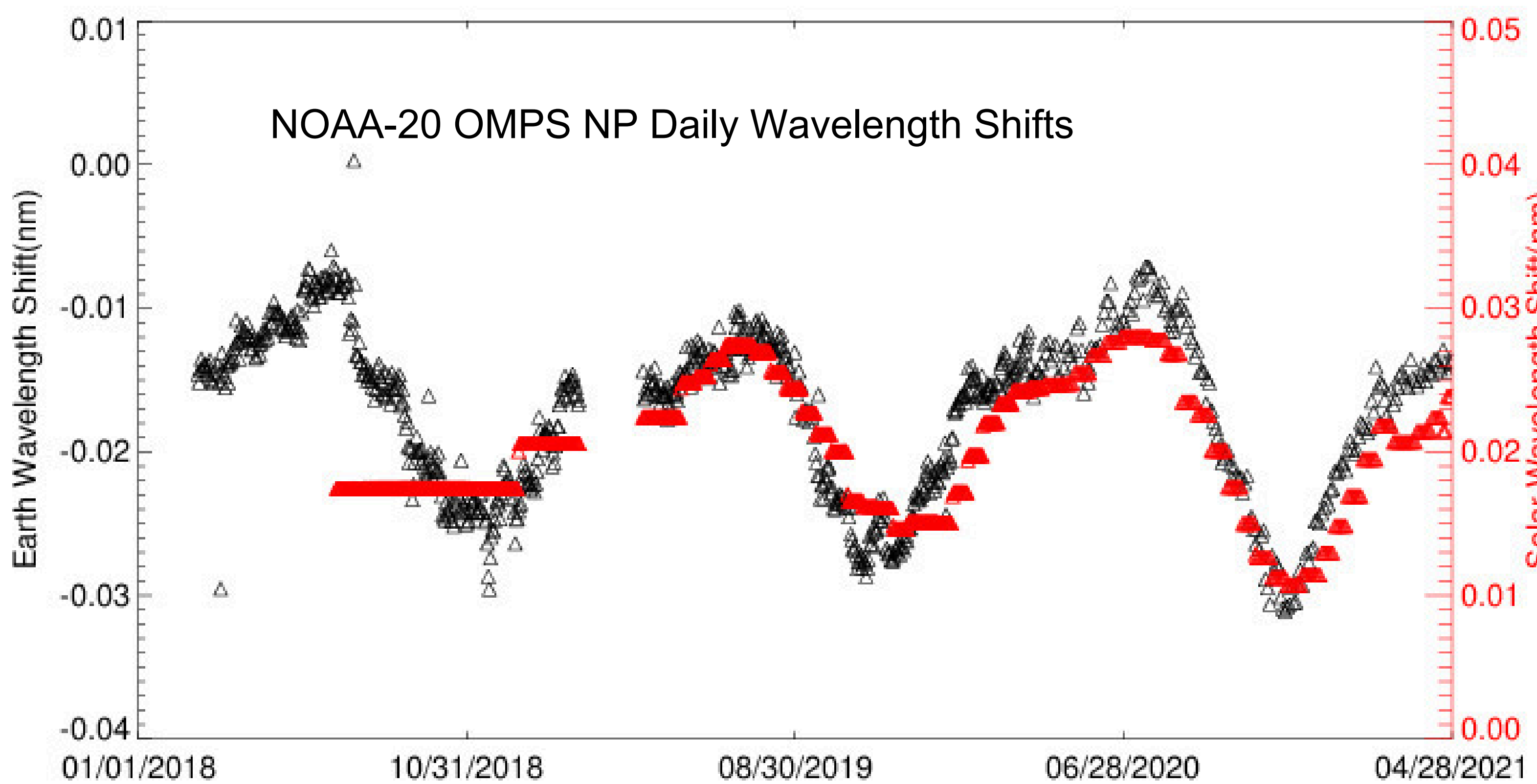
Channel Sensitivity to Wavelength Scale Errors

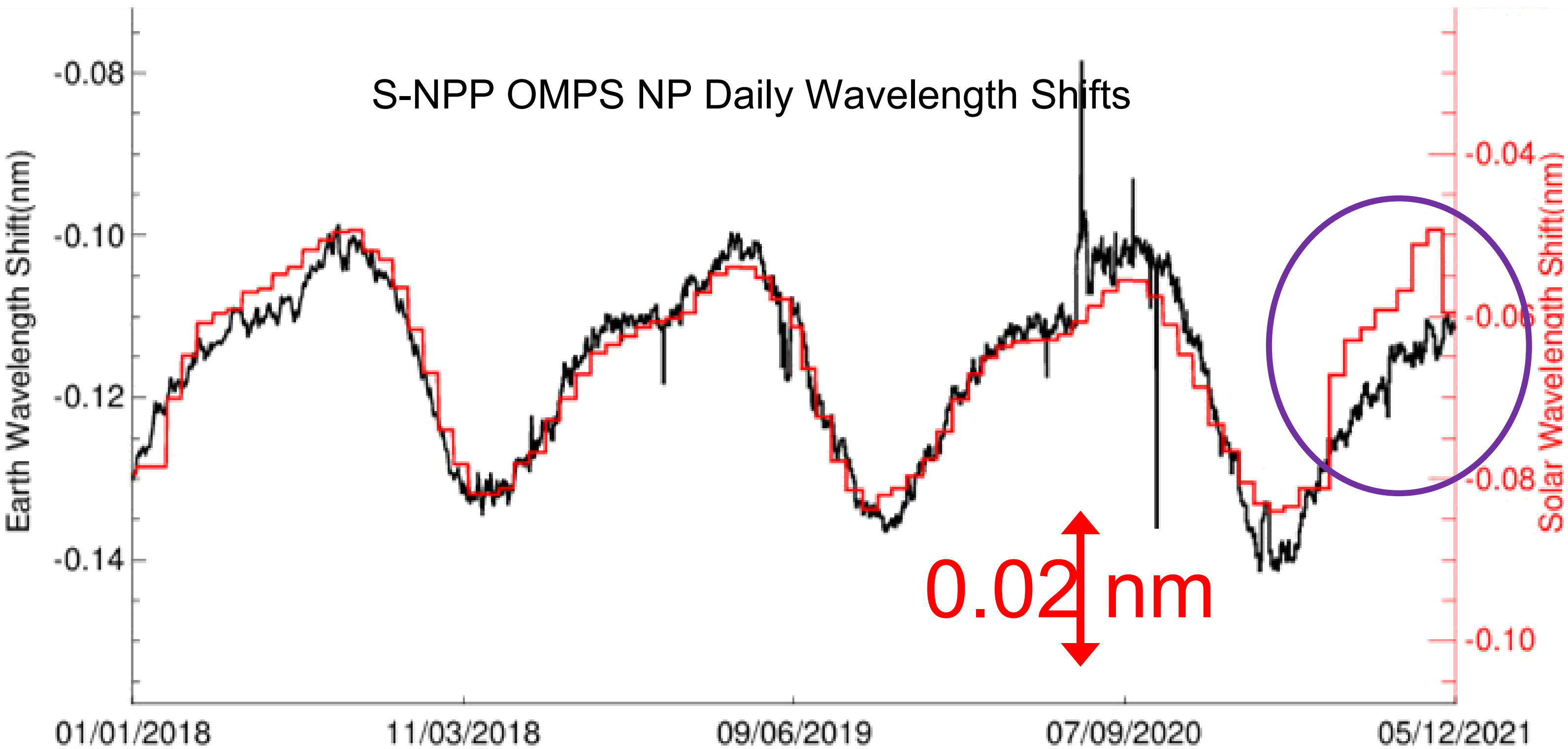


Retrieval Sensitivity to 0.04-nm shifts for 302 nm channel [50°N-Eq. solid, 50°S-Eq dotted]



The SDR Team is considering how to address the two-week lag in SDR Table updates. These lags are removed in reprocessings.





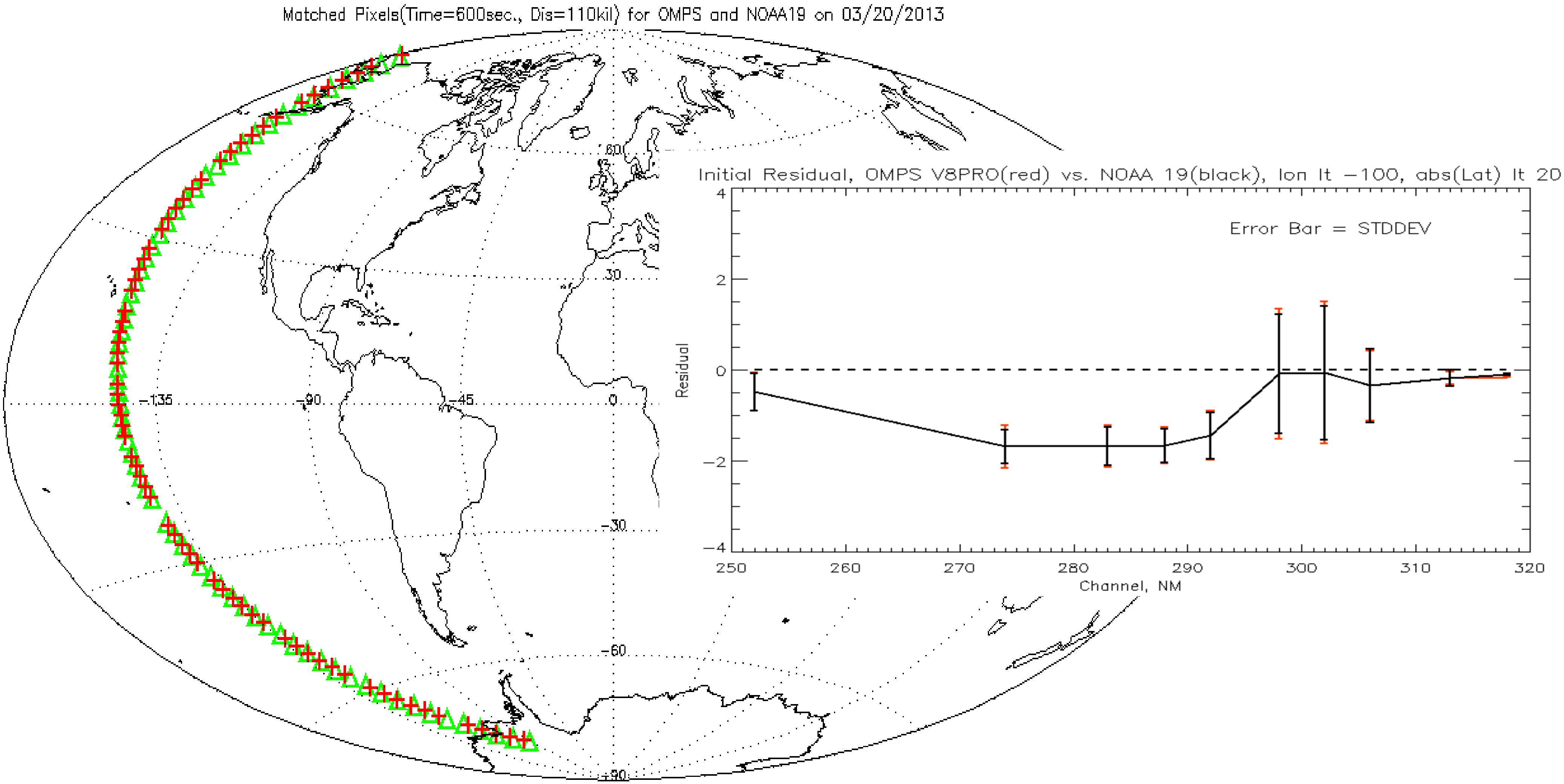
Shift in S-NPP wavelength scale in early 2021

S-NPP V8Pro Accuracy & Stability

Why do we compare NOAA-20 to S-NPP?

- Comparisons with chasing orbits (Opportunistic Formation Flying) for S-NPP with NOAA-19 SBUV/2 results for 2013.
- Soft calibration adjustments to force agreement of S-NPP with NOAA-19 SBUV/2.
- Reference diffuser measurements to track throughput degradation.
- Reprocessing of S-NPP SDR and EDR through 2020 with daily solar to account for degradation, wavelength shifts and solar activity.
- Creation of overpass data set from reprocessed data for comparison to ground-based ozone profiles.

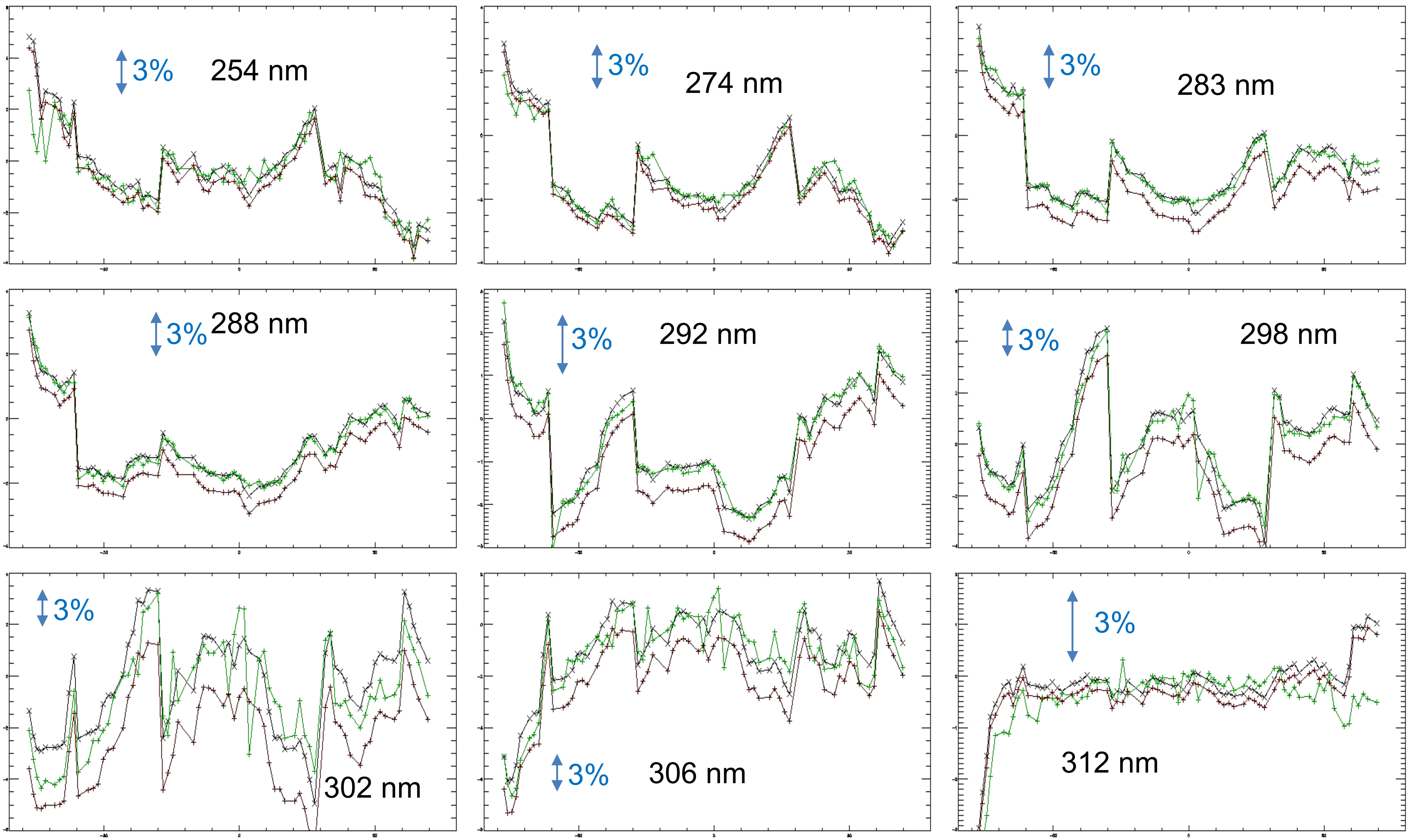
Matching orbit on 3/20/2013 for S-NPP OMPS and NOAA-19 SBUV/2



V8Pro Initial Residuals along Chasing Orbit

Red and Black S-NPP OMPS (Before and After), Green NOAA-19 SBUV/2.
Jumps at 30N/S and 60 N/S where climatologies switch latitude bins.

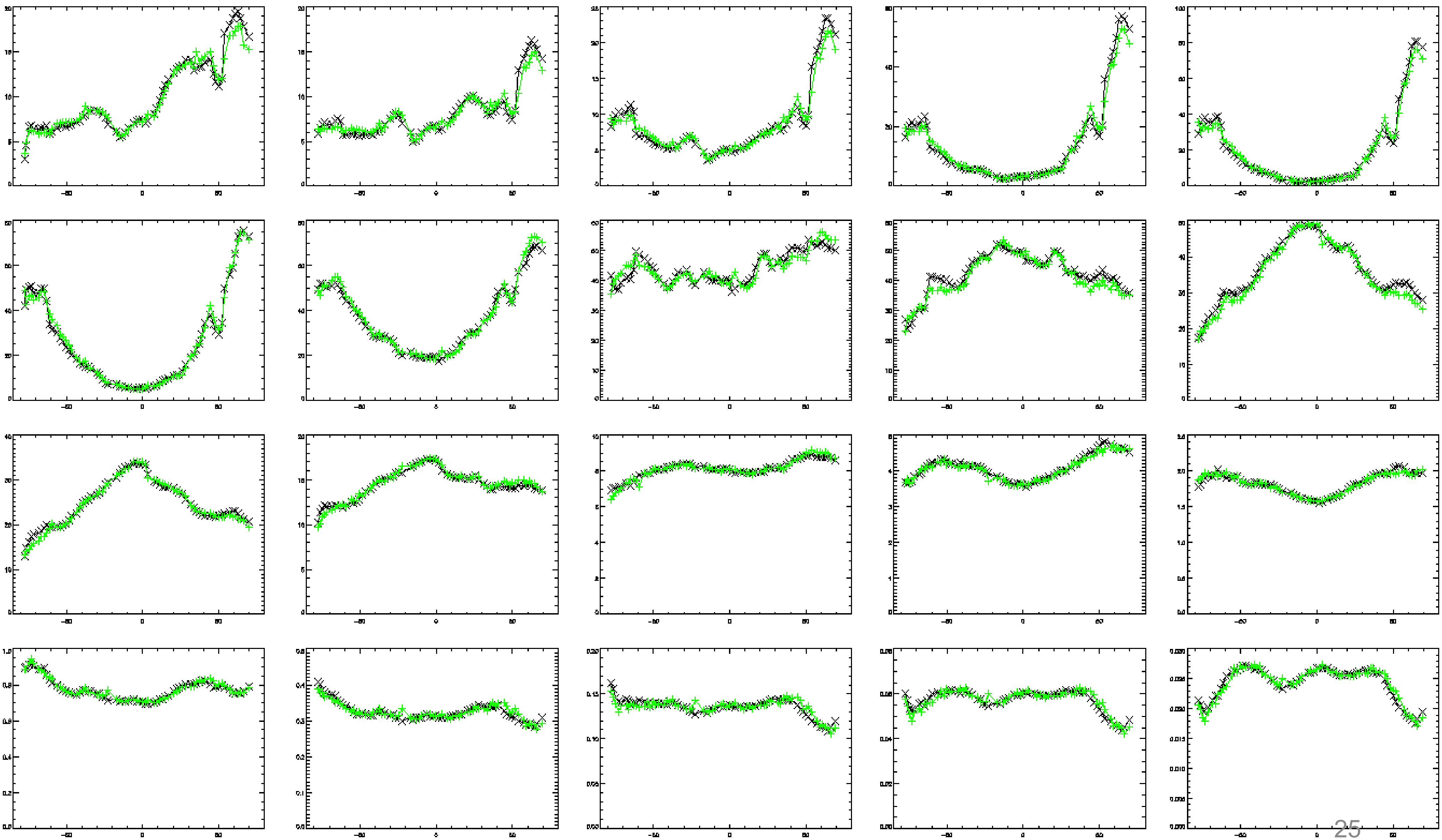
Adjustments: 254 0.4; 274 0.3; 283 0.6; 288 0.5; 292 0.5; 298 1.1; 302 2.3; 306 1.3; 312 0.3



Changes at 30N/S and 60N/S are changes in profile climatologies.

V8Pro Layer Ozone, Bottom to Top

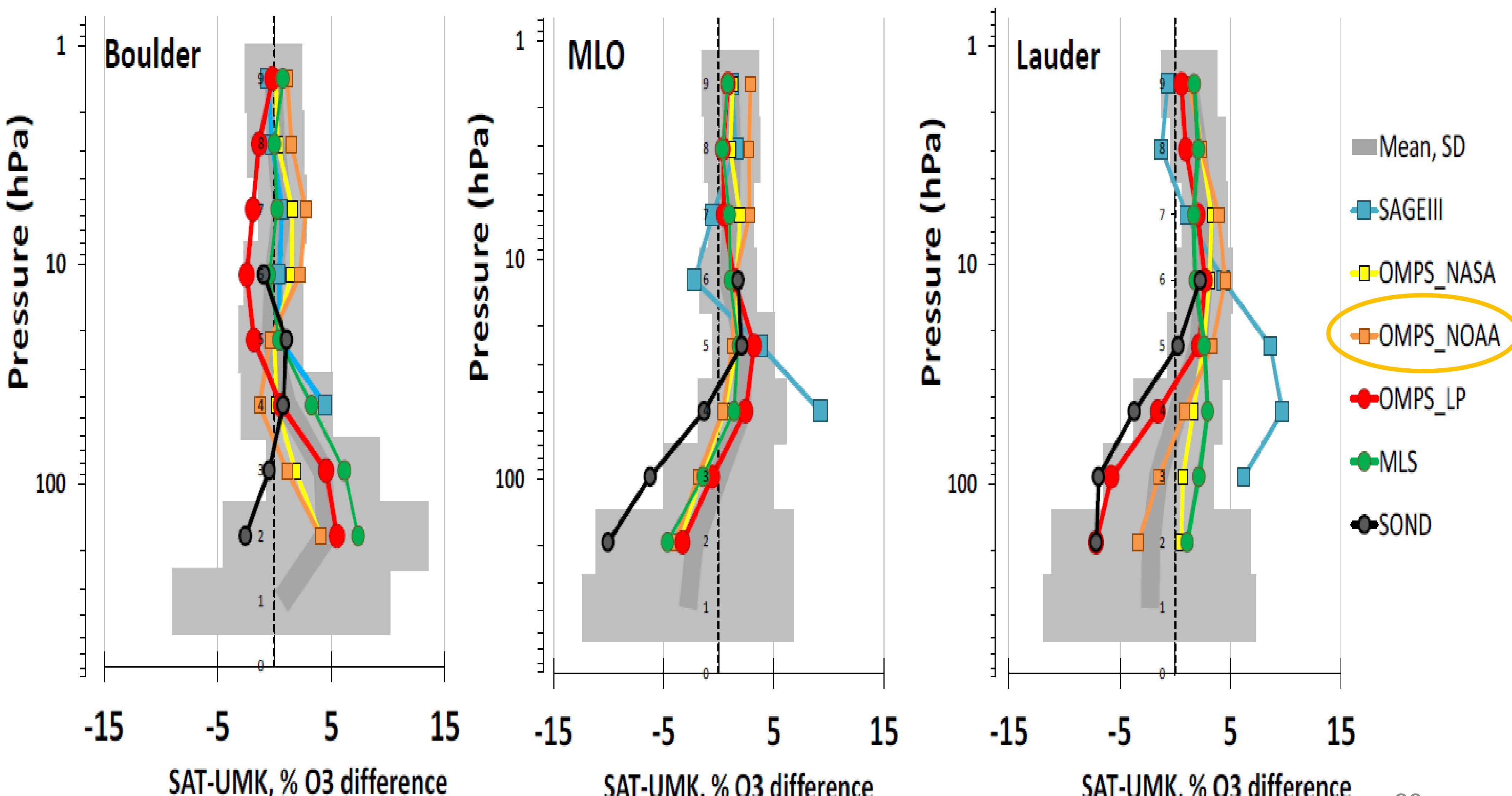
Bottom to top, Black S-NPP OMPS (After Adjustment) and Green NOAA-19 SBUV/2.



Umkehr profile algorithm optimized for stray light corrections,
by I. Petropavlovskikh et al., in preparation 5/2021,

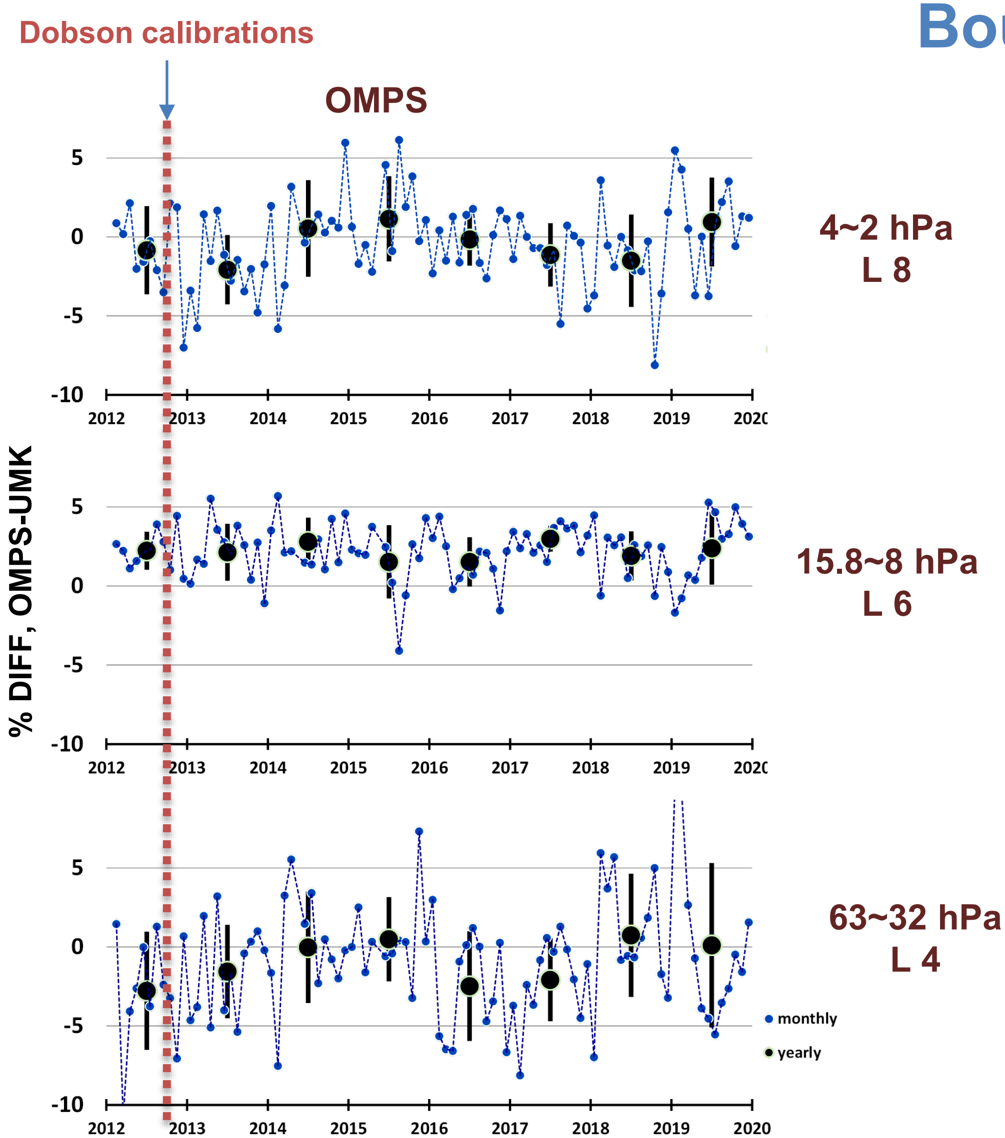
2014 -2020

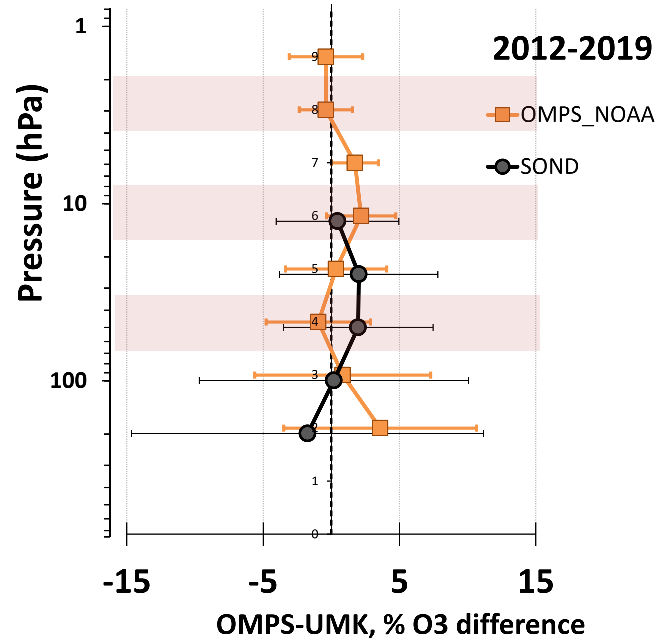
Updated for Lauder
2017 Optimization

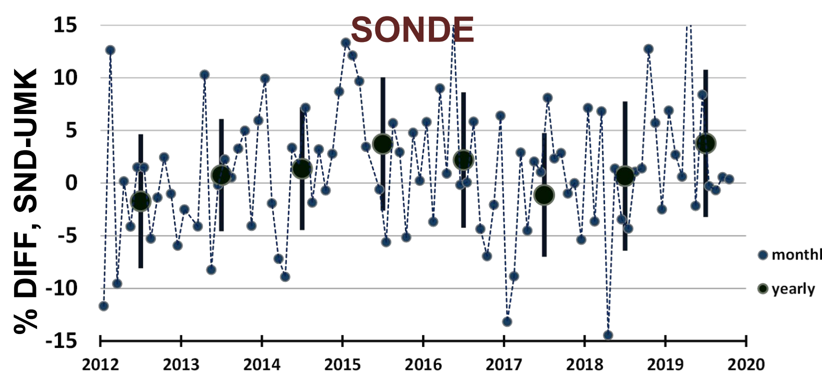


S-NPP V8Pro CDR Umkehr, Boulder CO

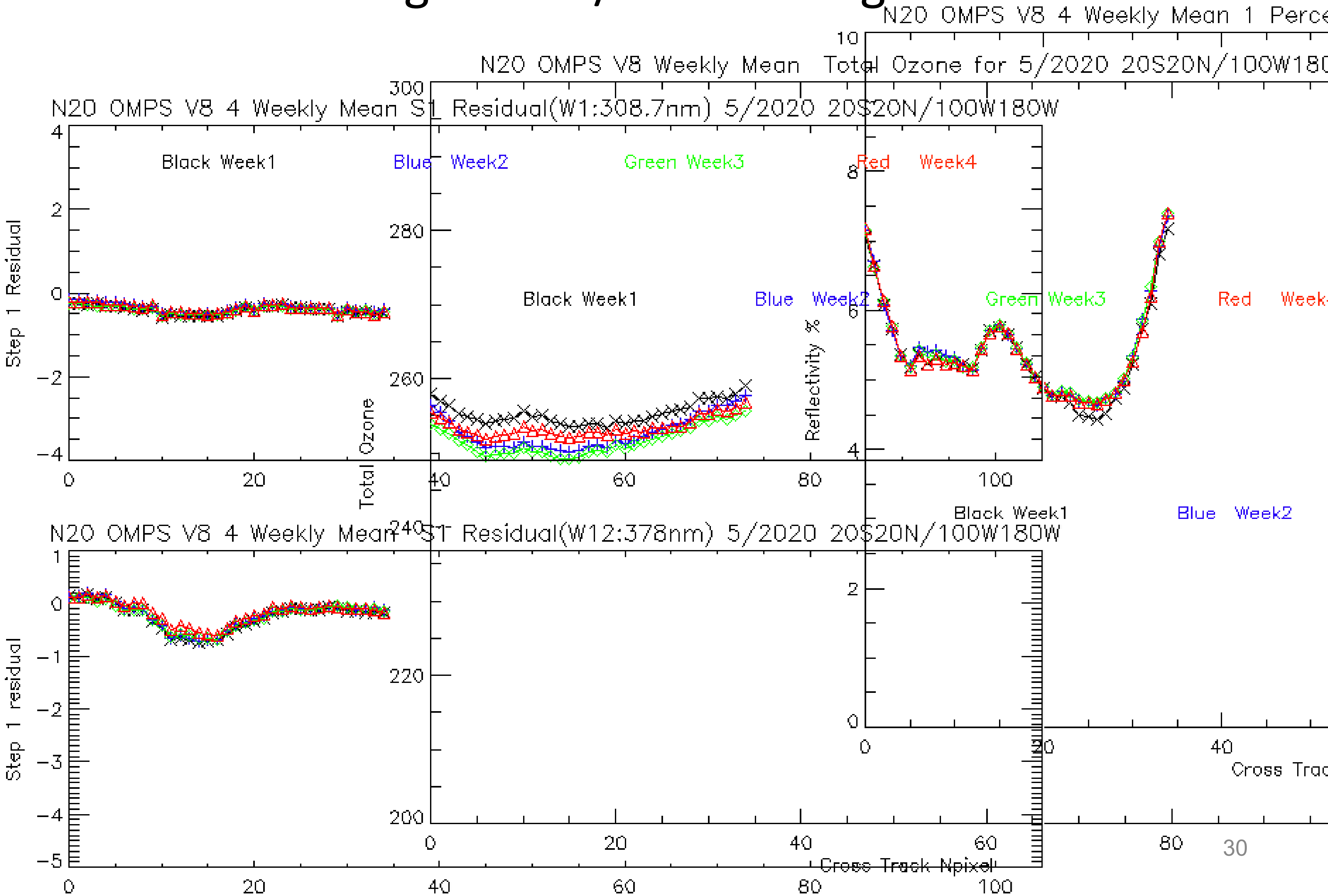
Boulder







NOAA-20 NM SDR features are stable away from algorithm / table changes



V8Pro Algorithm Refinement Stories

1. Degradation Updates – Dual tables (V3R3)
2. Filter to remove outliers and improve SNR (V3R3)

   Compare final residuals variability, Nearest-Neighbors Double-Differences, new SAA flag and ICVS monitoring
3. Improved Bandpass representation (V8Pro V4R0). On NDE development system 4/30/2021.

   Higher fidelity generation of RT tables

   Higher fidelity in internal single scattering forward model

   Correction for the code error for N20 Wavelength scales.
4. Improved Wavelength Scale from SDR (V3)

   Only N20 OMPS NP SDR has changed since provisional.
5. Model for N20 SDR Solar Stray Light correction at IDPS.
6. Interpolation errors – will be reduced with future table changes with satellite-dependent bandpass adjustments for channel locations relative to wavelength scales.

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

V8Pro Versions from NDE processing

NPP V3R0 started with the following granule:
V8PRO-EDR_v3r0_npp_s201709281322197_e201709281322571_c201709281519090.nc
NPP V3R1 started with the following granule:
V8PRO-EDR_v3r1_npp_s201805030901340_e201805030902114_c201805032036240.nc
NPP V3R2 started with the following granule:
V8PRO-EDR_v3r2_npp_s201809261418209_e201809261418583_c201809261527020.nc
NPP V3R3 started being output from NDE OPS starting with the following granule:
V8PRO-EDR_v3r3_npp_s202004161235290_e202004161236064_c202004161621040.nc
NPP V4R0 at NDE ready to move to I&T.

N20 V3R0 started with the data on Jan 17 2018.
N20 V3R1 started with the following granule:
V8PRO-EDR_v3r1_j01_s201803051819349_e201803051820124_c201803052110040.nc
N20 V3R2 started on Aug 16th, 2018.
N20 V3R3 started being output from NDE OPS starting with the following granule:
V8PRO-EDR_v3r3_j01_s202001221544286_e202001221545060_c202001221857090.nc
N20 V4R0 at NDE ready to move to I&T.

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

Summary of Main Changes for V8Pro Versions (3/3)

From V3R3 to V4R0

1. Modified scripts and codes to add option for running J02 for V8Pro algorithm, added required tables and ancillary files for J02.
2. Replaced old RT tables and triangular slit internal bandpass models with new RT tables and new higher-fidelity forward models.
3. Updated soft-calibration for aerosol channel of S-NPP retrievals and make the averaged AI at Equatorial Pacific equal to zero. Set soft-calibrations for both N20 to agree with NPP. Set J02 to be zero at start of the mission.
4. Rename some tables and ancillary files' filename to agree with npp/j01/j02 conventions
5. Corrected coding error in calculation of the NOAA-20 wavelength scale for OMPS NP channels.

From V4R0 to V4R1

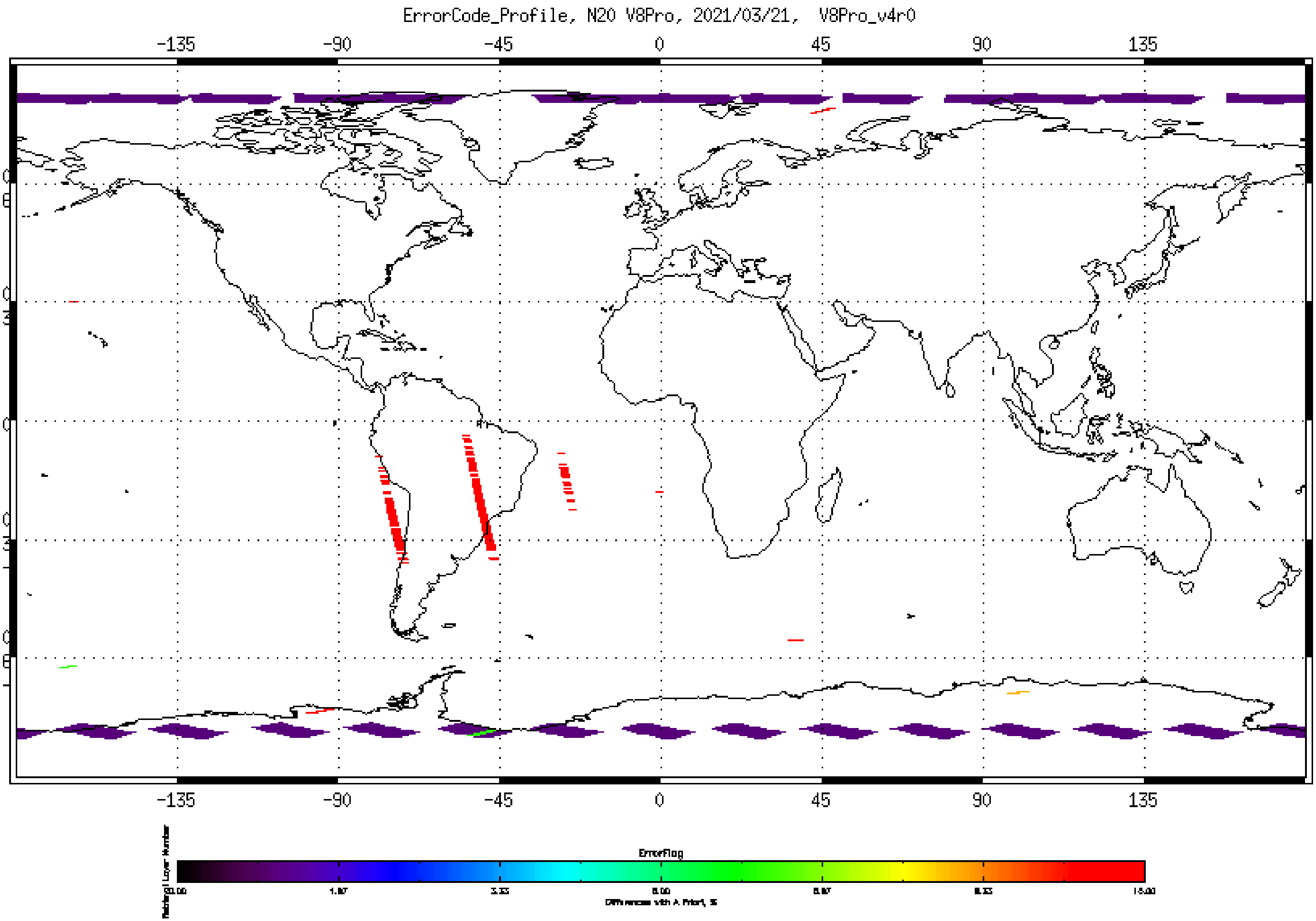
1. Revise soft calibration adjustment tables once SDR team identifies wavelength scale table situation for March 2021.
2. Revise radiative transfer and bandpass tables for channel locations to reduce interpolation errors.

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

V8Pro Profile Error Code and Descriptions

Profile Error Code	Description
0.0	Good retrieval
1.0	SZA > 84 degrees
2.0	|Step3O3 – Profile Total| > 25 DU
3.0	Average |Final Residual| for retrieval channels > threshold
4.0	|Final residue| greater than 3 times instrument error
5.0	|Retrieved - a priori| greater than 3 times a priori error
6.0	Non-convergent solution
7.0	Stray light anomaly
8.0	Initial residue >18.0 N-value units or upper level profile anomaly
9.0	Total ozone algorithm failure
+10.0	10 is added - to the flag values to designate descending portions of the orbit. The unit's value is unchanged.
+20.0 or +40.0	Thresholds on number of deviations from the polynomial fit. +20 for >30%, +40 for >60%.

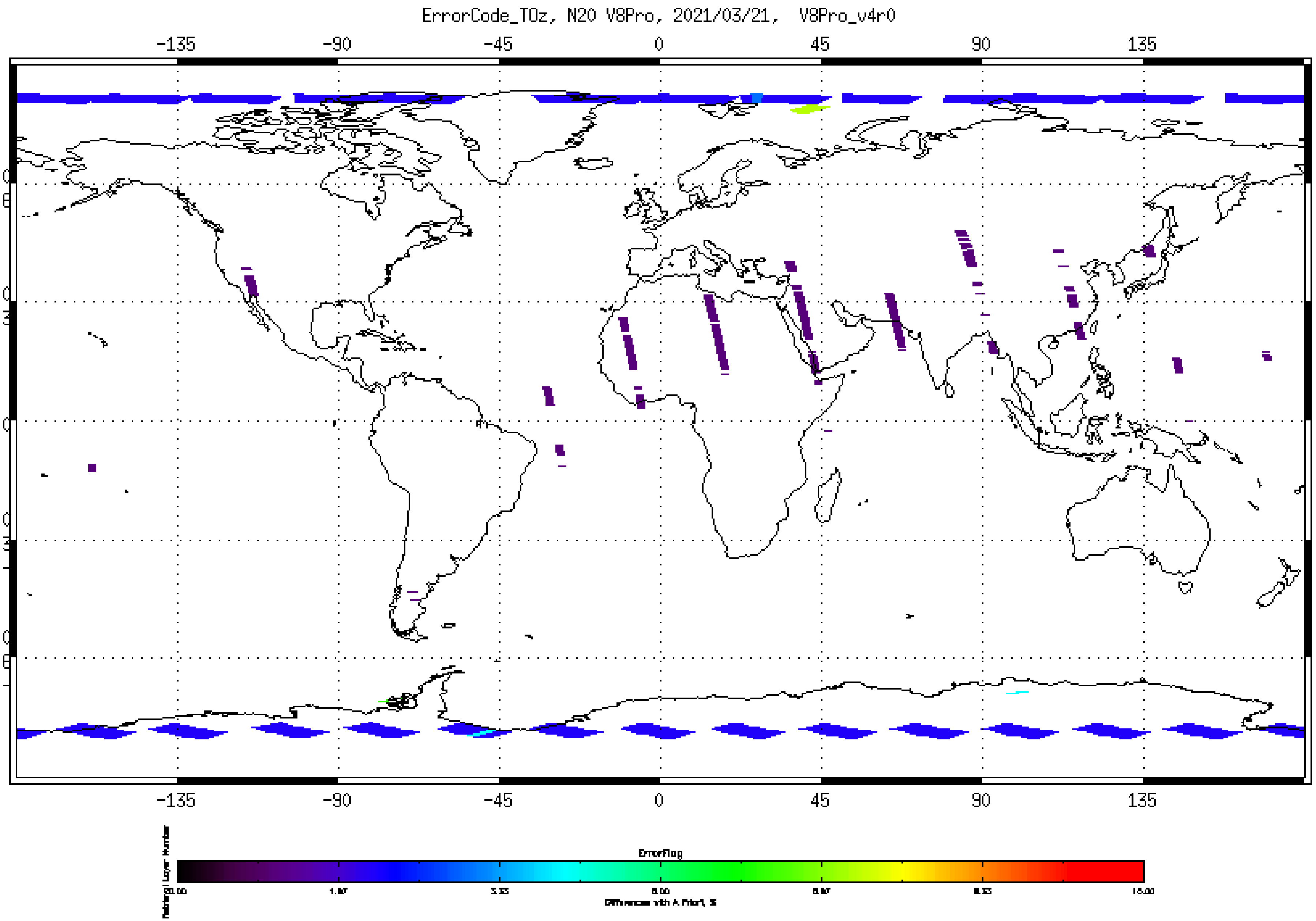
Profile Ozone Error Flags N20



V8Pro Total Ozone Error Code and Descriptions

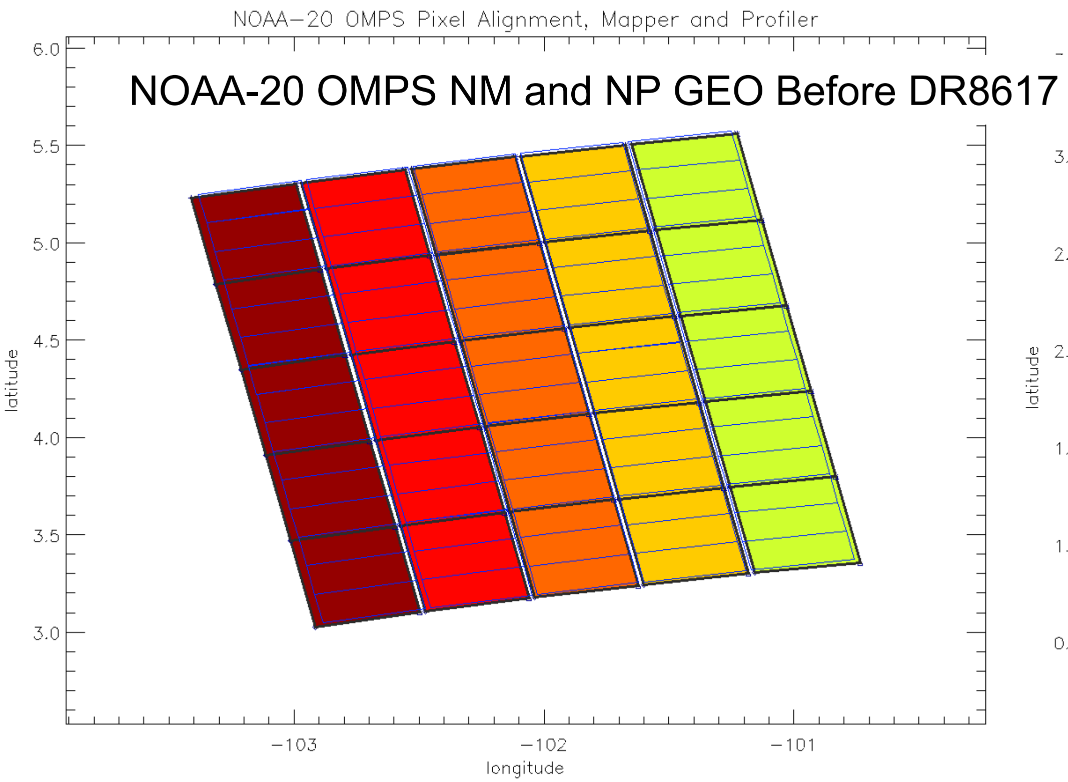
Total Ozone Error Code	Description
0.0	Good retrieval
1.0	High Aerosol Index
2.0	SZA > 84 degrees
3.0	|380 nm residue| greater than limit (Not Used)
4.0	Ozone inconsistency
5.0	SO2 Contamination
6.0	Step 1 ozone iteration did not converge
7.0	Any channel residue greater than 16 or bad radiance
8.0	Spare
9.0	Spare
+10.0	10 is added to the flag values to designate descending portions of the orbit. The unit's value is unchanged.

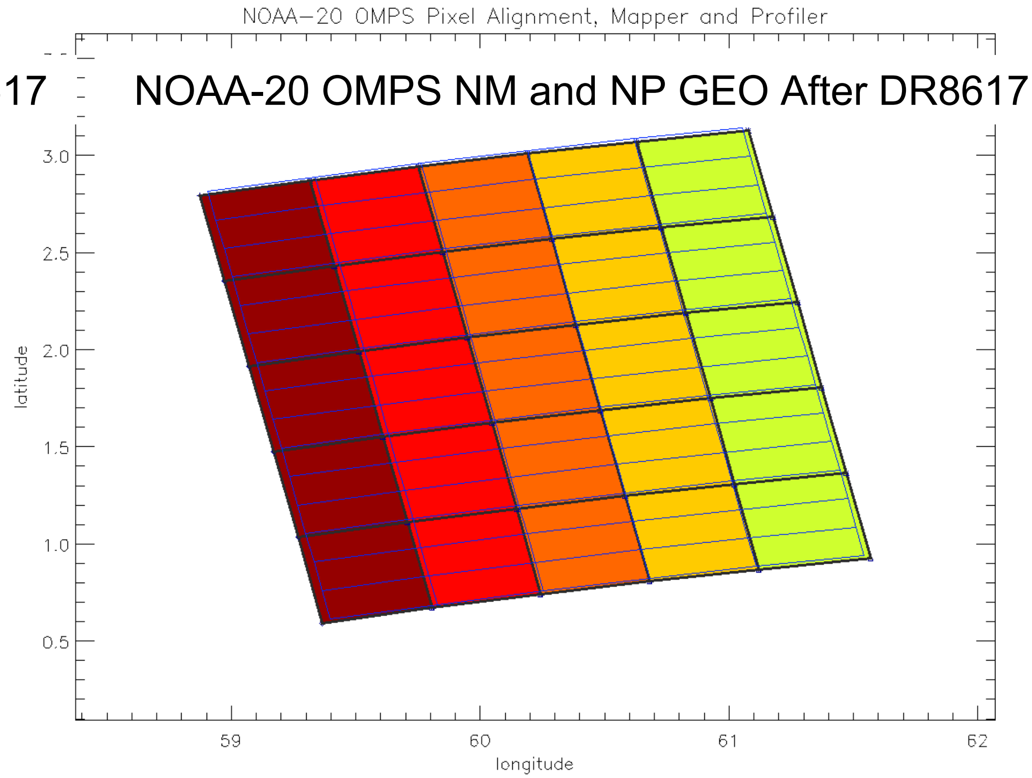
Total Ozone Error Flags N20



Matchup GEO between OMPS NM and NP

The ground pixel corner geolocation is modified. The first image below shows the ground pixels for one 37-second granule for OMPS-NP and OMPS-TC. The gaps between each FOV are about 2.4km.





V8Pro v3r3 Refinements

A. Dual Adjustment Tables
- Provides Old (Current) and New (Updated) soft calibration tables with the option to interpolate between them to smooth the transition at the request of data assimilation applications. File names will have creation dates.

B. Metadata improvements.
- Additional fields are added to metadata to be consistent with NDE requirements and to provide better information. These include the NDE production site, NDE production environment, and the adjustment table's file name.

C. Area-Weighted FOV Averages
- When the NOAA-20 OMPS NM goes to [10,10,10,10, 5, 10, 5, 10, 10, 10, 10] pixel aggregation, we will want to have area-weighted values computed in the glueware. This refinement provides the code to calculate and use the relative sizes of the FOVs.

D. Remove the use of 340 nm channel for reflectivity.
- Code updates to switch from 340 nm channel to 331 nm channel for some reflectivity calculations for consistency with the NASA V8Pro implementation.

E. Code Fixes
- Averaging Kernels: Change OMPS V8Pro product configuration for the averaging kernels to agree with the SBUV/2 relative response ones.
- Mixing ratio inconsistency in amount and pressure order.
- Terrain Pressure maximum and minimum extended to include Dead Sea and Mt. Everest.
- Descending orbit data are not processed – fixed by changing corner order in Glueware.

F. Changes to handle OMPS NM SDR sizes up to 30 scans x 140 cross-track FOVs per granule.

G. Outlier Detection Filter and Information Concentration (F&IC)
- Implements a combination of median filter and 10- to 12-wavelength polynomial fits of the radiance / irradiance ratios for the shorter ozone profile channels to reduce measurement noise, remove outliers and identify PMCs.

V8Pro v4r0 Refinements

A. Internal Single Scattering Bandpasses
   – Single Scattering forward model and Jacobians use latest SDR Team bandpasses at higher spectral resolution.

B. Multiple Scattering Bandpasses
   – Radiative Transfer Tables were computed with the same improved bandpasses used in the single scattering code.

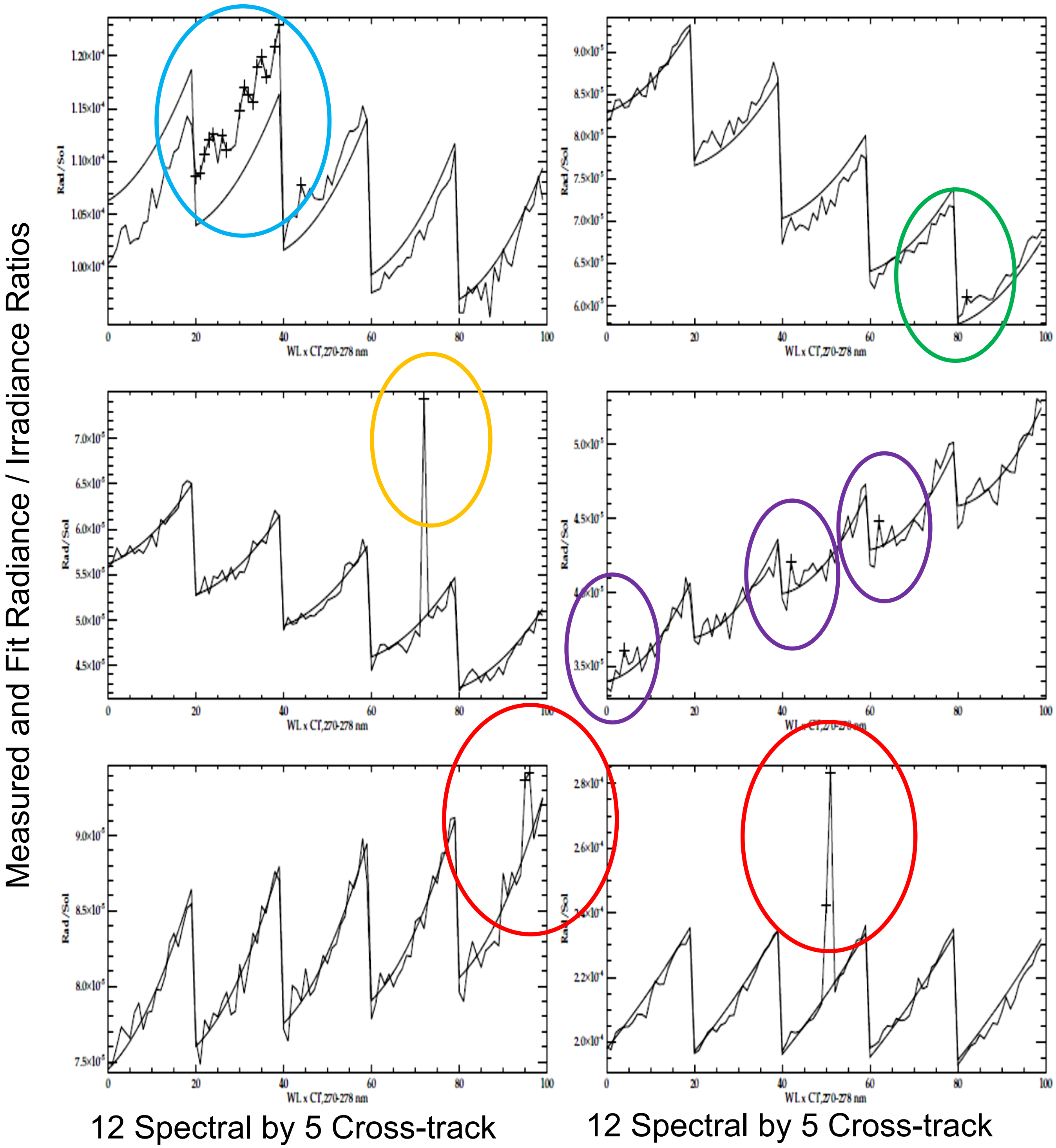
C. Code Improvements
   – Glueware is ready for higher spatial resolution (smaller FOV up to 30x241) data from J02 OMPS NM.

D. Error Code Addition
   – Deviations from v3r3 local fits are used to set flags for measurements with excessive numbers of deviations. Primarily a second check on the SAA flag. ICVS is tracking the SAA geographic distribution with time.

Precision Considerations

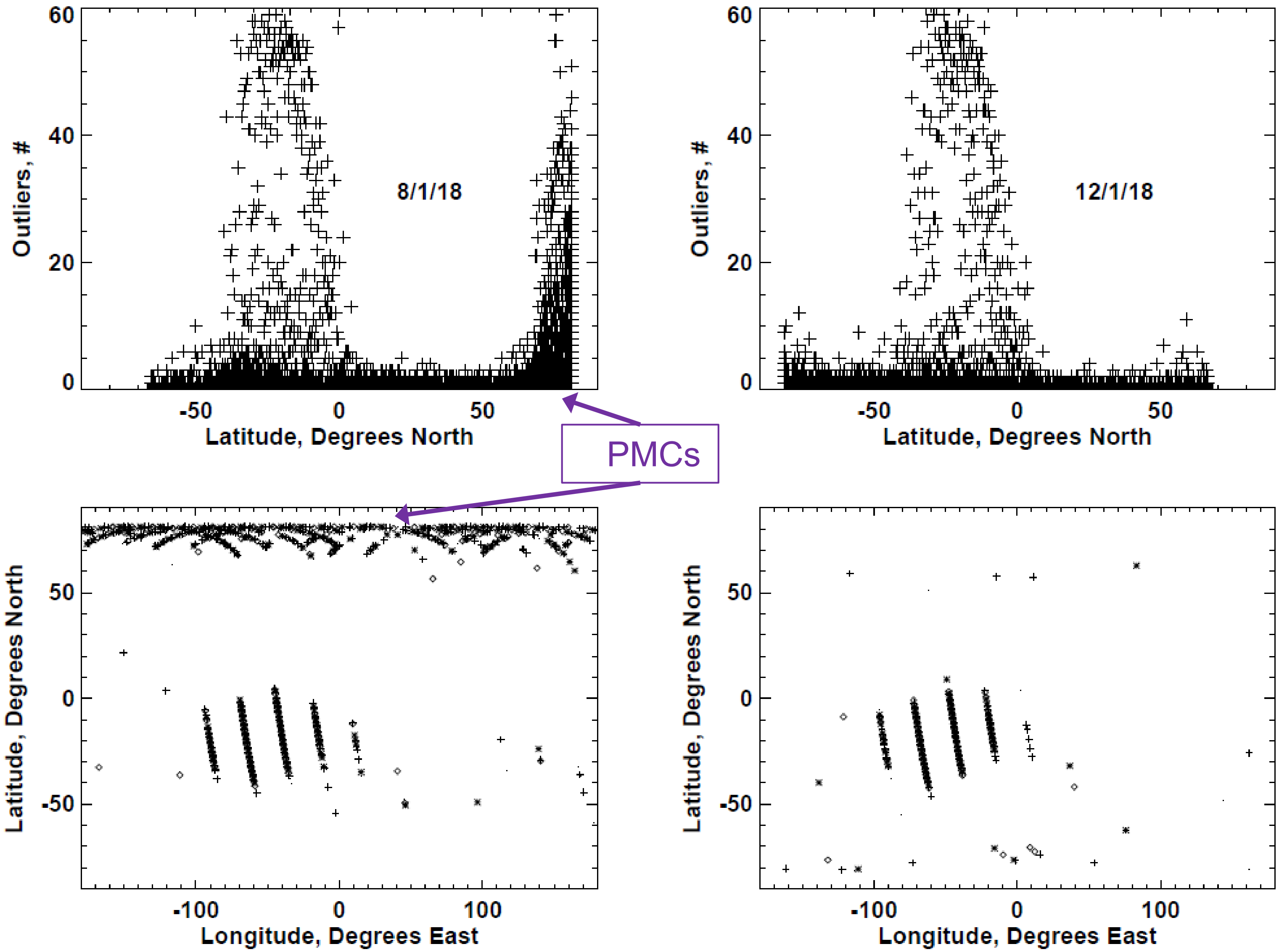
- NOAA-20 OMPS NP SNRs are consistent with the smaller FOV (5 times cross-track, 5 times along-track).
- V8Pro for NOAA-20 combines five cross track into single cross-track but keeps along-track resolution.
- V8Pro V3R3 includes fits of radiance / irradiance ratios in wavelength for outlier detection and information concentration.
- This process reduces noise and identifies measurements corrupted by noise in the SAA or from scattering due to the presence of Polar Mesospheric Clouds (PMCs).

Outlier Detection & Filtering for NOAA-20 OMPS NP



Filter with a 4% threshold. A "+" indicates a bad value. Orange - a single spike. Red - two spikes. Purple - three spikes for the same spectral row. These all occurred in the SAA. Blue - high latitude, summer hemisphere, Polar Mesospheric Clouds (PMCs) are present in at least one FOVs. Green - marginal case due to PMCs, or noise, or a charged particle hit in the auroral oval.

NOAA-20 2-D Filter Comparison for 274 nm

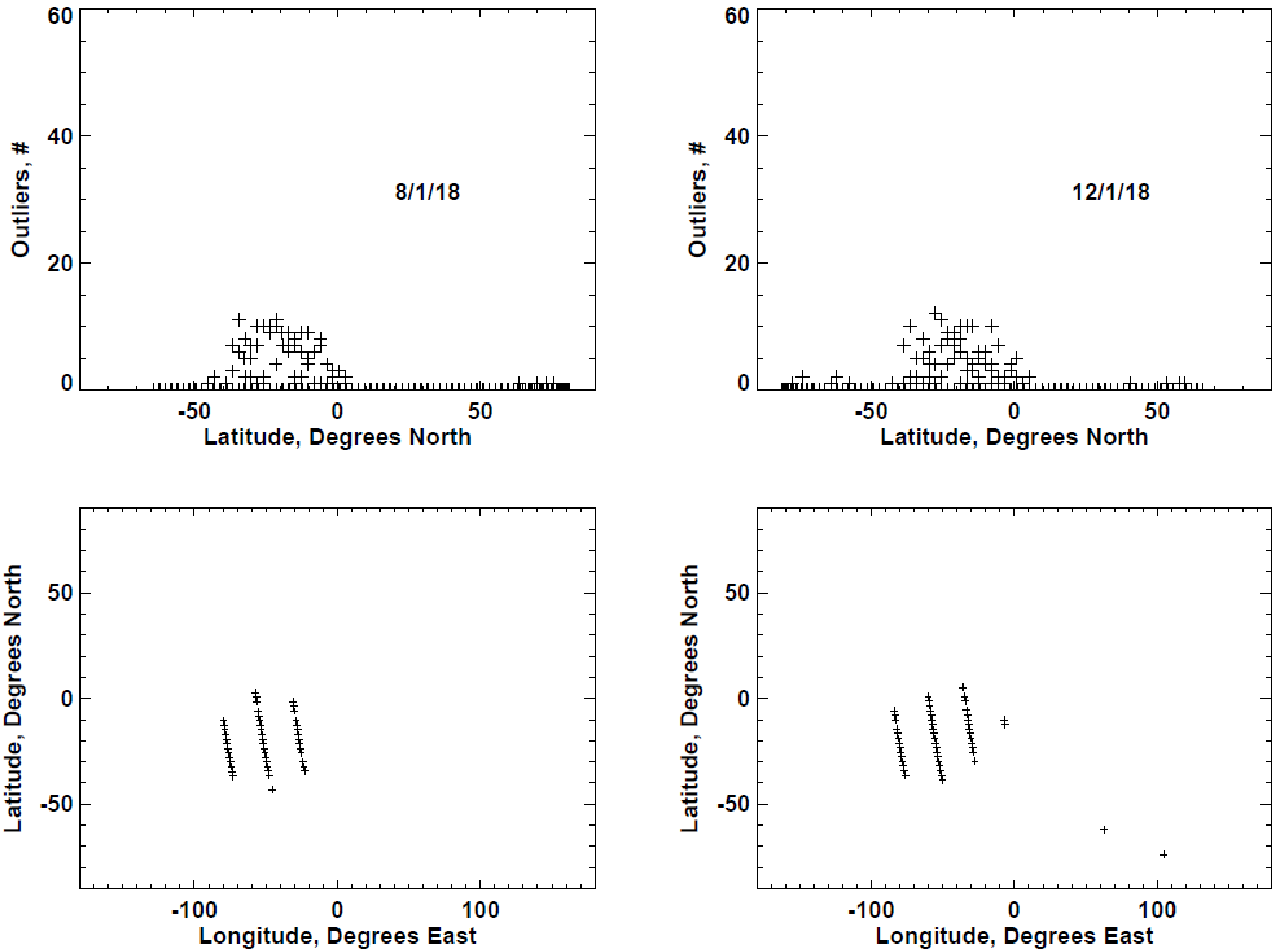


Number and location (for scans with five or more replaced values) of outliers for two days of NOAA-20 OMPS NP SDR data. Twelve wavelength intervals around 273 nm were used and each five cross-track FOV scan was fit with a linear regression using a quadratic model in wavelength and a linear model in cross-track FOV number.

The filter process used an initial difference from a median test of the albedos followed by an iterative removal of terms using the absolute radiance differences from the fit.

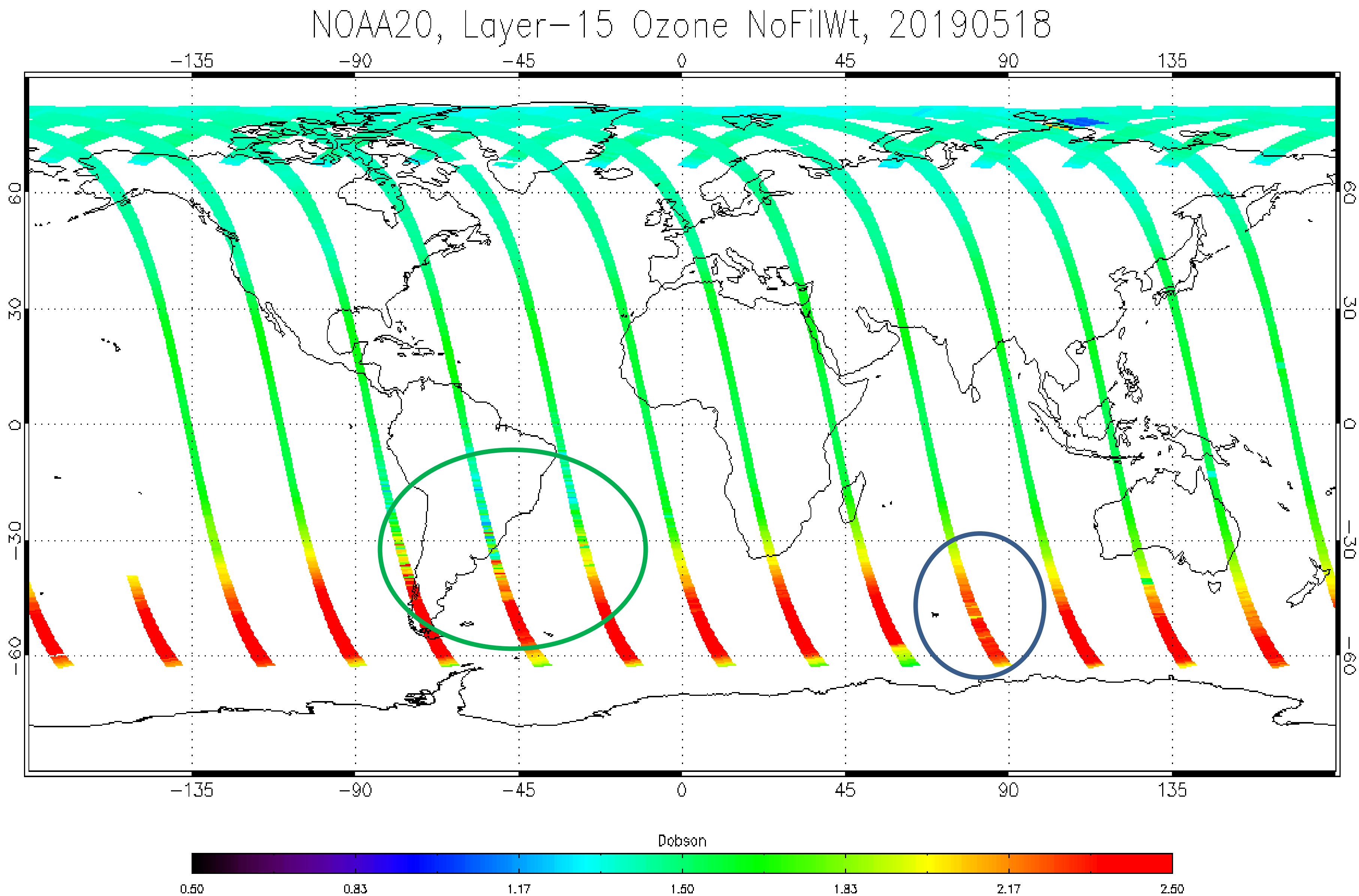
The IDL code to calculate the fits is in the note pages.

S-NPP 2-D Filter Comparison for 274 nm

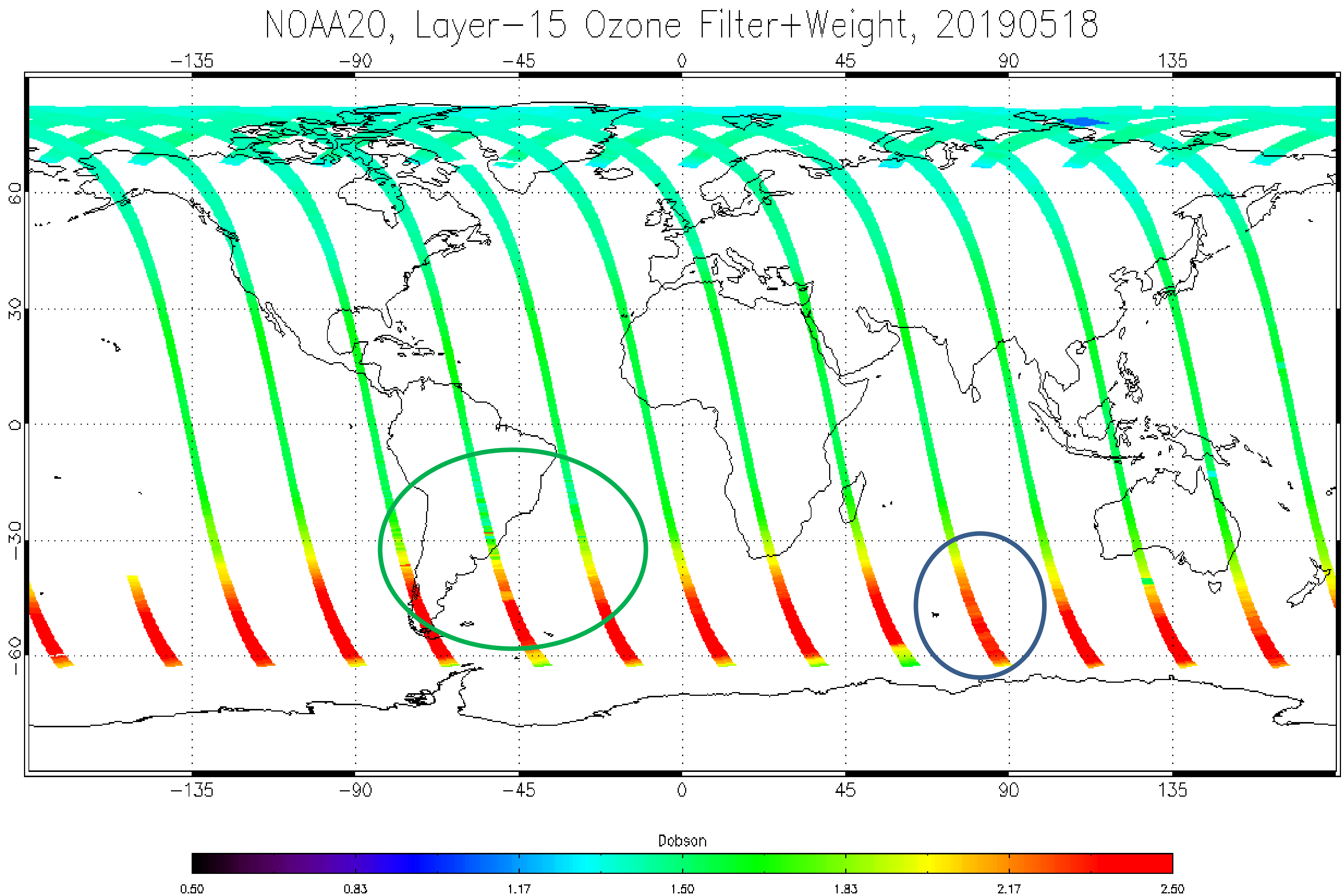


Number and location (for scans with more two or more replaced outliers) of outliers for two days of S-NPP OMPS NP SDR data. Twelve wavelength intervals around 273 nm were used. The radiance/irradiance ratios for each spectral interval were fit with linear regression using a quadratic model in wavelength.

The filter process used an initial difference from a median test of the albedos followed by and iterative removal of data values using the absolute radiance difference from the fit.



NOAA-20 OMPS V8Pro results for May 18, 2018 without measurements outlier detection and filtering.

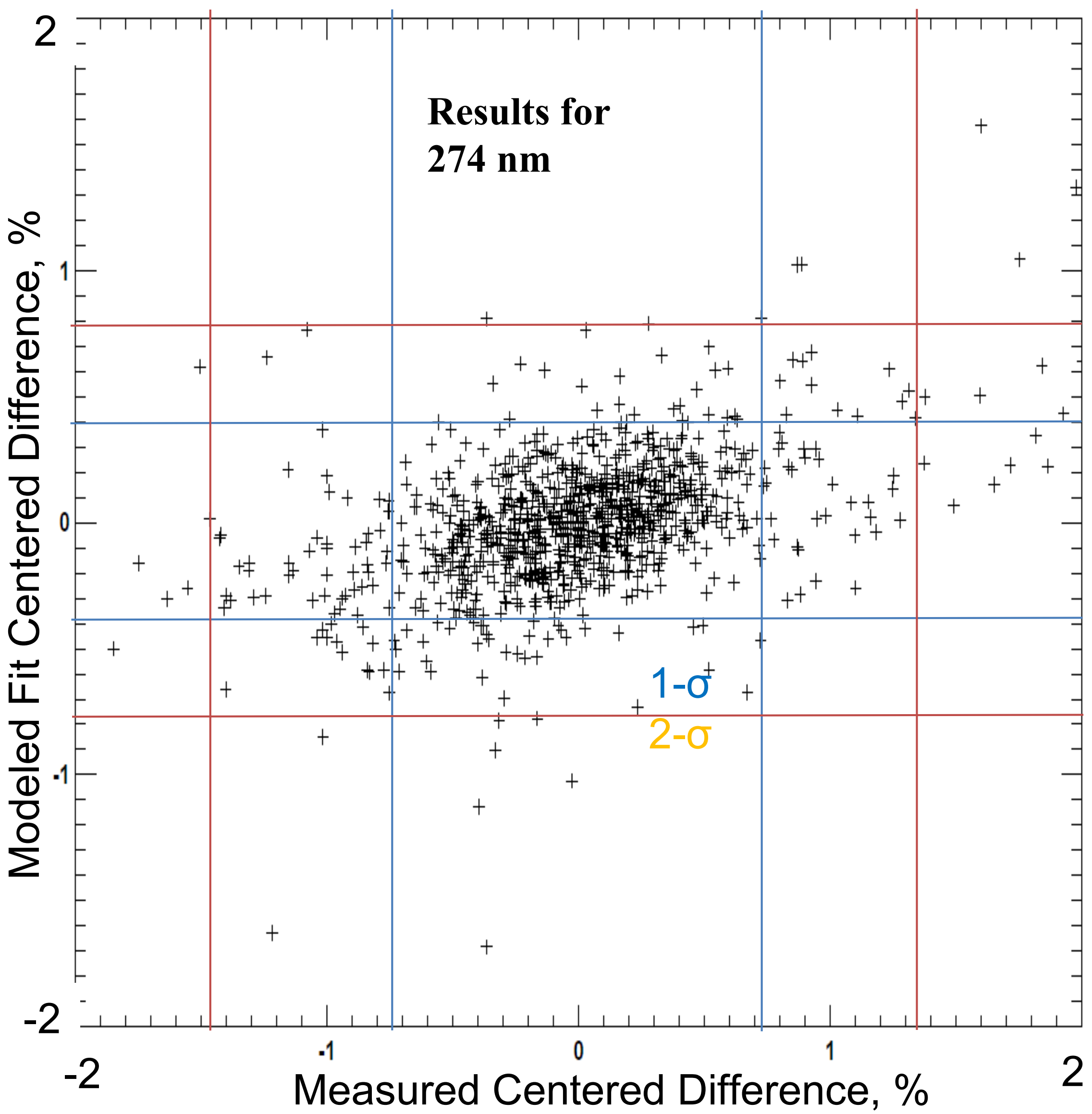


NOAA-20 OMPS V8Pro results for May 18, 2018 with measurements outlier detection and filtering.

```
Final Residual Variations by Channel for 3/31/2019
versus 3/31/2020 NOAA-20 OMPS NP (and 3/30) (0-30N)
```

	253	274	283	288	292	298
N20-V3R2	0.588	0.042	0.110	0.049	0.110	0.110
N20-V3R3	0.190	0.013	0.032	0.046	0.074	0.051
NPP-V3R3	0.314	0.011	0.032	0.029	0.032	0.037
N20-V3R2	0.539	0.036	0.103	0.056	0.116	0.109
N20-V3R3	0.222	0.015	0.035	0.048	0.071	0.050
NPP-V3R3	0.313	0.013	0.028	0.023	0.032	0.037

Nearest Neighbor Centered Differences Noise Reduction Estimates



The along-track values at the V8Pro wavelengths for the middle (3rd) scan of five in a granule were compared to the averages of the 2nd and 4th ones. The plot to the left compares the percent differences for the measured results to the those for the model fits for the 274 nm channel.

RMS Differences

nm	ModFit	Measured
253	1.04%	1.73%
274	0.39%	0.73%
283	0.32%	0.47%
288	0.26%	0.46%
292	0.14%	0.27%

The model results show reduced noise for this statistic.

Steps to Reconcile S-NPP & NOAA-20 OMPS SDRs

- NOAA-20 OMPS had ground to orbit wavelength shifts
  - The SDR team created new tables for NOAA-20 – wavelength scale and radiance and irradiance calibration for OMPS NP SDRs called Version 3. This version is in use at IDPS starting on August 21, 2020.
- NOAA-20 and S-NPP have significant differences in their bandpasses
  - The EDR team created new tables and revised the internal computations to better represent each instruments measured bandpasses in the forward models.
- NOAA-20 and S-NPP have significant differences in their N-values and these vary with latitude
  - The EDR team experimented with soft calibration adjustments to force agreement in the tropics.
  - The EDR team identified a solar stray light intrusion affecting the shorter channels in the Northern Hemisphere for NOAA-20. NASA OMPS Team (L.-K. Huang SSAI) has developed a correction.
  - The major portion (~70%) of the differences has been removed with the EDR wavelength scale code correction. Soft calibration adjustments are now successful.
  - Improve bandpass representation for interpolated channels are planned.

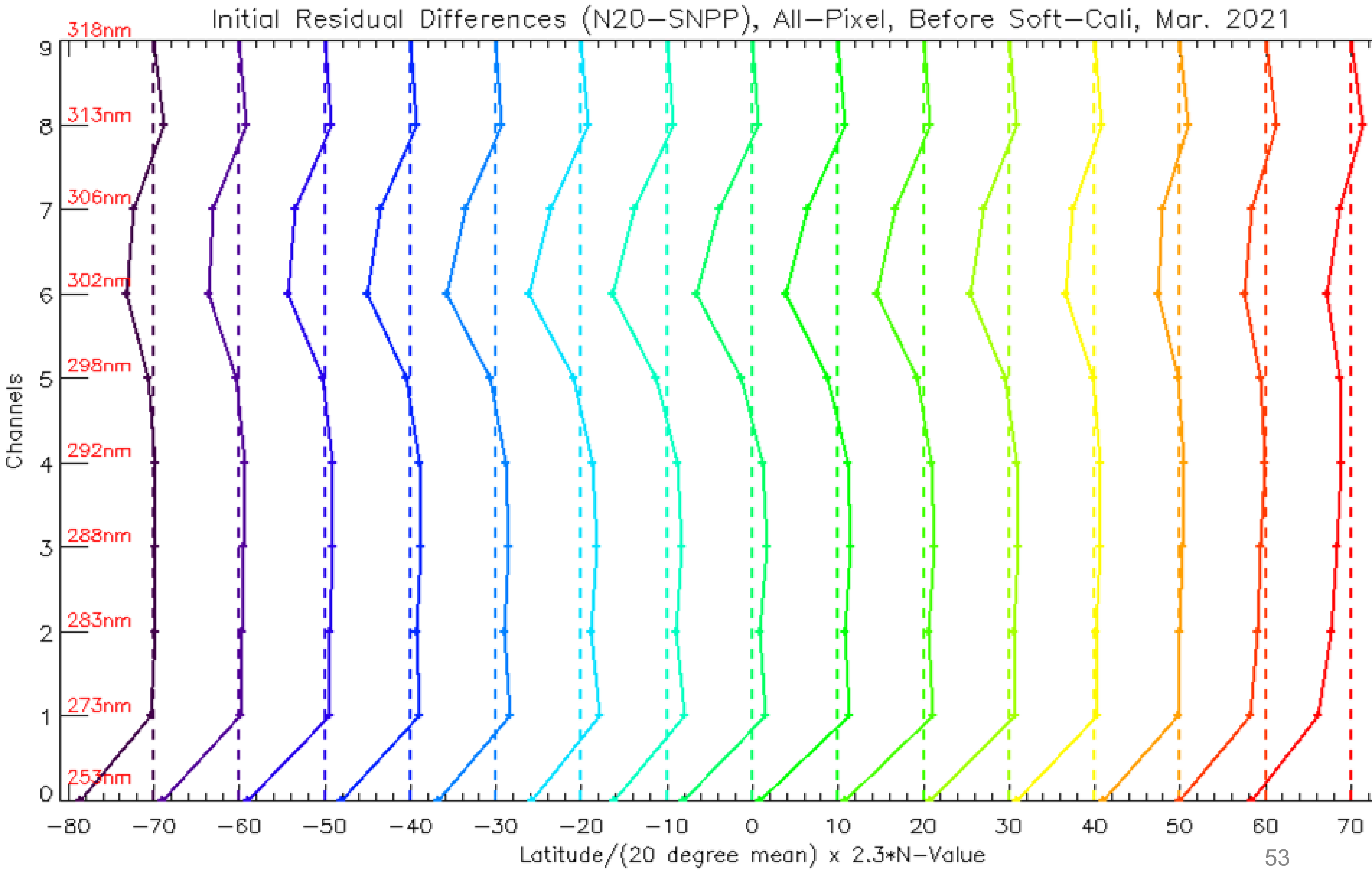
Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

Retrieval Differences reduced after Soft Calibration Adjustment

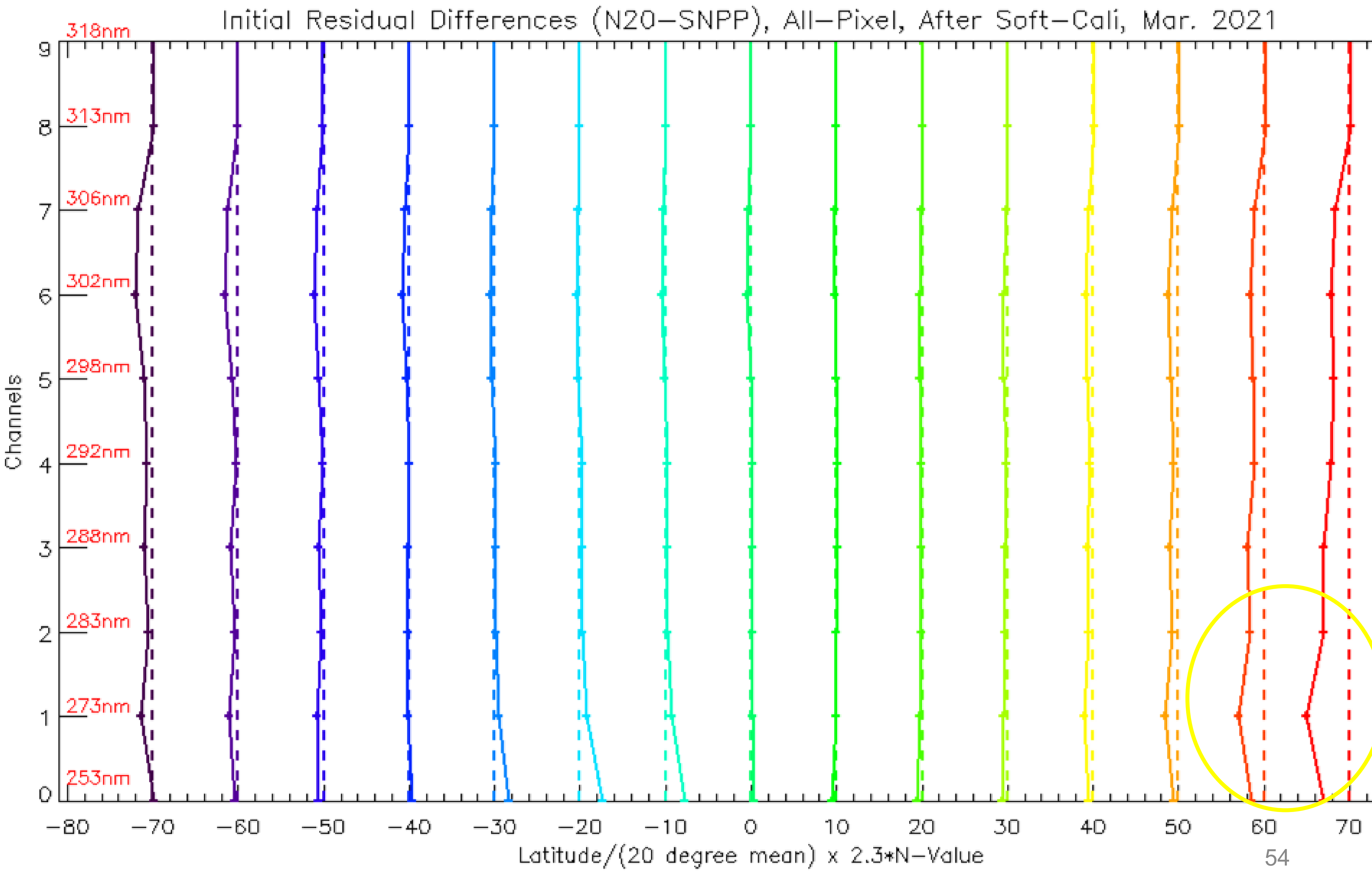
- The SDR Team provided NOAA-20 OMPS NP SDRs from off-line processing for their Version 3.
- The EDR Team used December 2019 and March 2020 data to check if this resolved the latitude-dependent measurement differences.
- The EDR Team examined the V8Pro V4R0 results with and without forced Equatorial agreement.
- March 2021 data were use to estimate the soft calibration adjustments necessary to create agreement between NPP and N20 V8Pro. These adjustments were delivered to NDE with the wavelength scale code patch.*

*Requires the application of the IBSL correction in the Northern Hemisphere for SZA > 62°.

Global Zonal Mean Comparison of Initial Residuals between NPP and N20 before Soft Calibration with EDR Code Fix

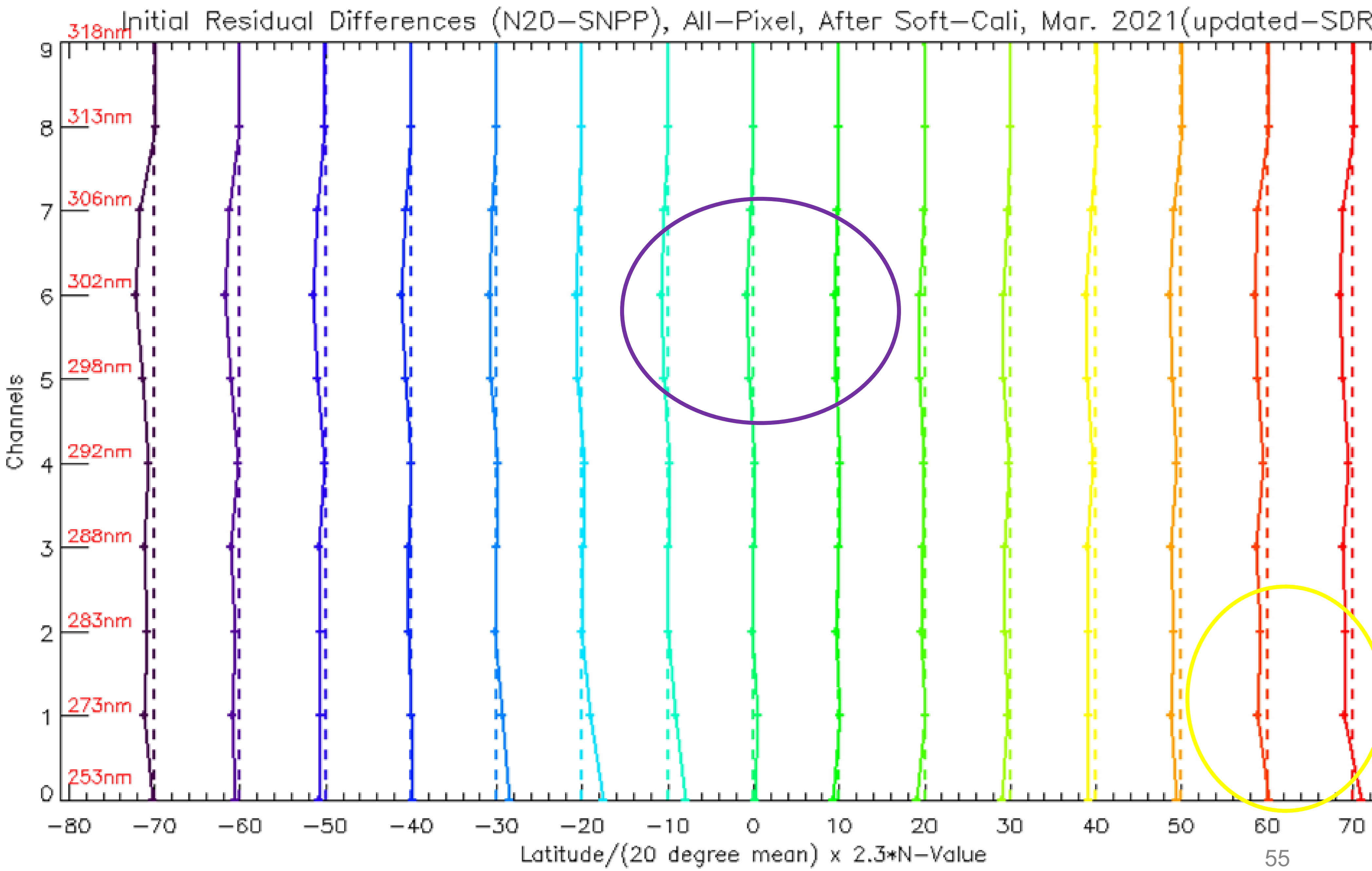


Global Zonal Mean Comparison of Initial Residuals between NPP and N20 after Soft Calibration w/o New SDR (λ & IBSL)



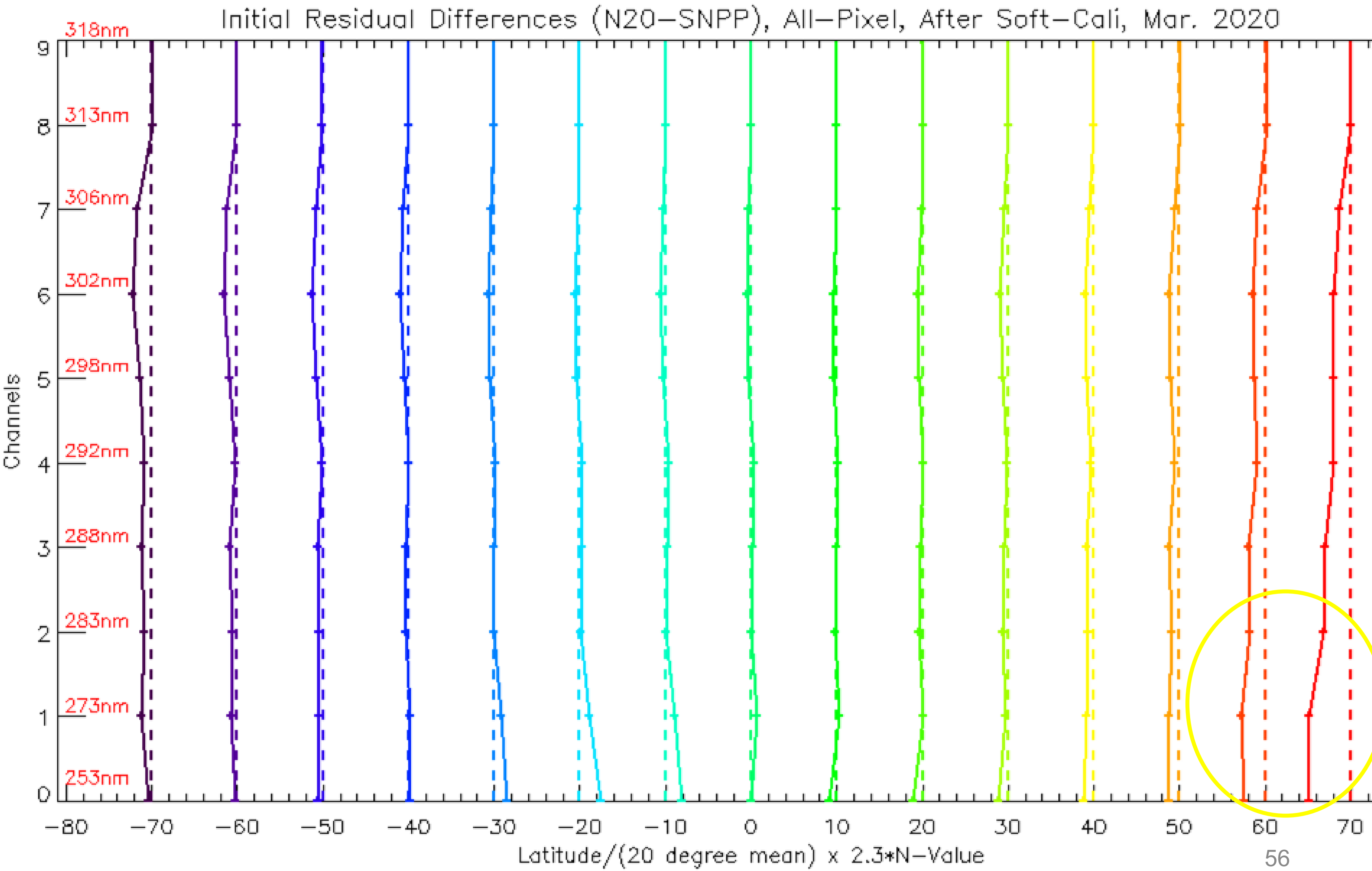
Pre-exiting Results | Current/Newer Results | Future Results | Unsolved Problems

Global Zonal Mean Comparison of Initial Residuals between NPP and N20 after Soft Calibration with New SDR (λ & IBSL)

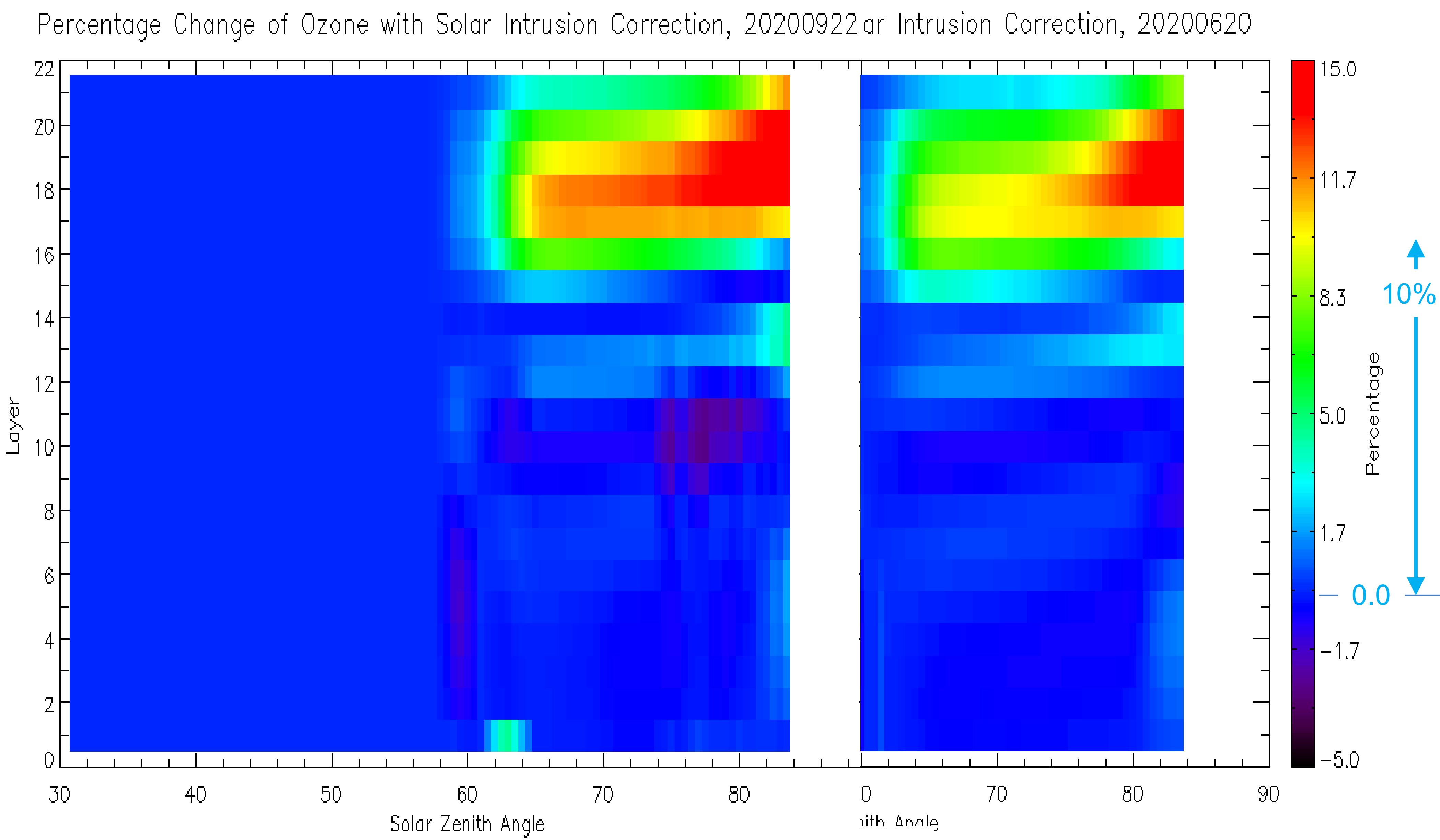


Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

Global Zonal Mean Comparison of Initial Residuals between NPP and N20 for 3/2020 after Soft Calibration for 3/2021

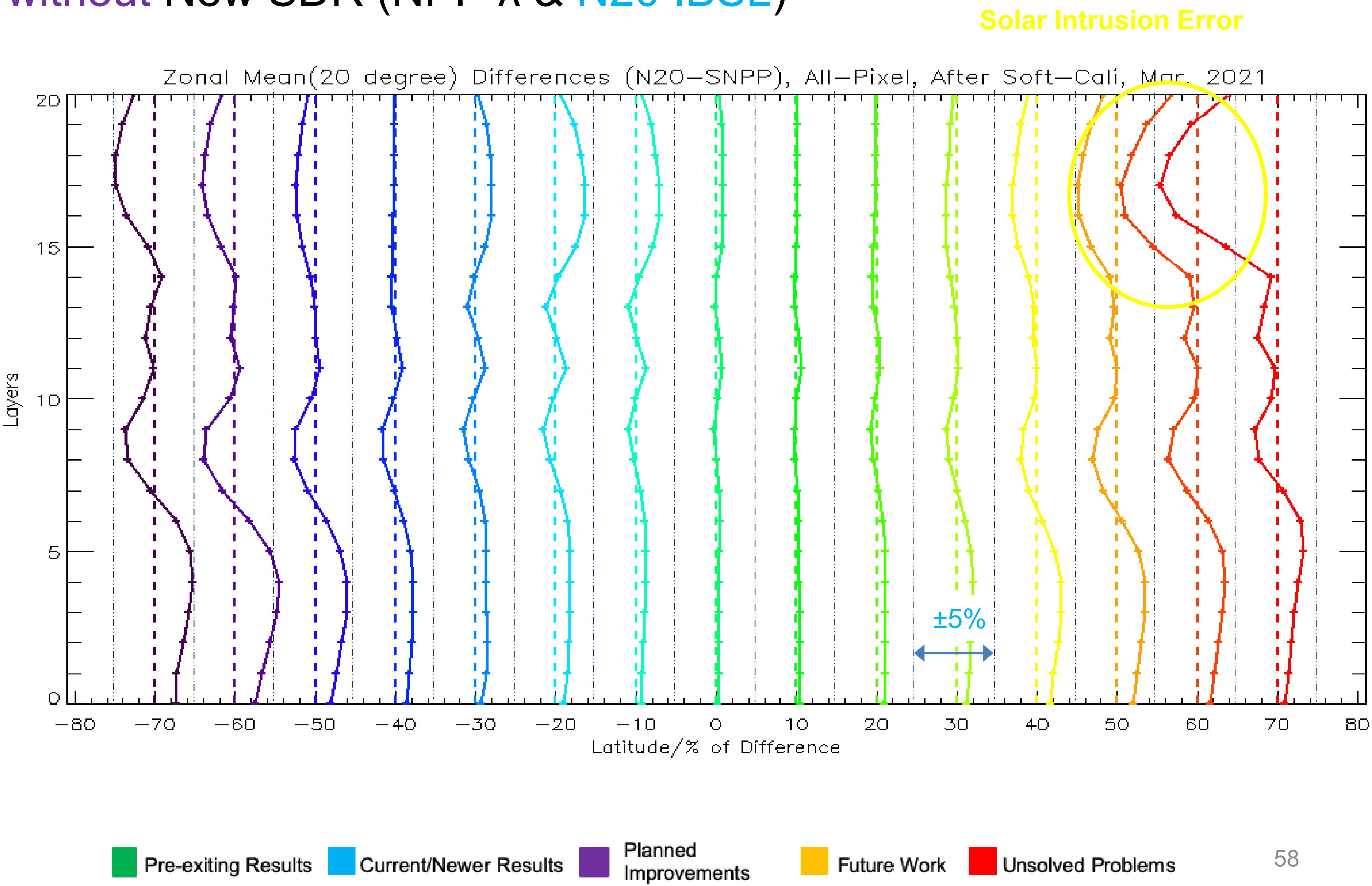


Changes in the N20 Northern Hemisphere Layer Ozone from the Solar Intrusion Correction

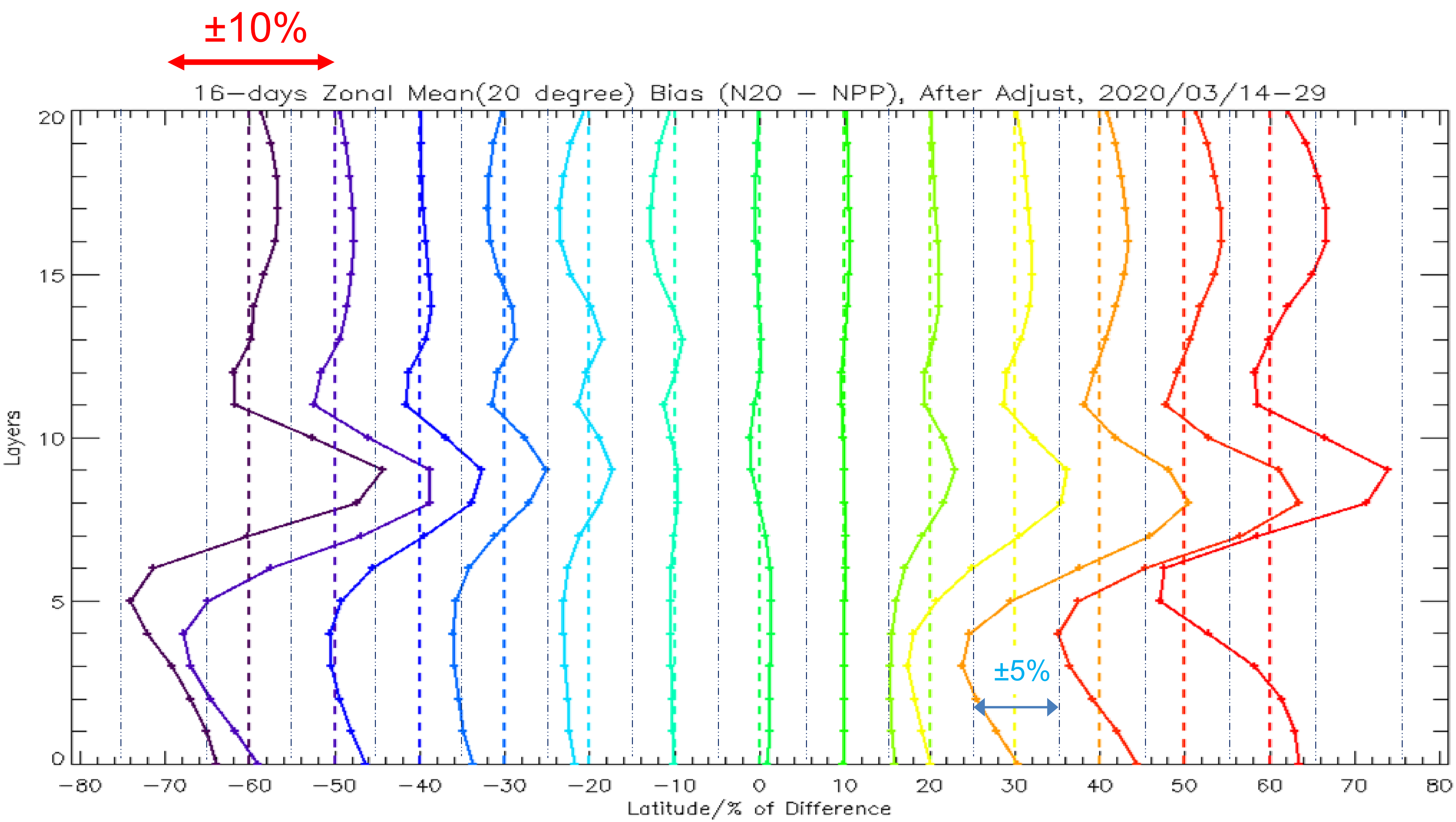


SZA, Degrees

Global Zonal Mean Comparison of Retrieved Profiles between NPP and N20 after Soft Calibration with Code Fix for 3/2021 without New SDR (NPP λ & N20 IBSL)



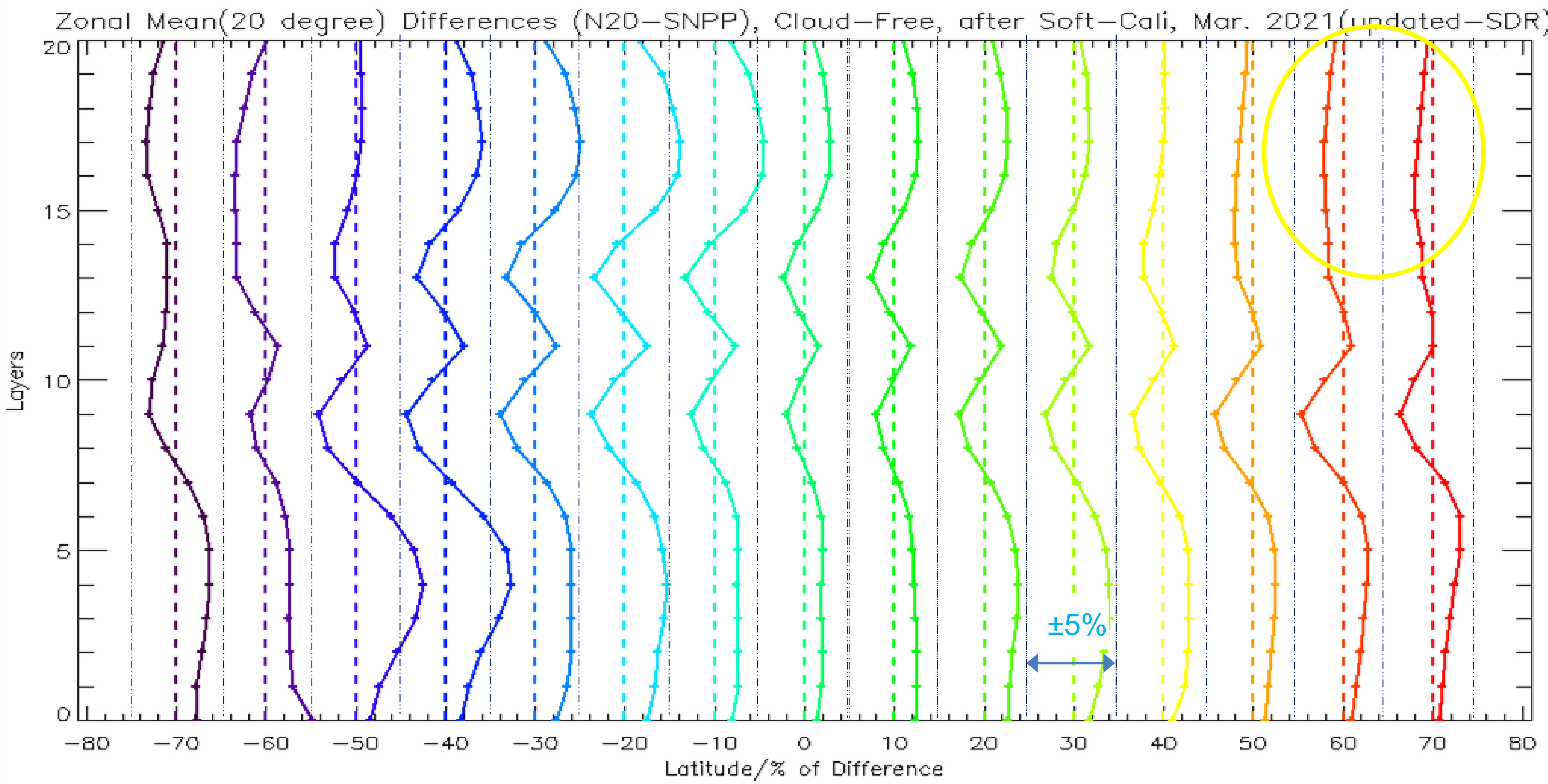
Zonal mean differences Adjusted Retrieved Ozone Profiles with EDR error for 21 layers (~3 km)



RESULTS SHOWN AT LAST REVIEW

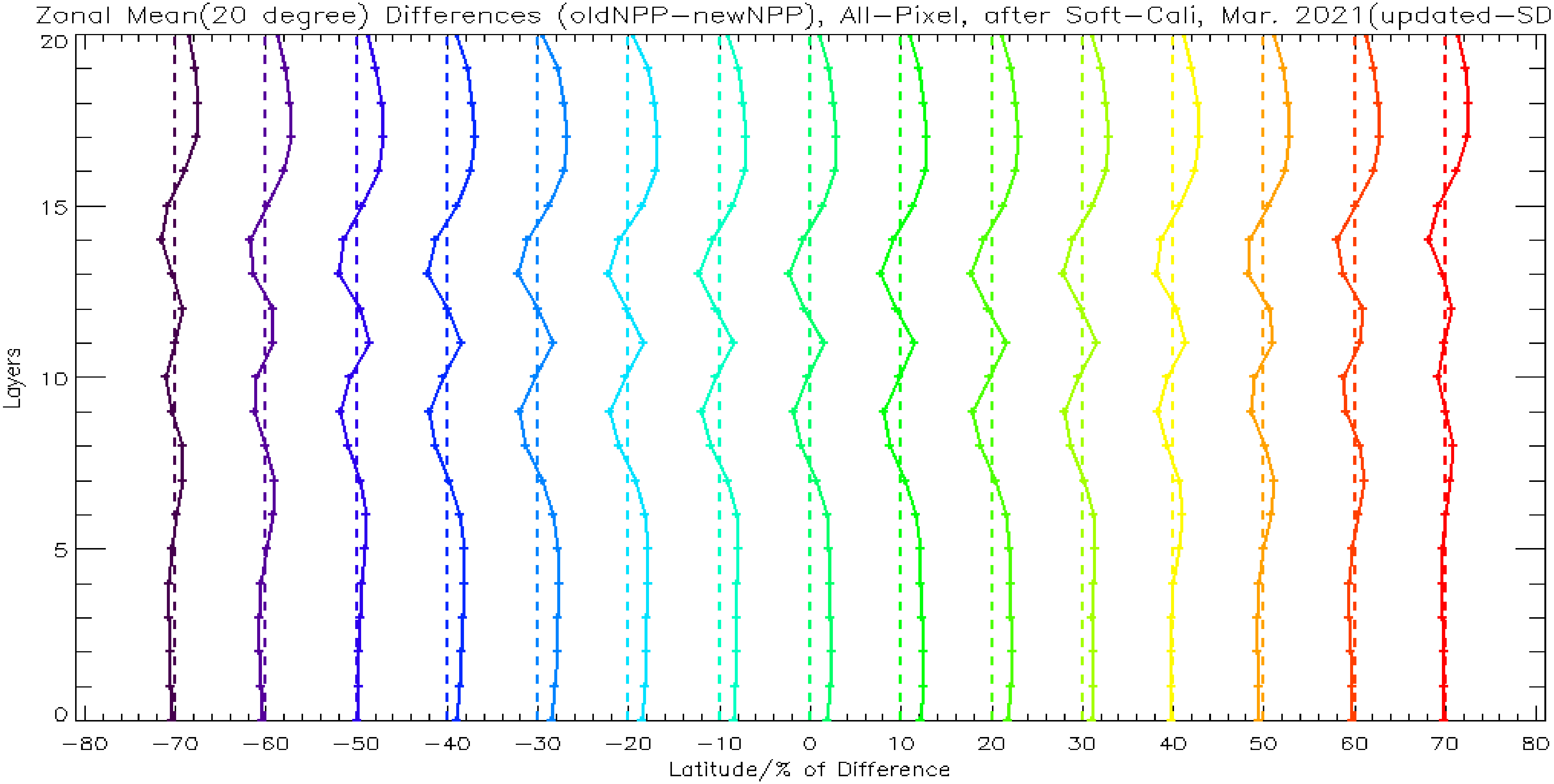
Global Zonal Mean Comparison of Retrieved Profiles between NPP and N20 after Soft Calibration with Code Fix for 3/2021 with New SDR (NPP λ & N20 IBSL)

Solar Intrusion Corrected

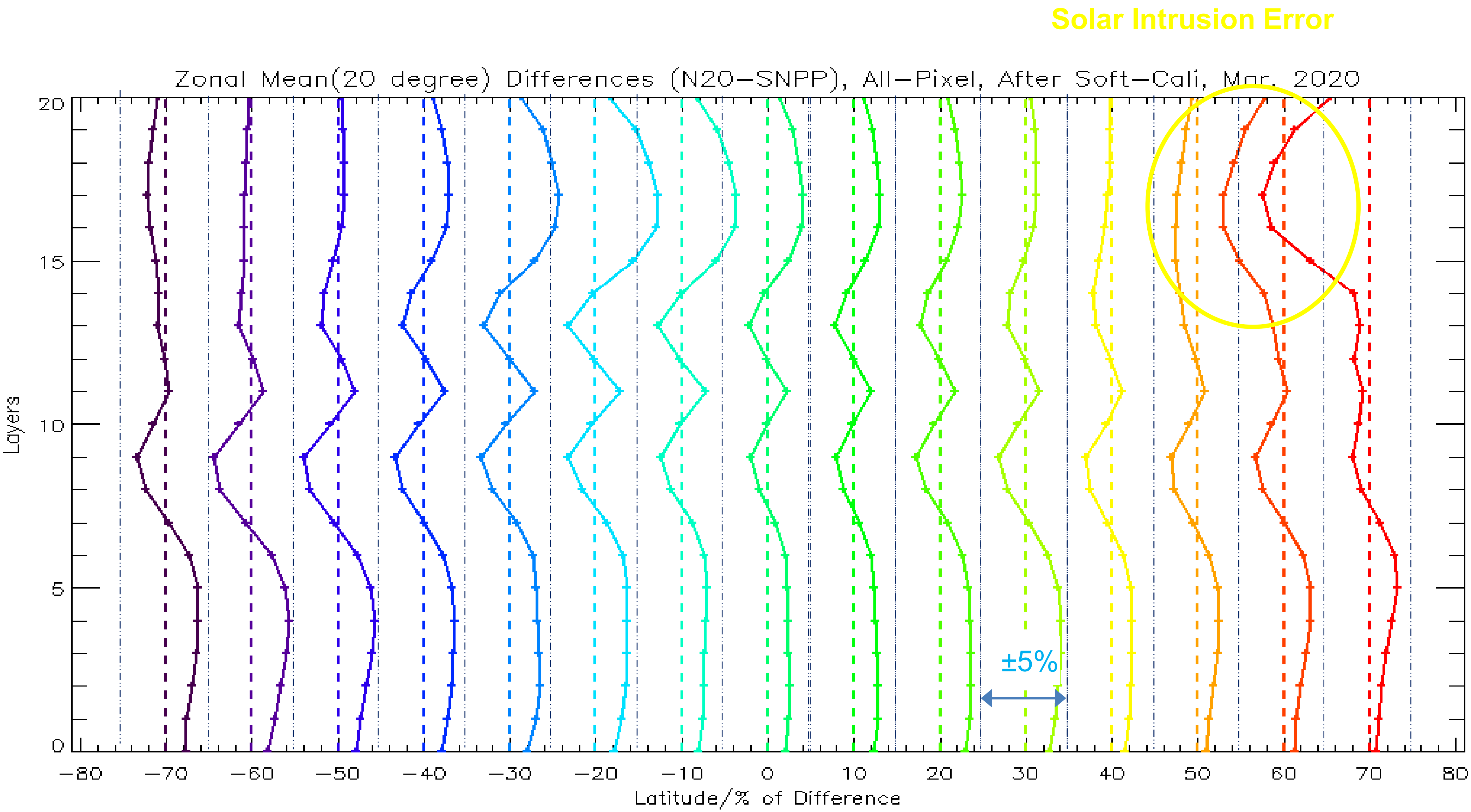


Pre-exiting Results
Current/Newer Results
Future Results
Unsolved Problems

Global Zonal Mean Comparison of Retrieved Profiles between NPP operational with error versus offline without error

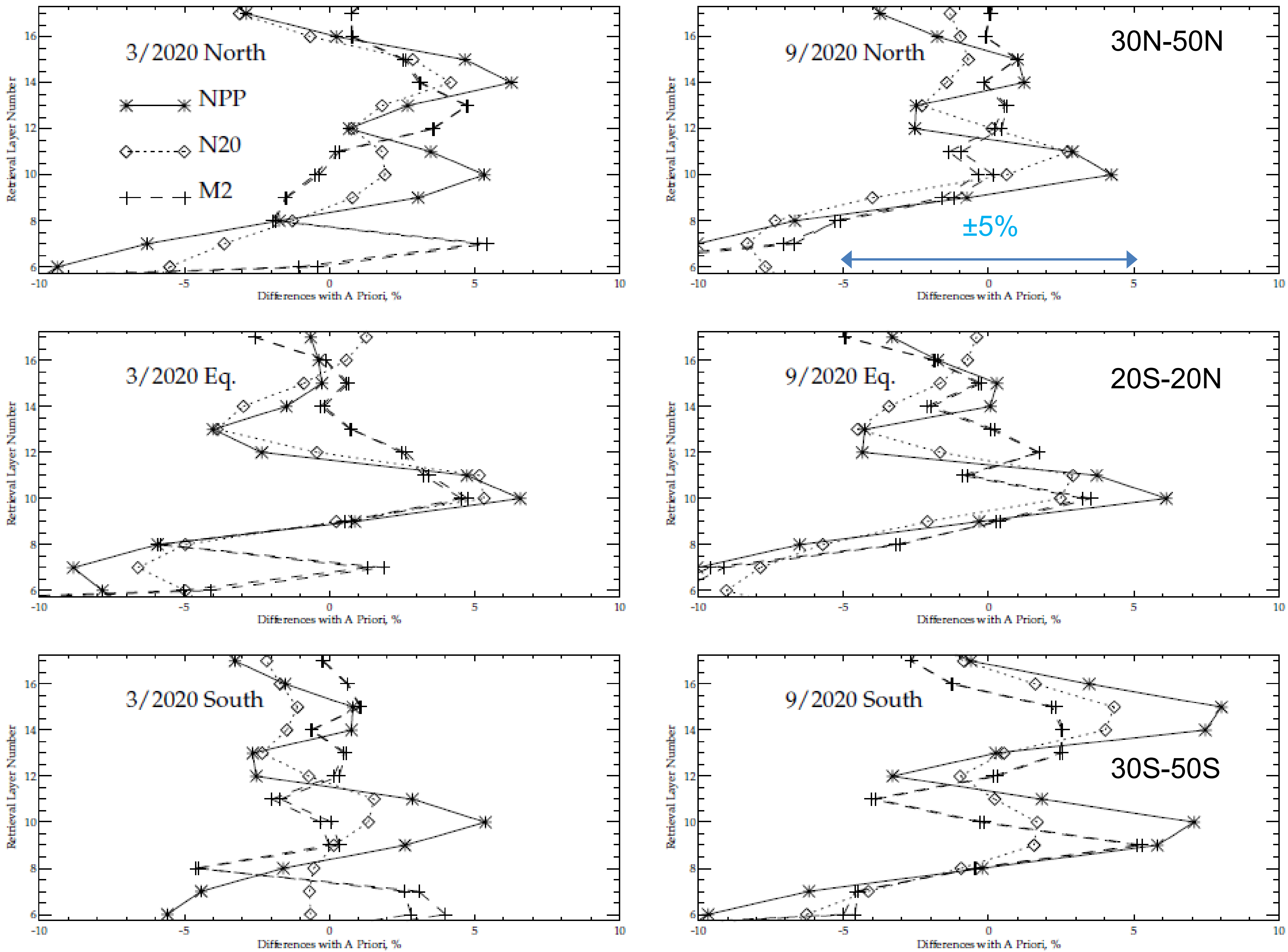


Global Zonal Mean Comparison of Retrieved Profiles between NPP & N20 after 3/2021 Soft Calibration with Code Fix for 3/2020



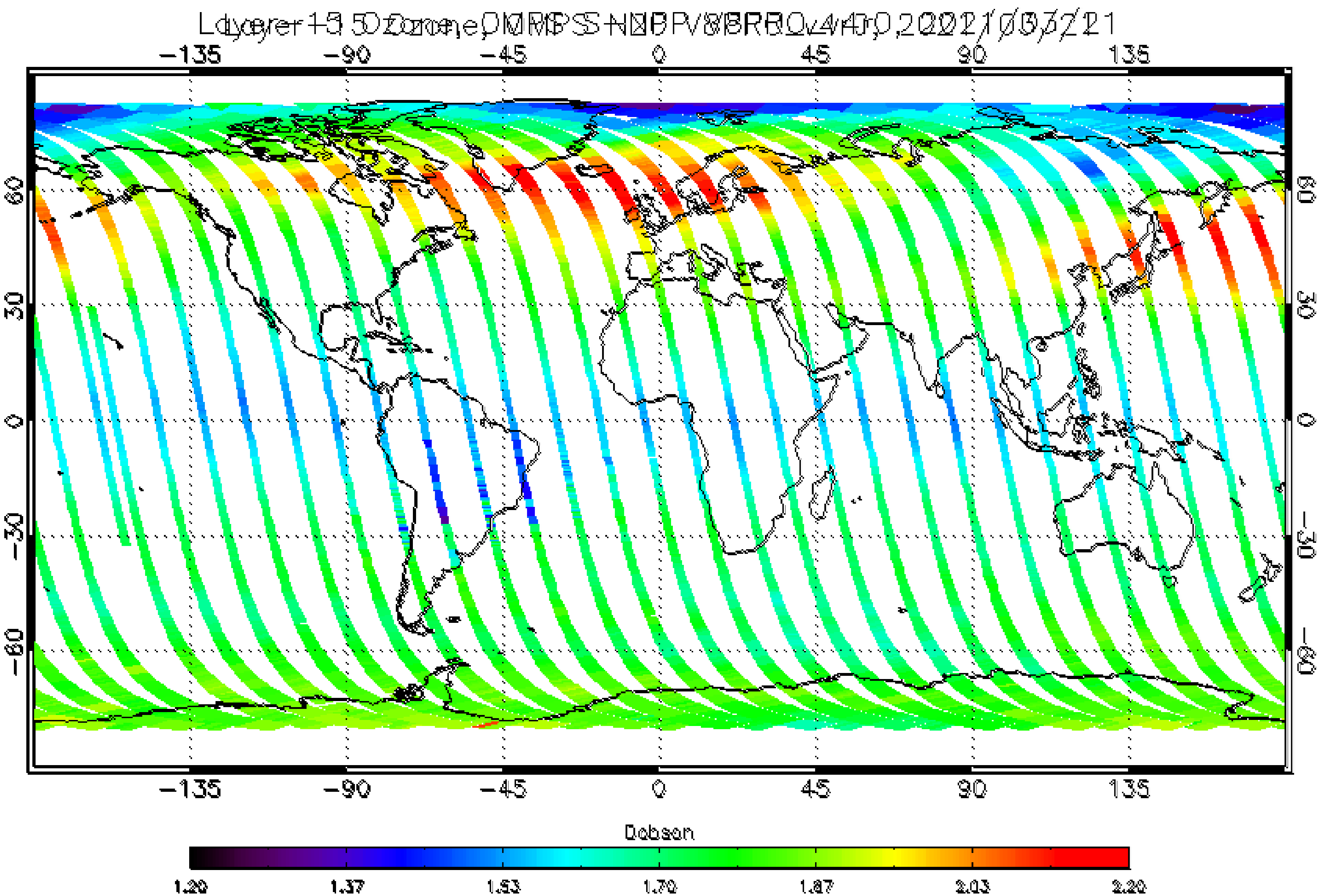
Comparisons to MERRA2

V8Pro Layers 6 to 17



Profile Differences with *A Priori*, %

Layer 15 STAR Offline N20 & NPP

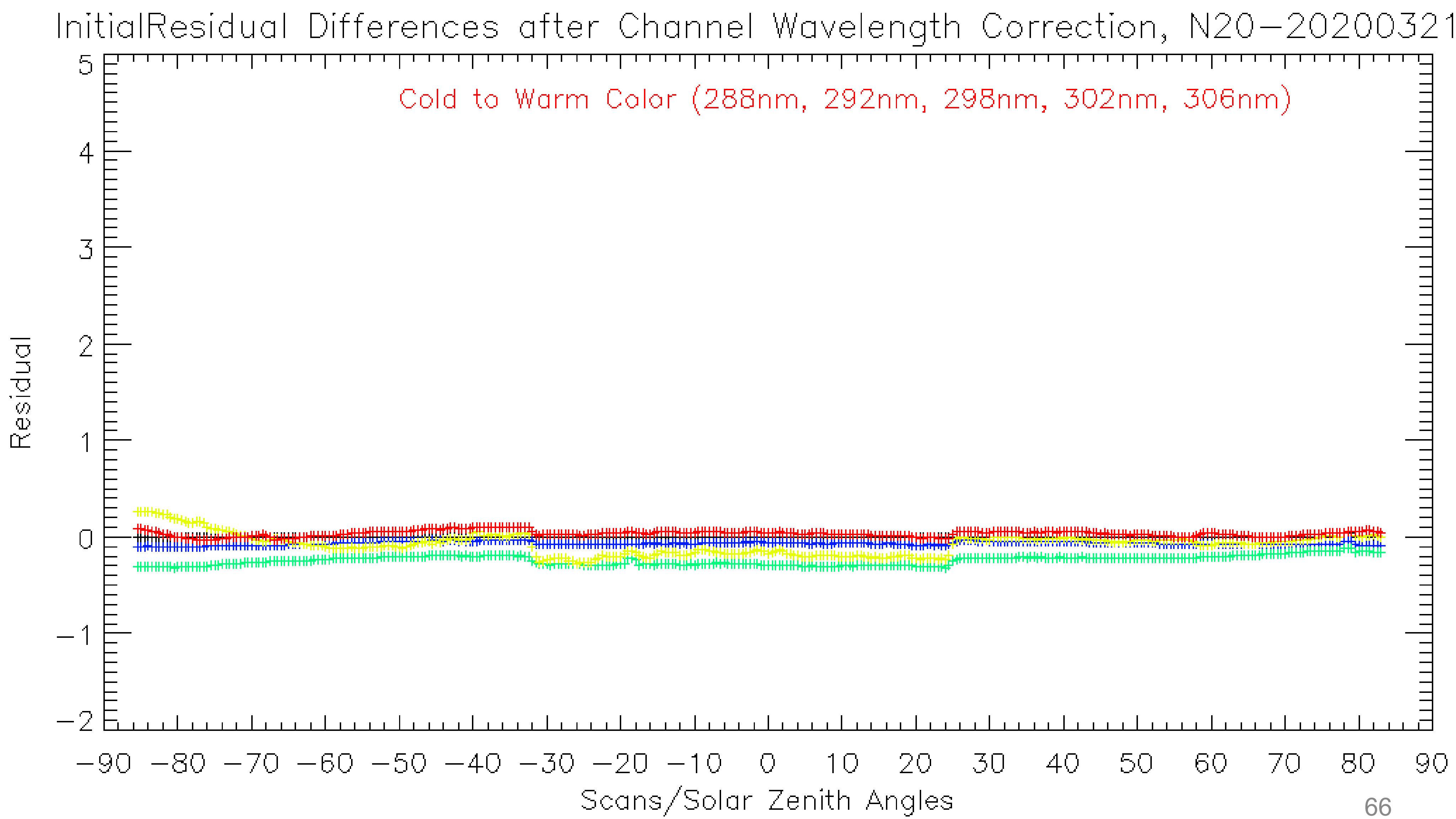


Why don't N20 and NPP agree better?

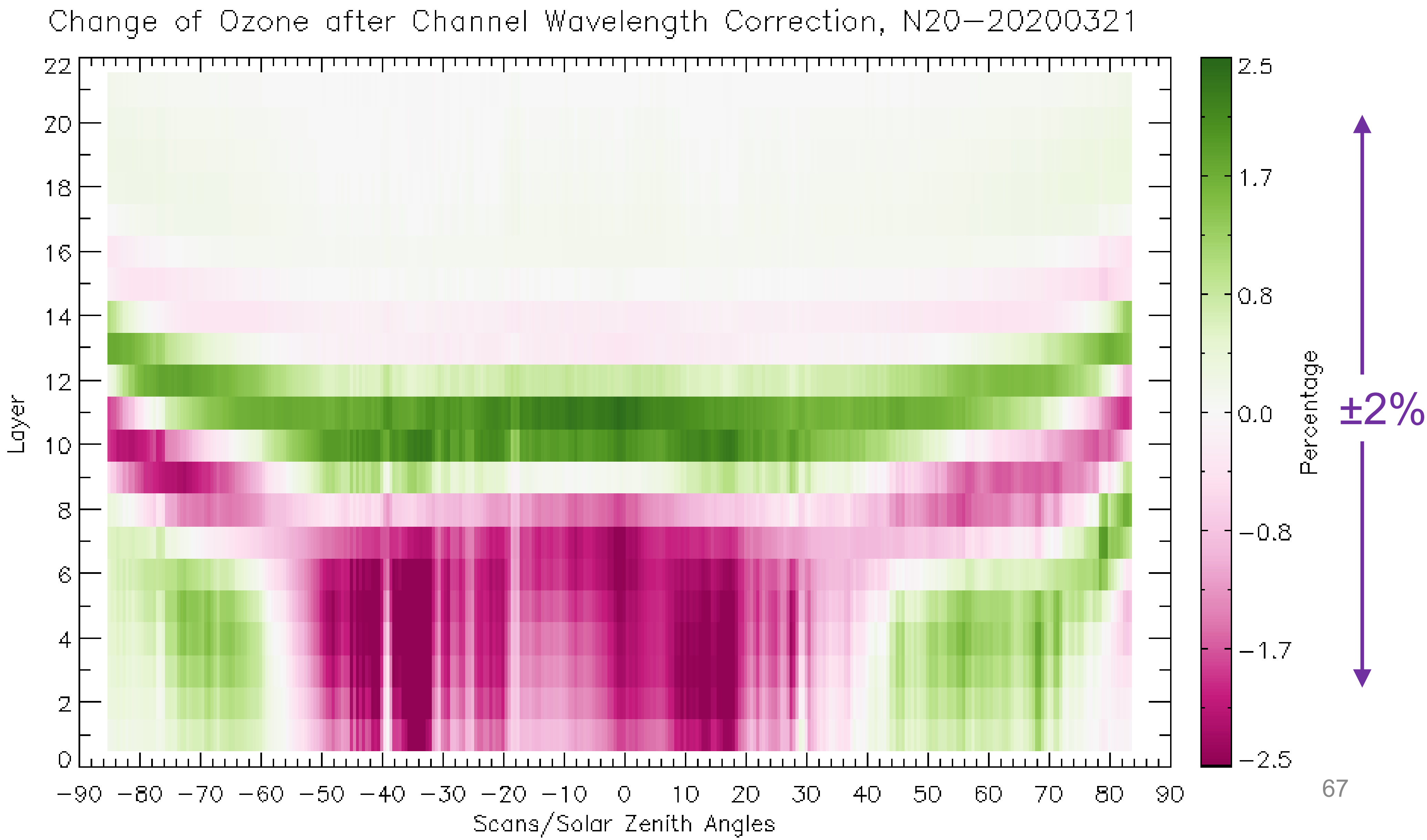
- Wavelength scale
  - Shifts from ground to orbit on the order of 0.1 nm.
  - SDR teams have revised scales for both satellites.
  - The latest wavelength and calibration tables for NOAA-20 OMPS NP were implemented at IDPS on 8/21/2020.
  - There is a shift in the NPP SDR wavelength scale for 2/2021 to 4/2021.
- Bandpass (Spectral Response Functions - SRFs)
  - There are significant differences in the FWHM of the two OMPS NP sensors. The dichroics complicate the bandpass characterization.
  - SDR teams have revised SRFs for both satellites.
  - The EDR Team has implemented improved fidelity SRF models in both Radiative Transfer tables and internal forward models in V4R0.
- Straylight
  - The NOAA-20 OMPS NP has in-band stray light from solar intrusion in the Northern hemisphere for SZA > 62 degrees.
  - A correction has been developed, and it is in the queue at IDPS.
- Interpolation
  - Channels do not fall on pixel wavelength centers.
  - Wavelength scales vary with time; Channels location are fixed.
- Polarization
  - BATC System Engineering Reports (SERs) indicate differences in the polarization sensitivity between S-NPP and NOAA-20. No forward model refinements are used for polarization.

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

Study of the effects of channel interpolation for V8PRO: Initial Residual changes after accounting for moving channel locations to measured wavelengths (1/2)



Study on the effects of channel interpolation for V8PRO: Retrieved ozone changes. We will correct most of this error with the next table deliveries. The tables will adjust the bandpasses for the as-interpolated effective bandpasses. (2/2)



N20 V8Pro Validated Maturity Caveats

- NOAA-20 V8Pro adjustments can give good agreement with the S-NPP V8Pro
- The quality of the products changed with the newest SDR Version 3 tables installed at IDPS. (TTO was 8/21/2020)
- The V8Pro EDR products described in this presentation will not be available from NDE until after the operational implementation of the latest changes (v4r0 + patch in 4/2021).
- An IBSL correction for the SDRs has been developed. Its implementation provides agreement for the upper profile (Layers 12-21) in the Northern Hemisphere. It is at IDPS and will go into the next build.
- The bandpasses and radiative transfer tables will be adjusted for the interpolation to the channel locations.
- An improved adjustment table will be delivered now that the SDR wavelength shift for S-NPP OMPS NP for 3/2021 is resolved.

Pre-exiting Results | Current/Newer Results | Planned Improvements | Future Work | Unsolved Problems

Processing Environment and Algorithms

- Processing environment and algorithms used to achieve Validated maturity stage:
  - Algorithm version V8Pro_v4r0 offline processing at STAR with wavelength scale code fix using offline OMPS NP SDR_V3 and operational OMPS NM SDR as inputs.
  - Offline processing with the solar intrusion correction implemented for northern hemisphere above 60° SZA
  - DAP provided to ASSISTT for implementation at NDE July 2020. Patch with N20 wavelength scale code correction and new soft calibration adjustment table provided directly to NDE April 2021.

Required algorithm inputs

- Required Algorithm Inputs
  - Primary Sensor Data
    - NOAA-20 OMPS NM SDR and GEO
    - NOAA-20 OMPS NP SDR and GEO
  - Ancillary Data
    - Ozone and cloud top pressure climatologies.
  - Upstream algorithms
    - OMPS SDR (Version 3)
  - LUTs / PCTs
    - Multiple scattering correction RT Table
    - N-value Adjustment Table
    - High fidelity bandpass SRF

User Feedback

Name	Organization	Application	User Feedback - User readiness dates for ingest of data and bringing data to operations
C. Long H. Liu L. Ciasto L. Kouvaris	NCEP	O3 Assimilation for NWP, UV Index, and Monitoring.	Will not add NOAA-20 V8Pro BUFR to operational use with current disagreement with S-NPP for NDE products. Will make use for Ozone Hole monitoring in conjunction with S-NPP.
Irina P.	GML	Ground-based comparisons in NOAA AC4	Will wait for Solar IBSL corrections before using NOAA-20 V8Pro overpasses in the study for high northern latitudes. (Note: SDR reprocessing and IDPS CCR with the solar intrusion correction are proceeding.)

User Feedback

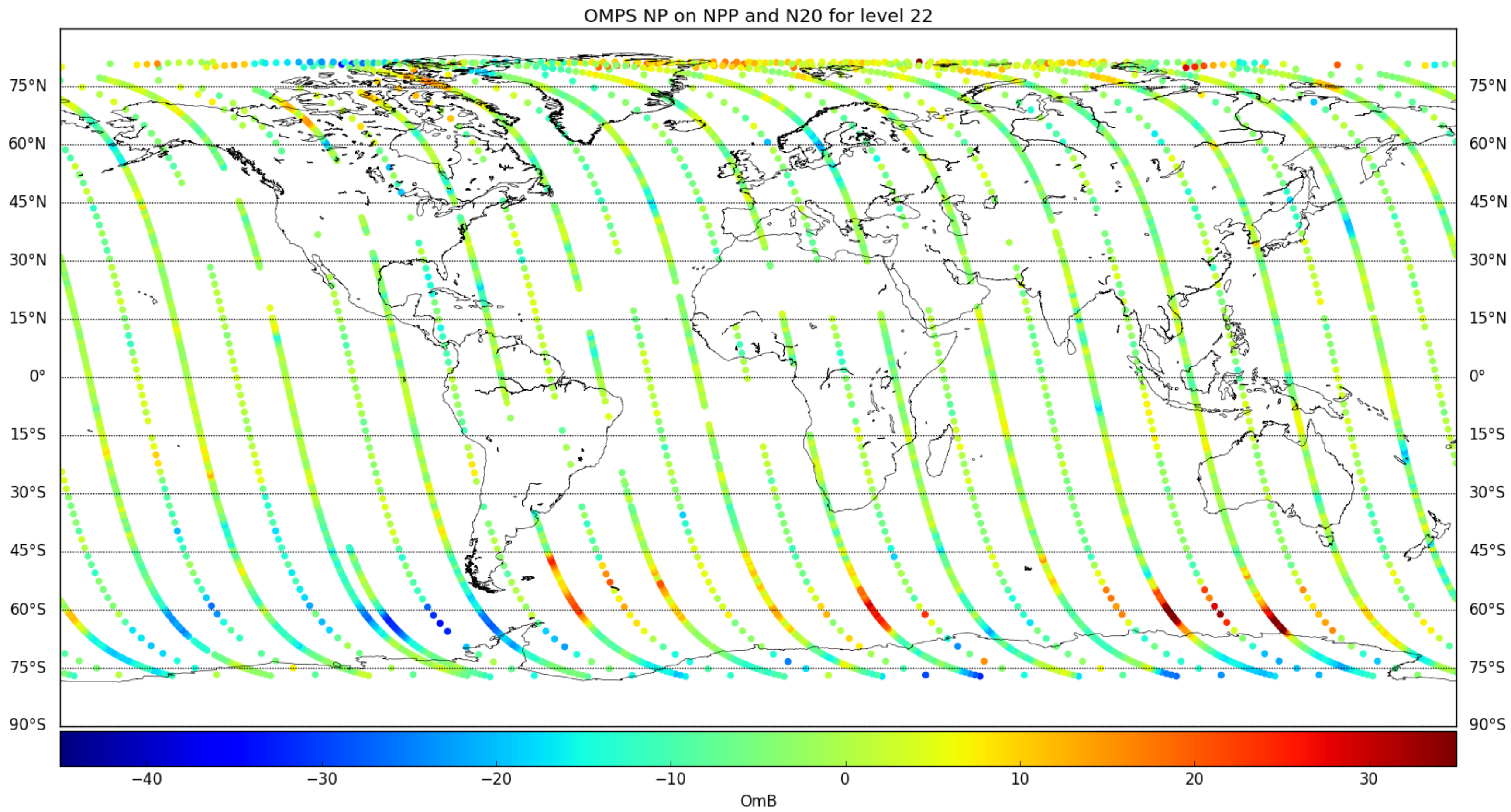
The V8PRO retrievals for the STAR offline processing with the latest updates delivered to NDE for September 2020 have been encoded into BUFR. The BUFR files were provided to NWS and ECMWF in April 2021.

NPP data:
ftp://ftp.star.nesdis.noaa.gov/pub/smcd/jpss-ait/V8PRO/npp/2020/09/

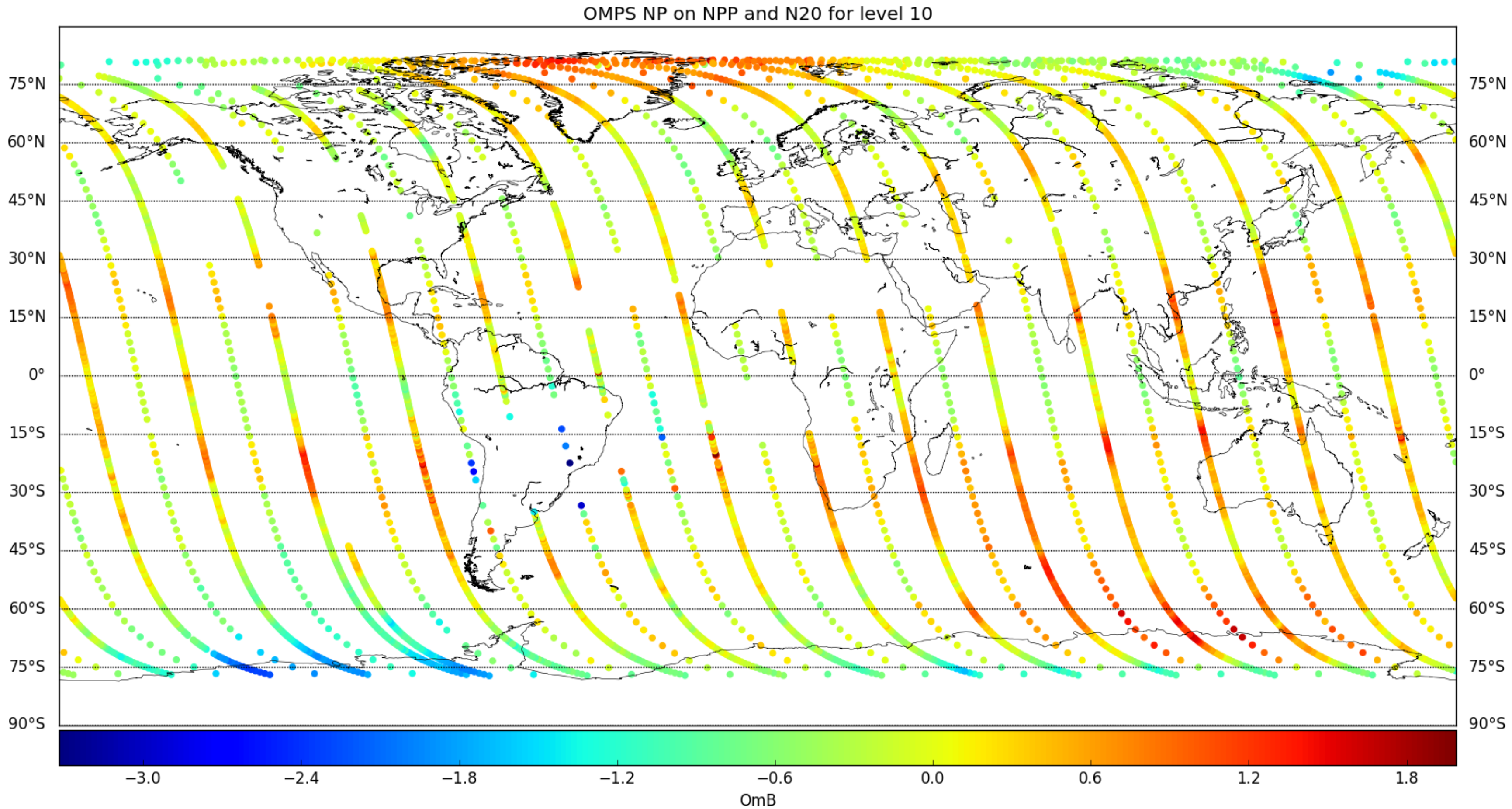
N20 data:
ftp://ftp.star.nesdis.noaa.gov/pub/smcd/jpss-ait/V8PRO/n20/2020/09/

From Louis Kouvaris: We have analyzed the data for Sept 13, 2020 and found much improved results and close matching to NPP. Attached (on the next three slides) are observed minus background plots for OMPS NP on N20 and NPP (level 10 and 22) and a scatter plot by latitude for the first cycle. Black is N20 and red is NPP. The distributions closely follow each other, though there does appear to be a slight bias between the two instruments. We plan to continue analyzing the data for the rest of the month.

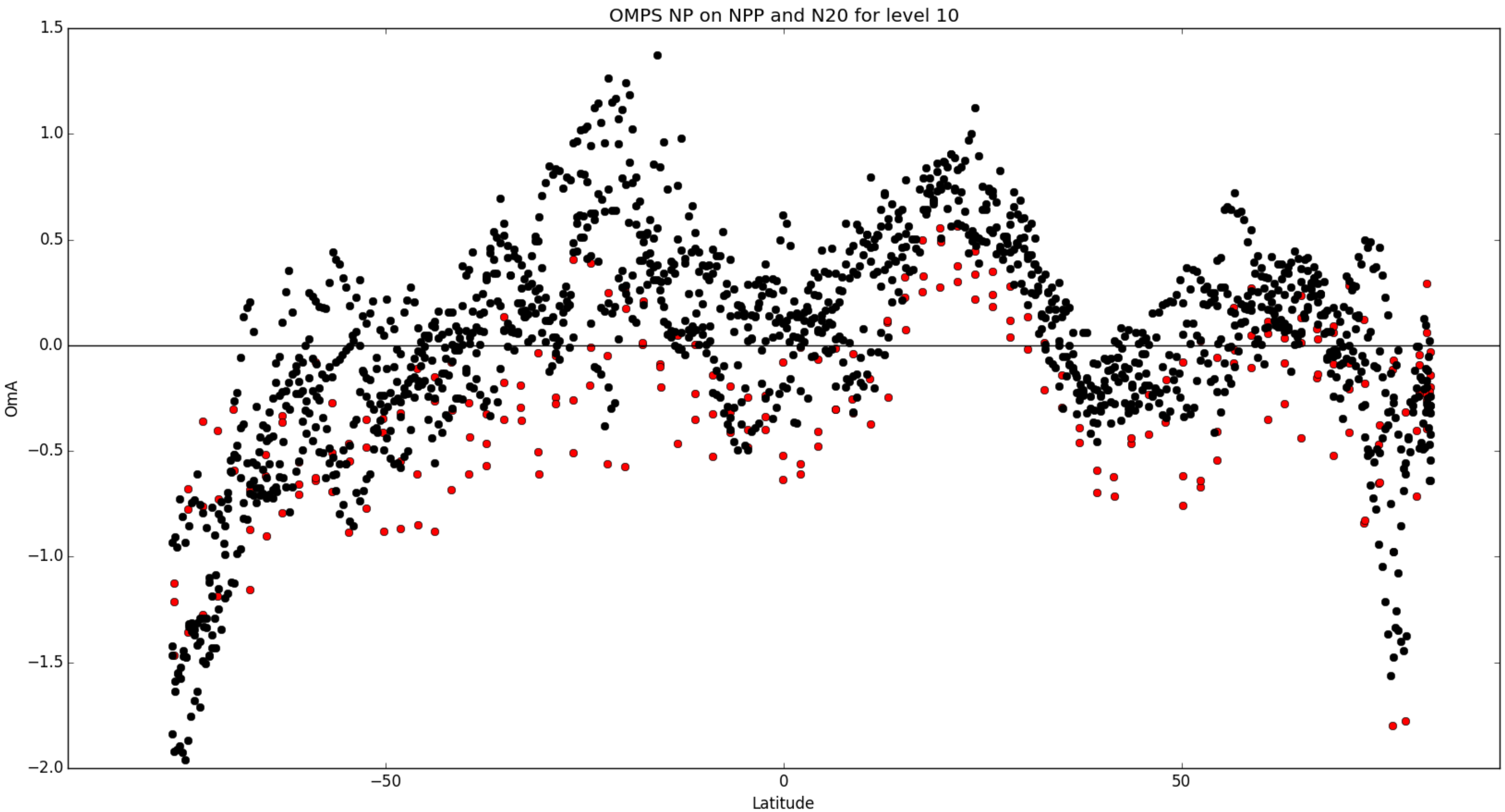
O minus B for level 22



O minus B for level 10



O minus B for level 10



Antje Inness ecmwf.onmicrosoft.com

- We've been struggling to understand why there are differences between N20 and NPP OMPS.

- We will halt our assimilation tests with the data until the product is more mature. And perhaps Eumetcast could attach a 'health warning' to the data? We had assumed the data quality would be ok as they were being distributed on Eumetcast.

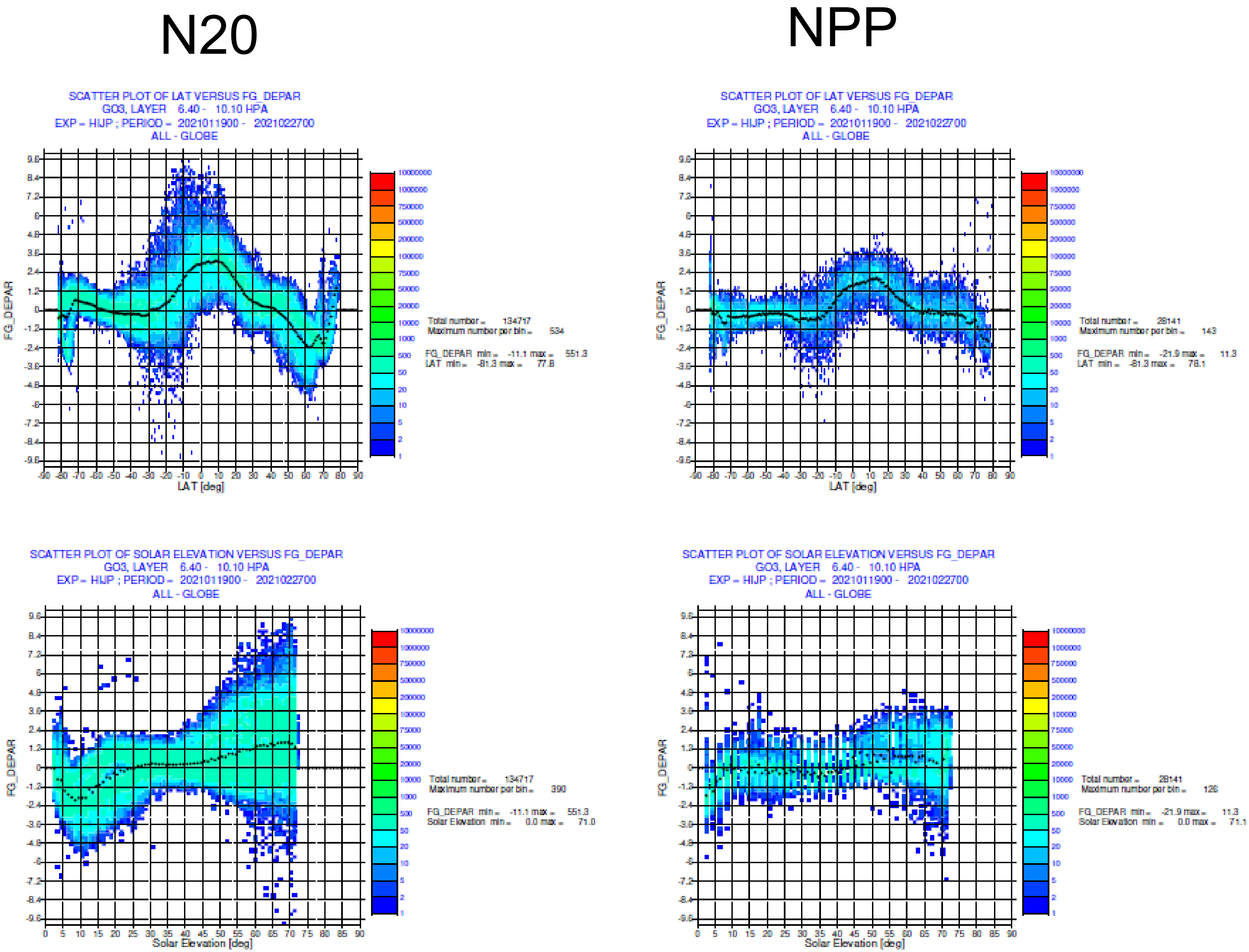


Figure 1: 6.4-10 hPa: Scatterplots of first-guess departures against latitude (top) and solar elevation (bottom) for N20 (left) and NPP (right)/OMPS.

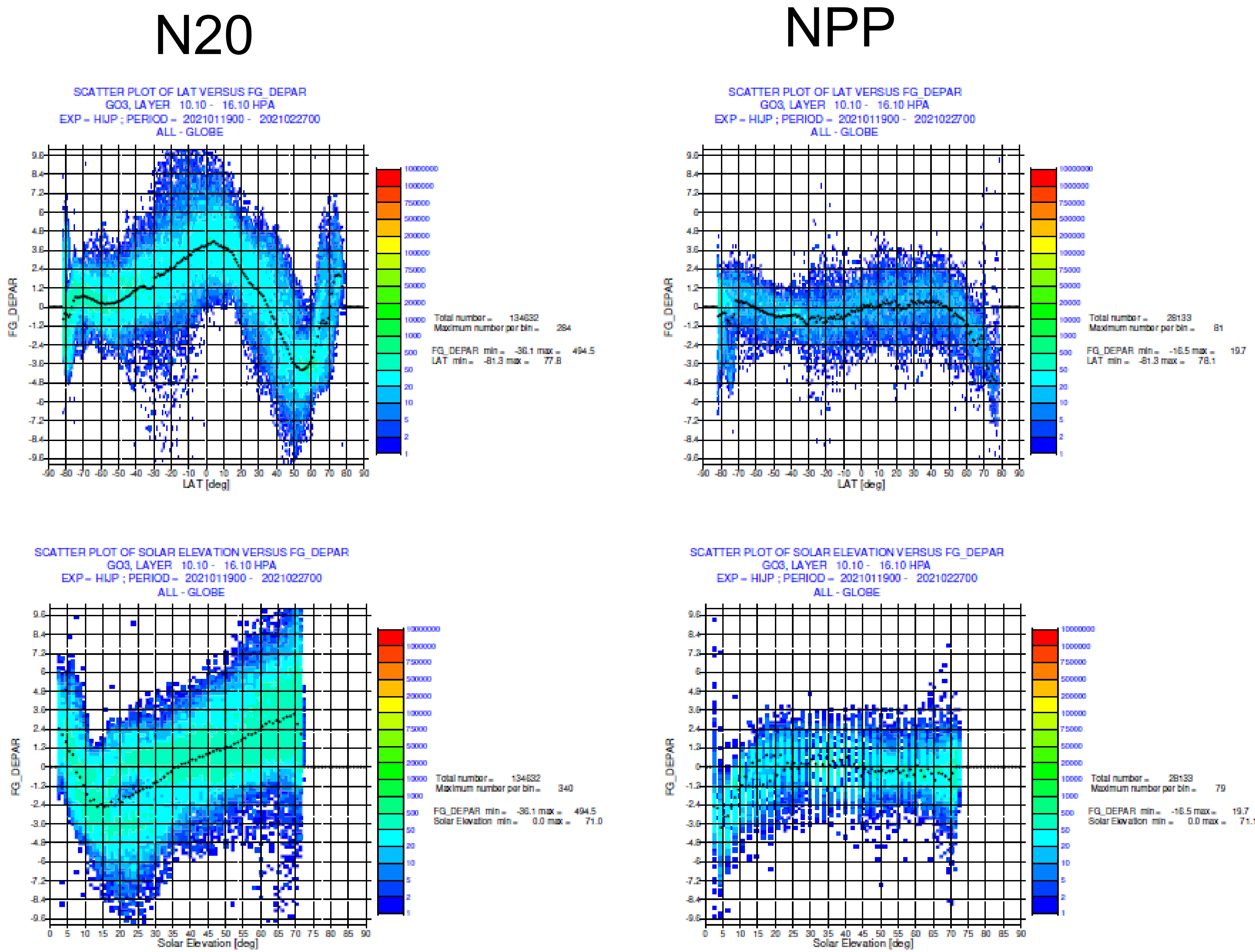


Figure 2: 10-16 hPa: Scatterplots of first-guess departures against latitude (top) and solar elevation (bottom) for N20 (left) and NPP (right) OMPS.

Downstream Product Feedback

Algorithm	Center	Product	Downstream Product Feedback - Reports from downstream product teams on the dependencies and impacts
V. Kapoor TOAST Blended Products	OSPO	Global Ozone Maps	Currently using S-NPP V8Pro. Ready to add NOAA-20 V8Pro with latest agreement. Will make a separate NOAA-20 based product (V8Pro and NUCAPS).
J. Wild CDR development	NCEP	O3 Trends / Ozone Layer Assessments	Will not add NOAA-20 to the Ozone Profile CDR record using S-NPP with current disagreement. Will wait for reprocessed SDRs with solar correction.

Risks, Actions, and Mitigations

Identified Risk	Description	Impact	Action/Mitigation and Schedule
Failure to get agreement	Soft calibration did not resolve differences between S-NPP V8Pro and NOAA-20 V8Pro for the longer wavelength channels that contribute to the lower half of the retrieved ozone profile.	Major	Agreement after wavelength scale code correction now meets performance requirements. One-line code patch and new adjustment table delivered directly to NDE April 2021.
Improvements waiting in the queue.	Multiple code and table changes are ready for implementation at NDE. A new adjustment table will be needed.	Major	Working with ASSISTT and NDE to implement new DAP for V8PRo v4r0 with code and table changes.
Stray light correction	Soft calibration adjustments will continue to evolve as further analysis is performed and IBSL corrections are implemented.	Major	Provided new adjustment table as a part of one-line code patch delivery directly to NDE. Tested with solar intrusion correction data sets.
Uncertainty in SDR wavelength scale	Soft calibration will change when the SDR wavelength scale shift for 2-4/2021 is resolved.	Medium	We will deliver a new adjustment table now that NPP wavelength is resolved.
Improved Model	Interpolation errors on the order of ±2% should be reduced.	Medium	We will deliver new bandpass and multiple scattering tables.

Documentation

Science Maturity Check List	Yes / No
ReadMe for Data Product Users (Validated)	Yes (NOAA-20)
Algorithm Theoretical Basis Document (ATBD)	In revision (V8Pro_v4r1)
Algorithm Calibration/Validation Plan	Yes (JPSS-1/2 Ozone)
(External/Internal) Users Manual	Yes (V8Pro)
System Maintenance Manual	Yes (V8Pro)
Peer Reviewed Publications (Demonstrates algorithm is independently reviewed)	Yes (V8Pro)
Regular Validation Reports (at least annually) (Demonstrates long-term performance of the algorithm)	At S-NPP and JPSS annual meetings and reviews

Check List – Validated Maturity

Provisional Maturity End State	Assessment
Product performance has been demonstrated over a large and wide range of representative conditions (i.e., global, seasonal).	Full profile product agreement with S-NPP V8Pro has been achieved at the ±5% level. Coupled with the validation of the S-NPP V8Pro at the ±5% level, the validation of NOAA-20 at the ±10% level is achieved.
Comprehensive documentation of product performance exists that includes all known product anomalies and their recommended remediation strategies for a full range of retrieval conditions and severity level.	Multiple complications have been addressed by the EDR and SDR teams and a correction for the IBSL has been developed.
Product analyses are sufficient for full qualitative and quantitative determination of product fitness-for-purpose.	Differences as a function of layer and latitude have been quantified. Retrieval precision has been improved and quantified.
Product is ready for operational use based on documented validation findings and user feedback.	With conditions as noted in this presentation and the Validated ReadMe.
Algorithm changes associated with anomalies have been documented, implemented, tested, and shared with the user community.	The presentations on V8Pro refinements described motivations and changes. These are documented in the Readme appendices and updates to the ATBD.
Product validation, quality assurance, & algorithm stewardship continue through the product lifetime.	

Pre-exiting Results · Current/Newer Results · Planned Improvements · Future Work · Unsolved Problems

Path Forward and Recommendation

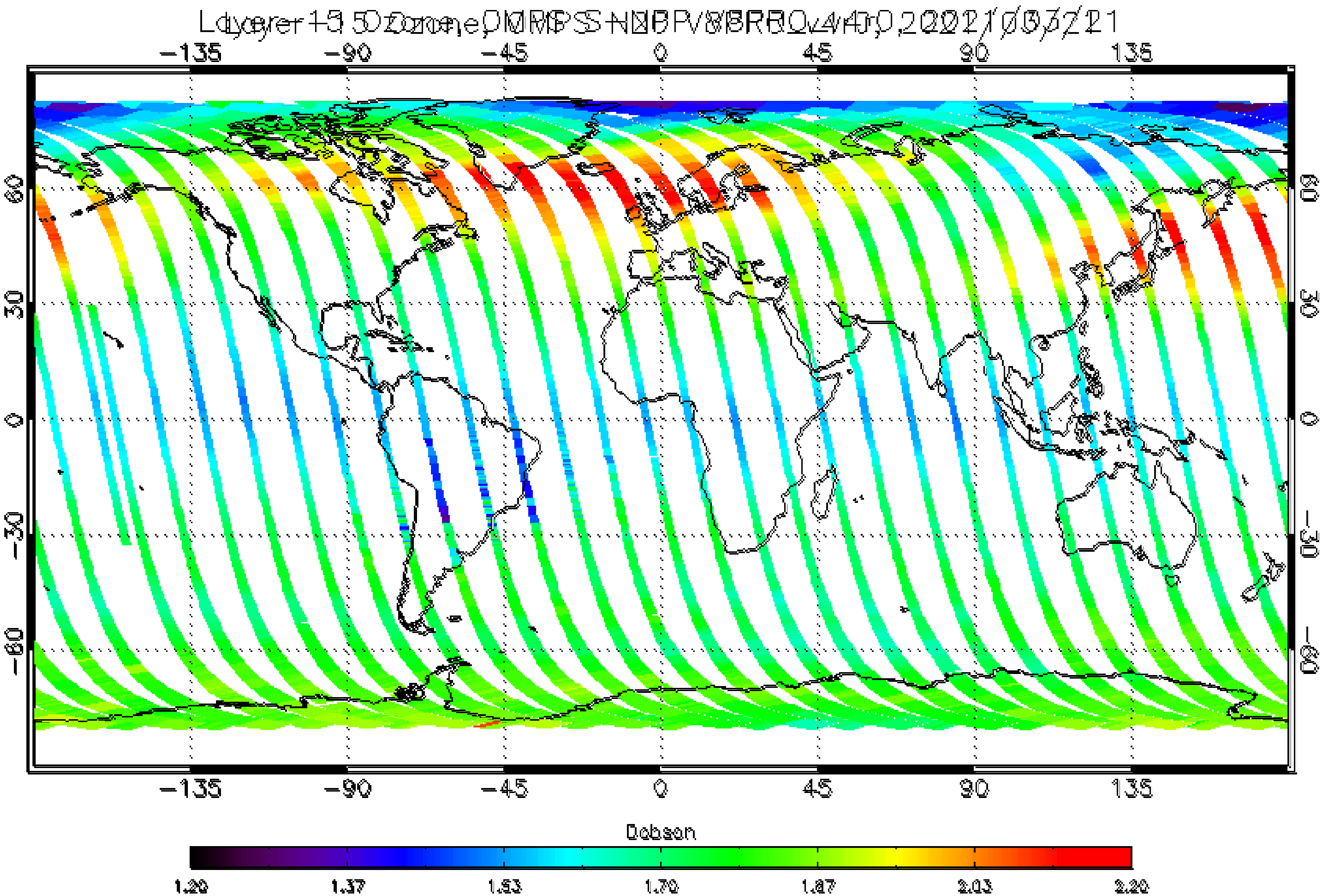
- Working with ASSISTT, OSPO and NDE to complete implementation of new code, and table and document changes.
- The SDR team is nearing completion of the implementation of the Solar IBSL within the V8Pro SDR ingest subroutines at IDPS.
- The Ozone EDR Team recommends validated maturity for the full product:
    - Full product performance relative to S-NPP is achieved globally.
    - Additional improvements in the agreement will take place with two planned changes.

Summary and Conclusions

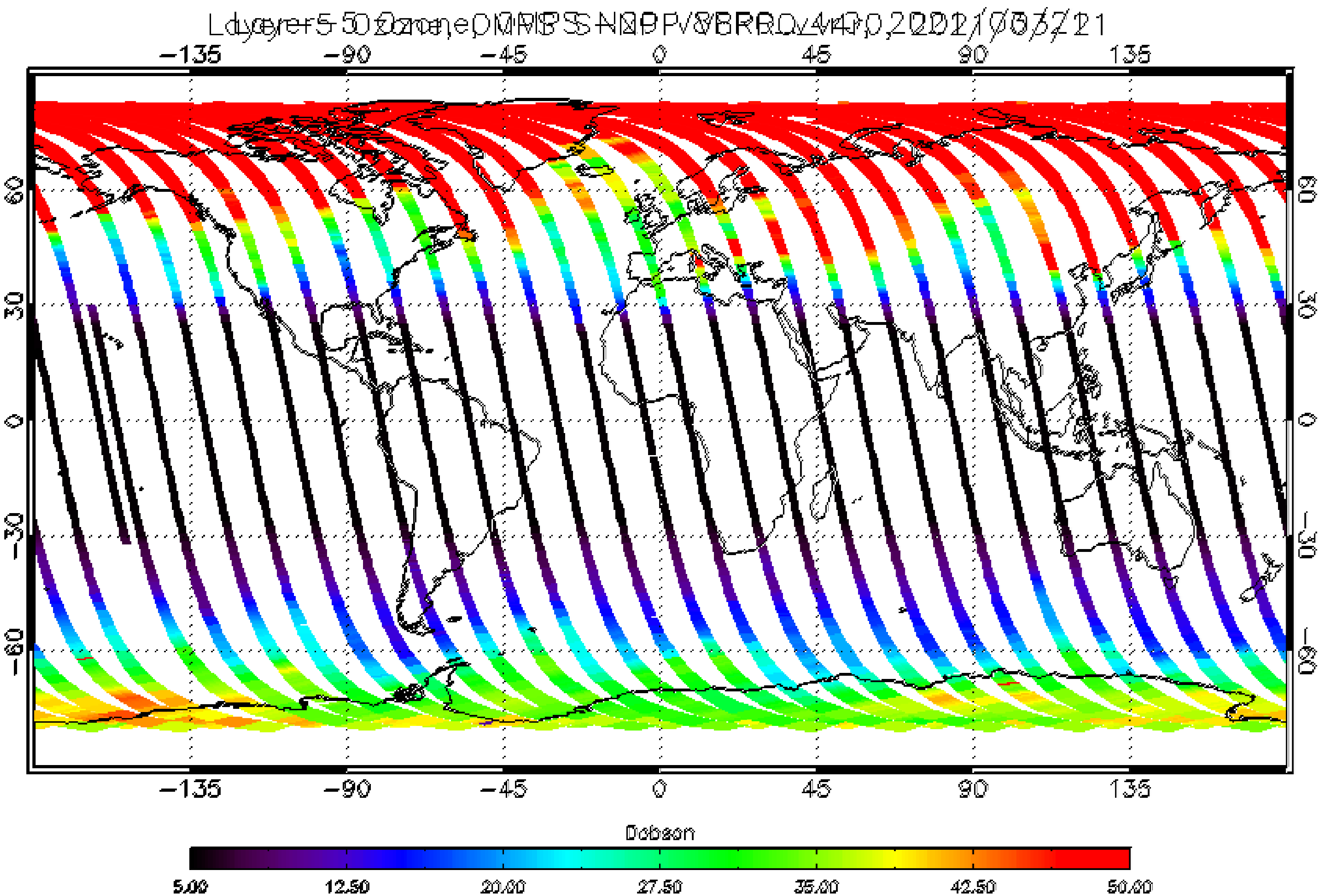
- The NOAA-20 OMPS NP & NM SDRs are performing well with measurement SNRs and stability similar to the S-NPP instruments.
- The code correction for the V8Pro and the new adjustment table are expected to be at NDE operations on June 7, 2021.
- The radiances for the shorter channels for the NOAA-20 OMPS NP deviate from those for the S-NPP OMPS NP in the Northern Hemisphere (SZA > 62) but the cause has been traced to IBSL and an SDR correction has been delivered to IDPS and is expected to become operational 7/21/2021.
- By implementing the IBSL correction and applying soft calibration to remove biases for the channels estimated over the tropics, the V8Pro V4R0 will provide good global agreement between the NOAA-20 and S-NPP products, and achieve validated performance.

Backup Material

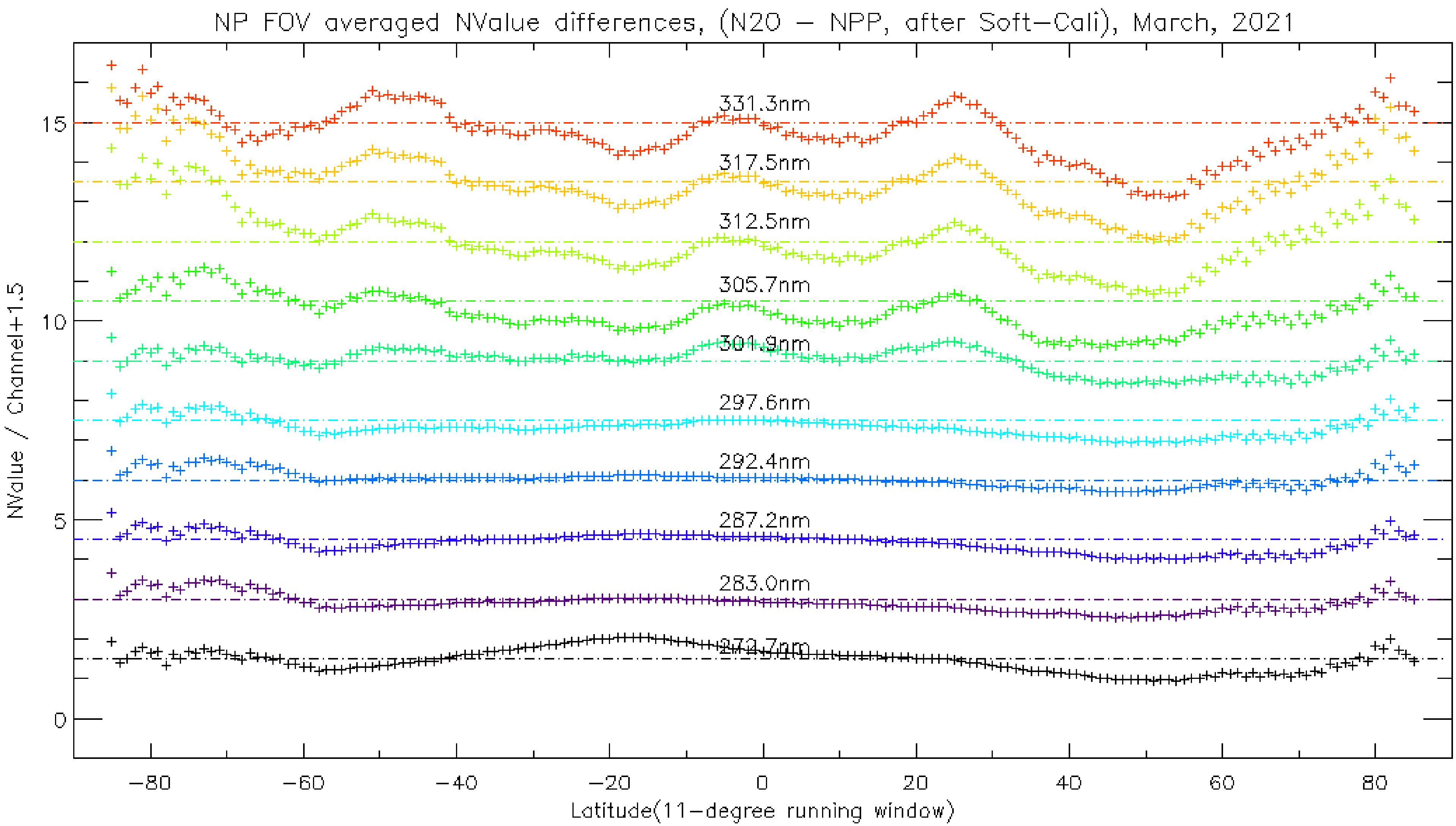
Layer 15 STAR Offline N20 versus



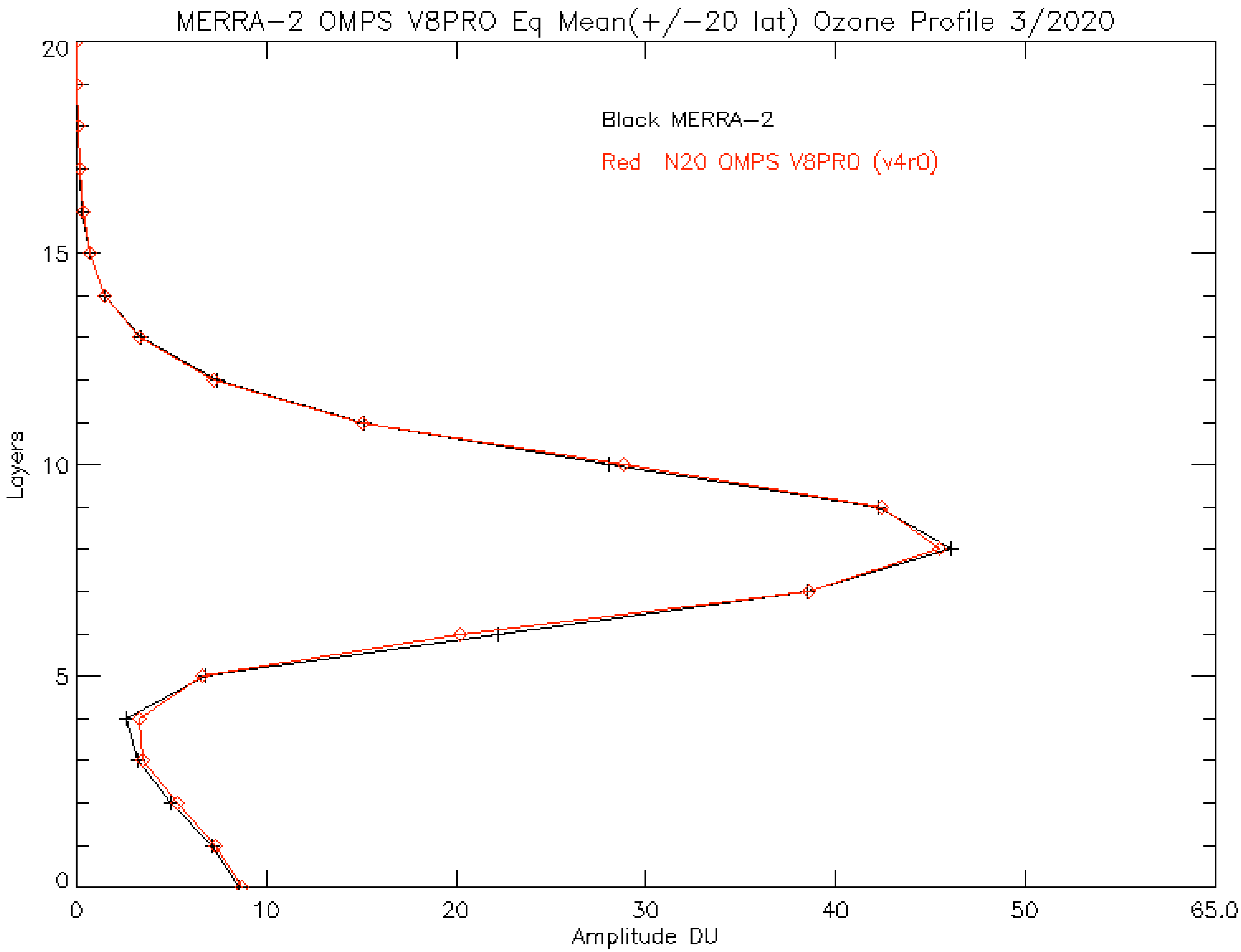
Layer 5 STAR Offline N20 versus N



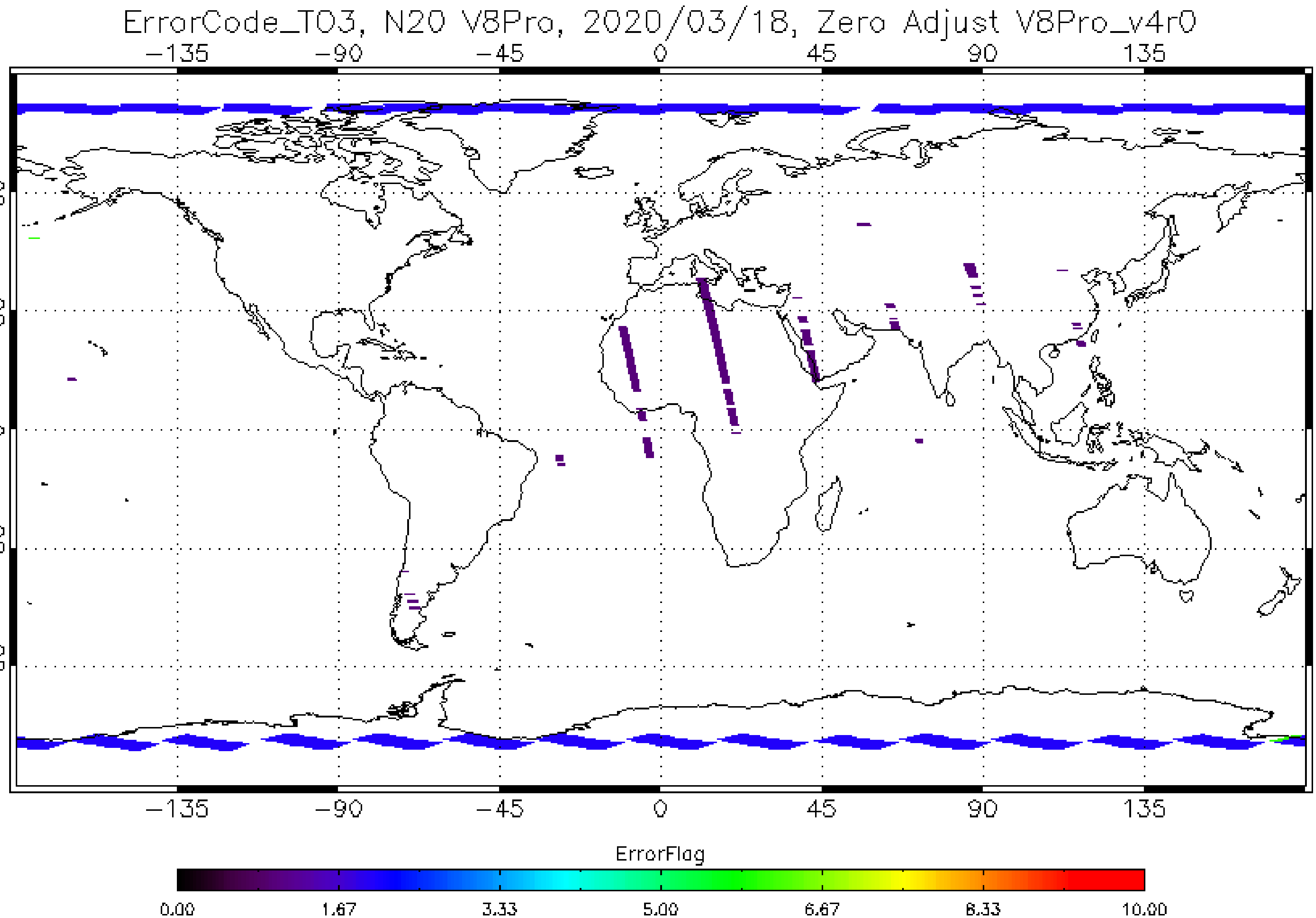
Offline N-Value Comparisons for 4/2021



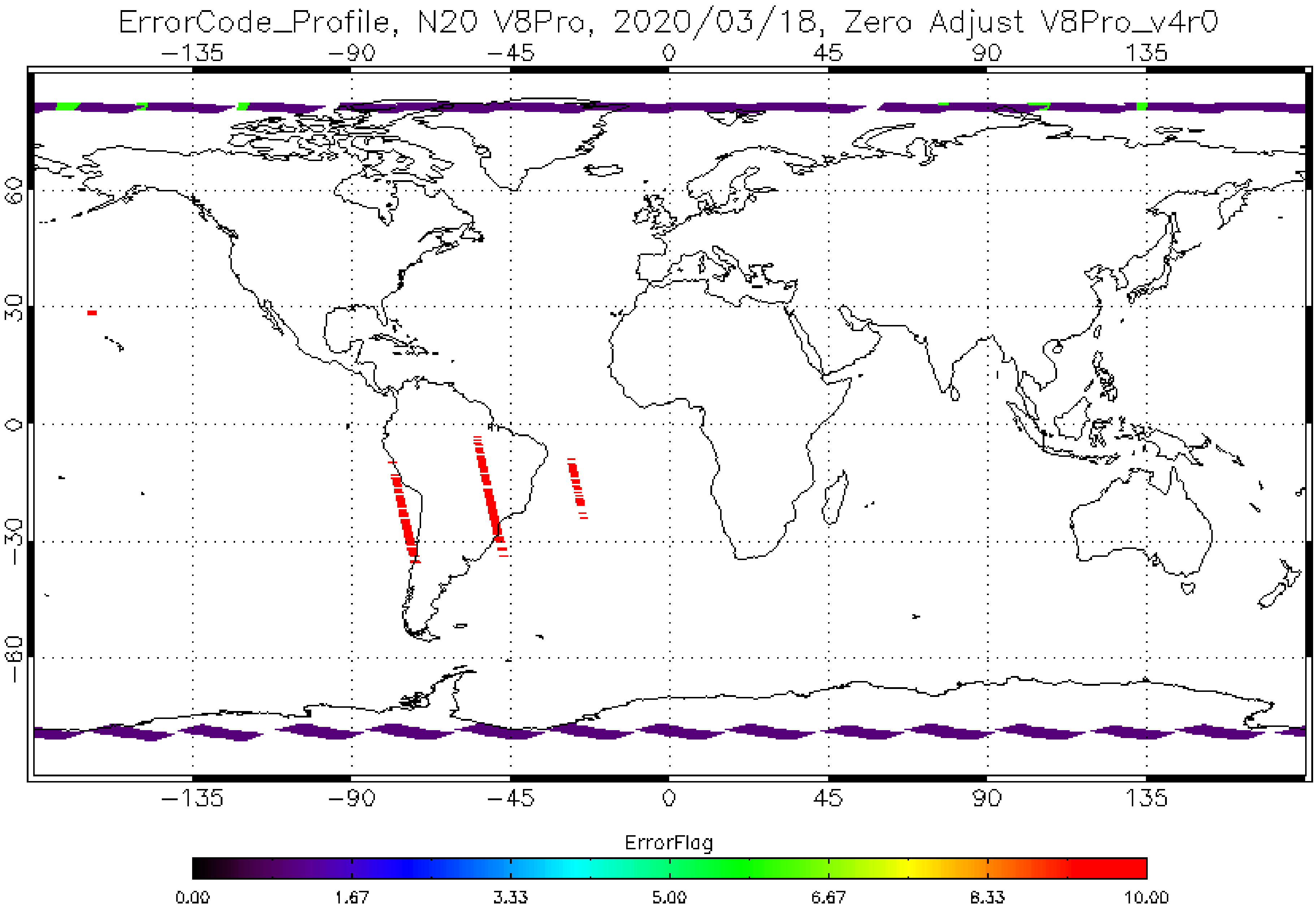
MERRA-2 Versus N20 Adjusted to NPP



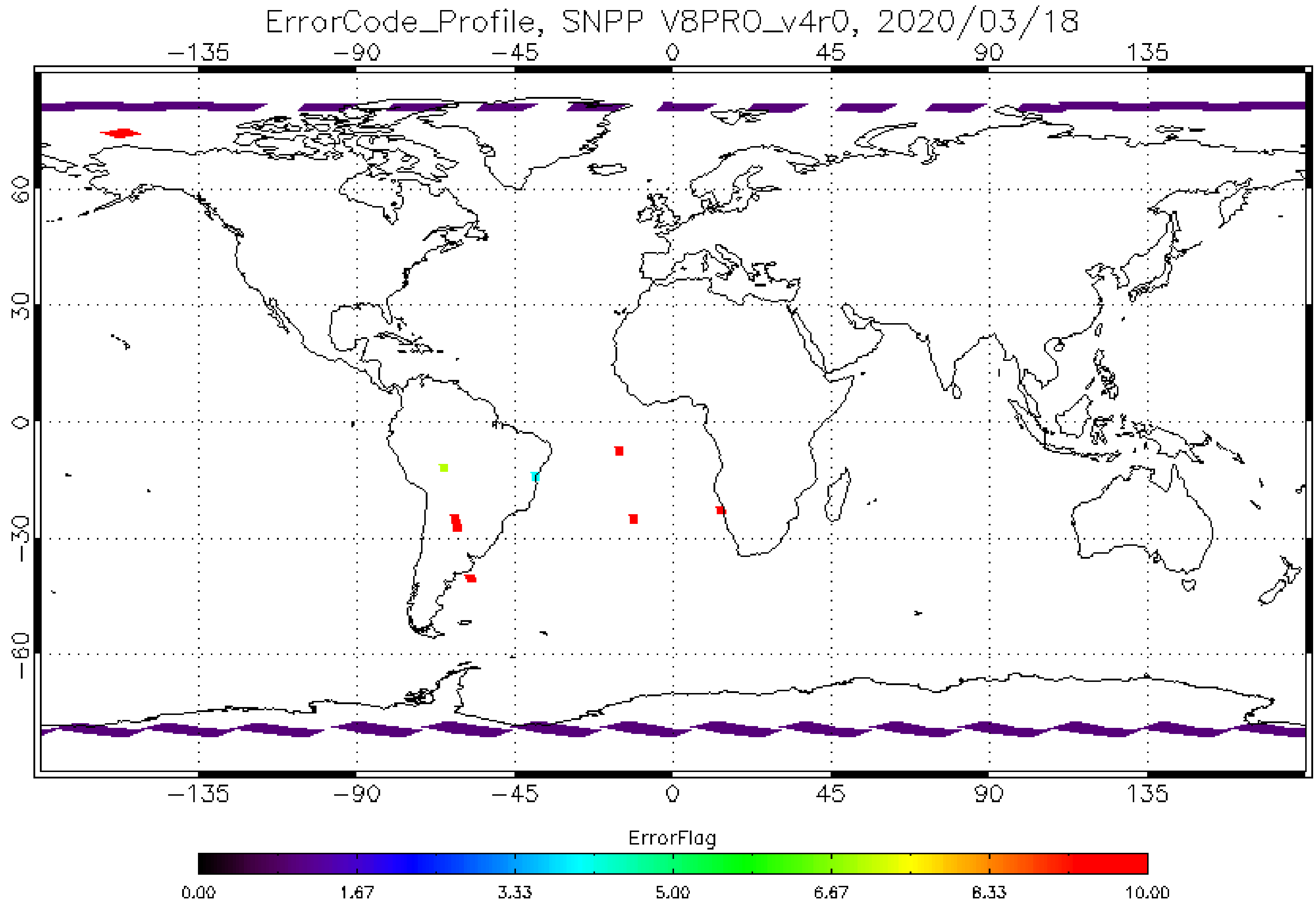
Total Ozone Error Flags N20



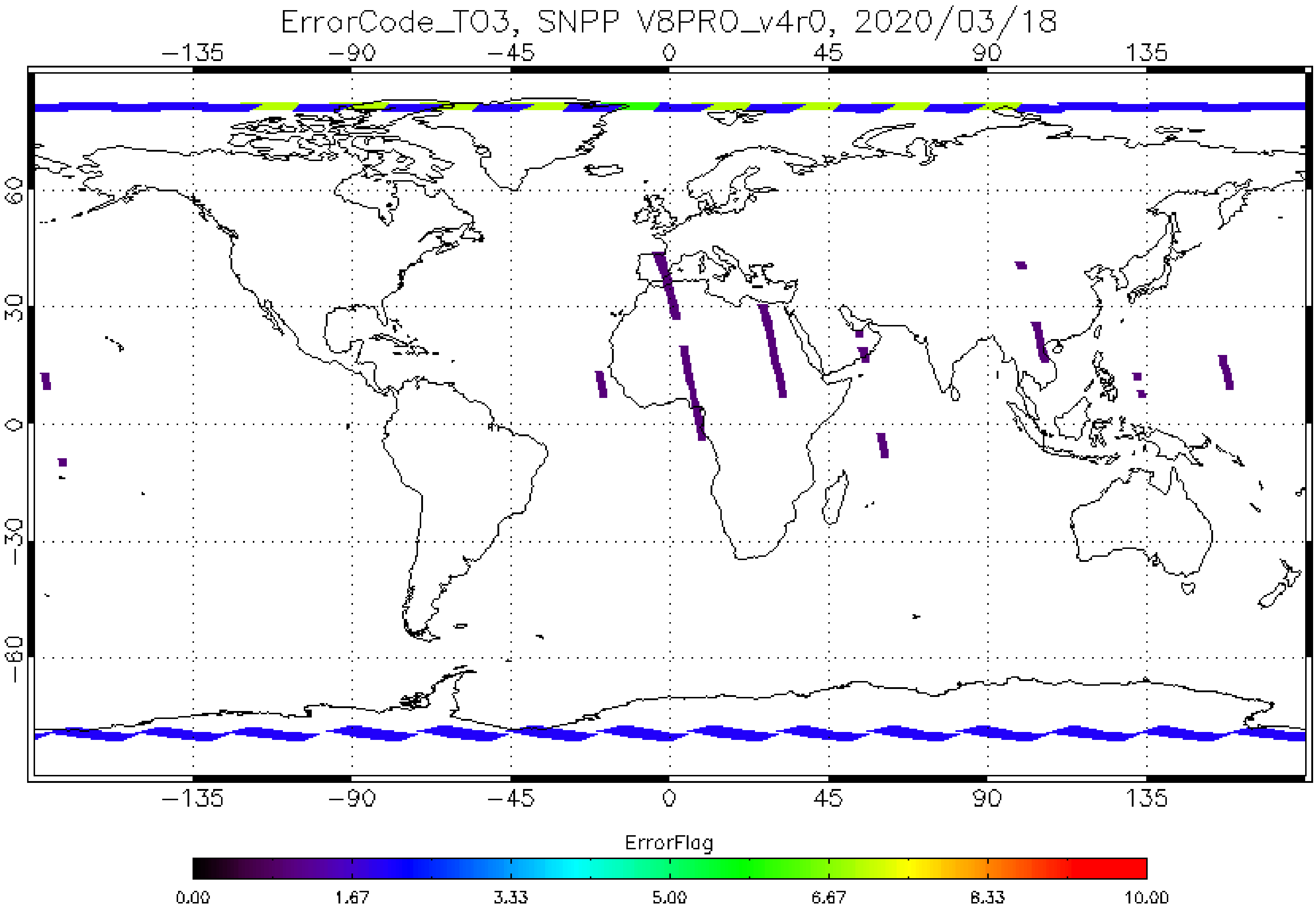
Profile Ozone Error Flags N20



Profile Ozone Error Flags NPP

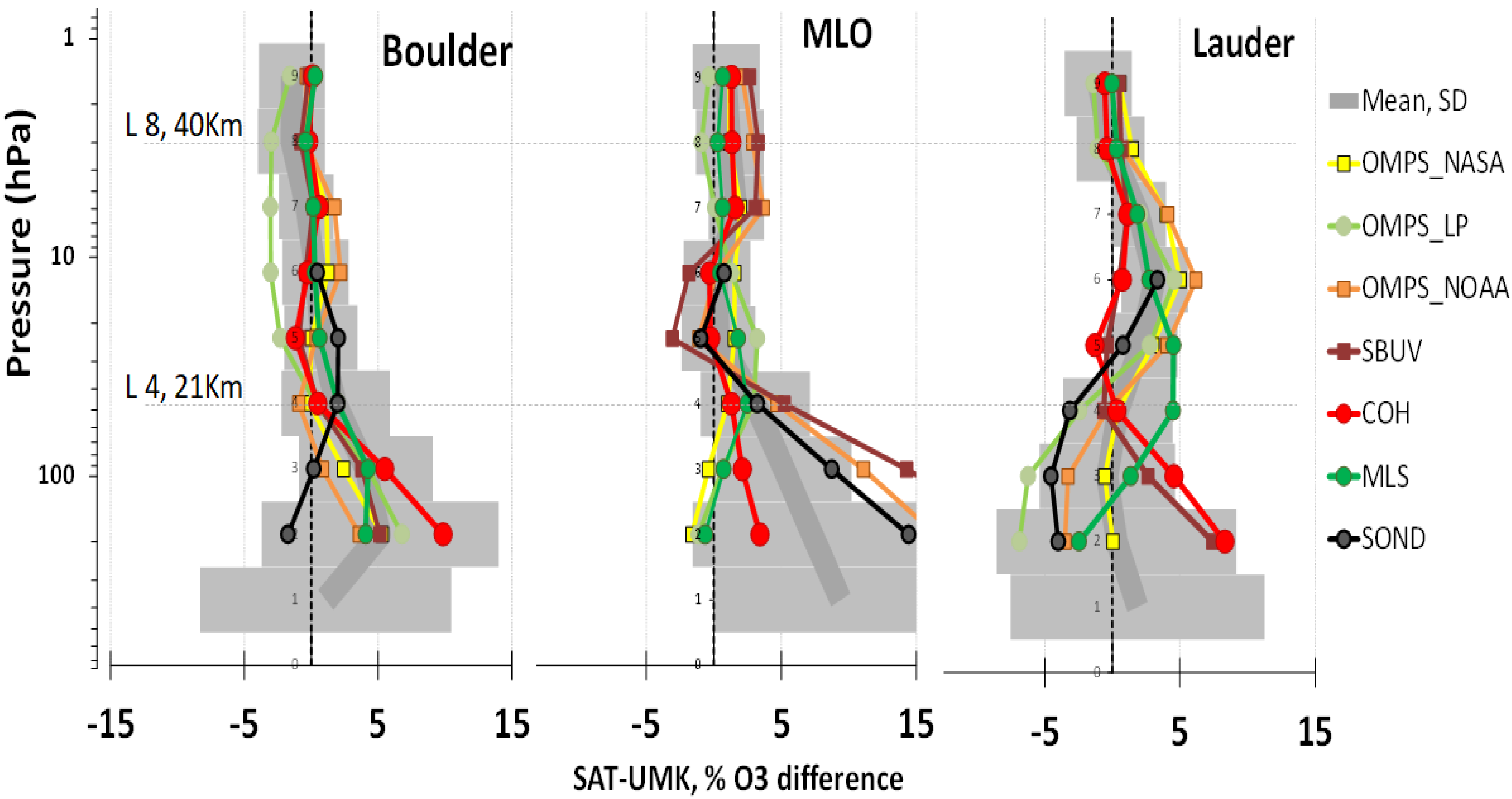


Total Ozone Error Flags NPP

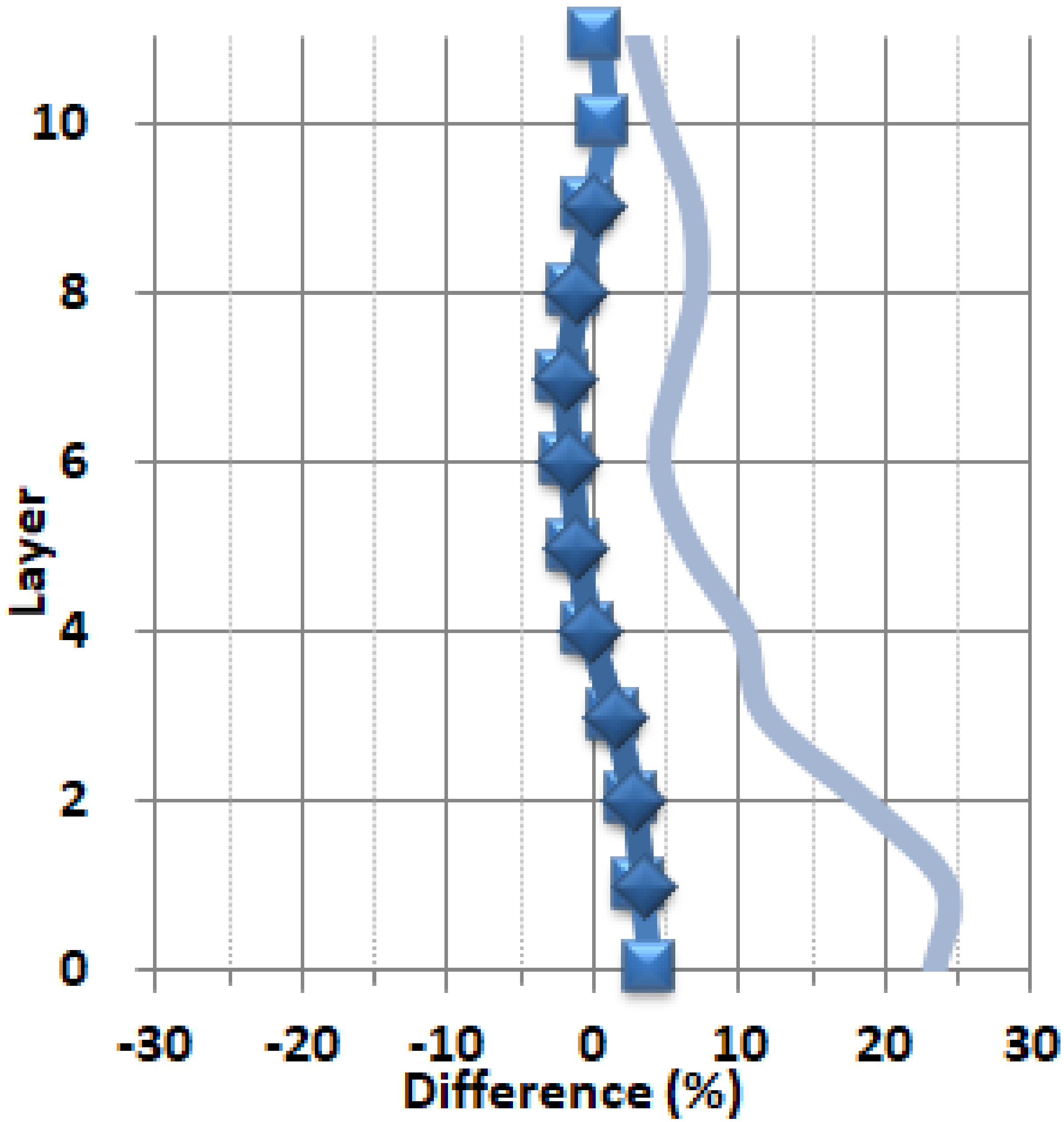


Umkehr profile algorithm optimized for stray light corrections,

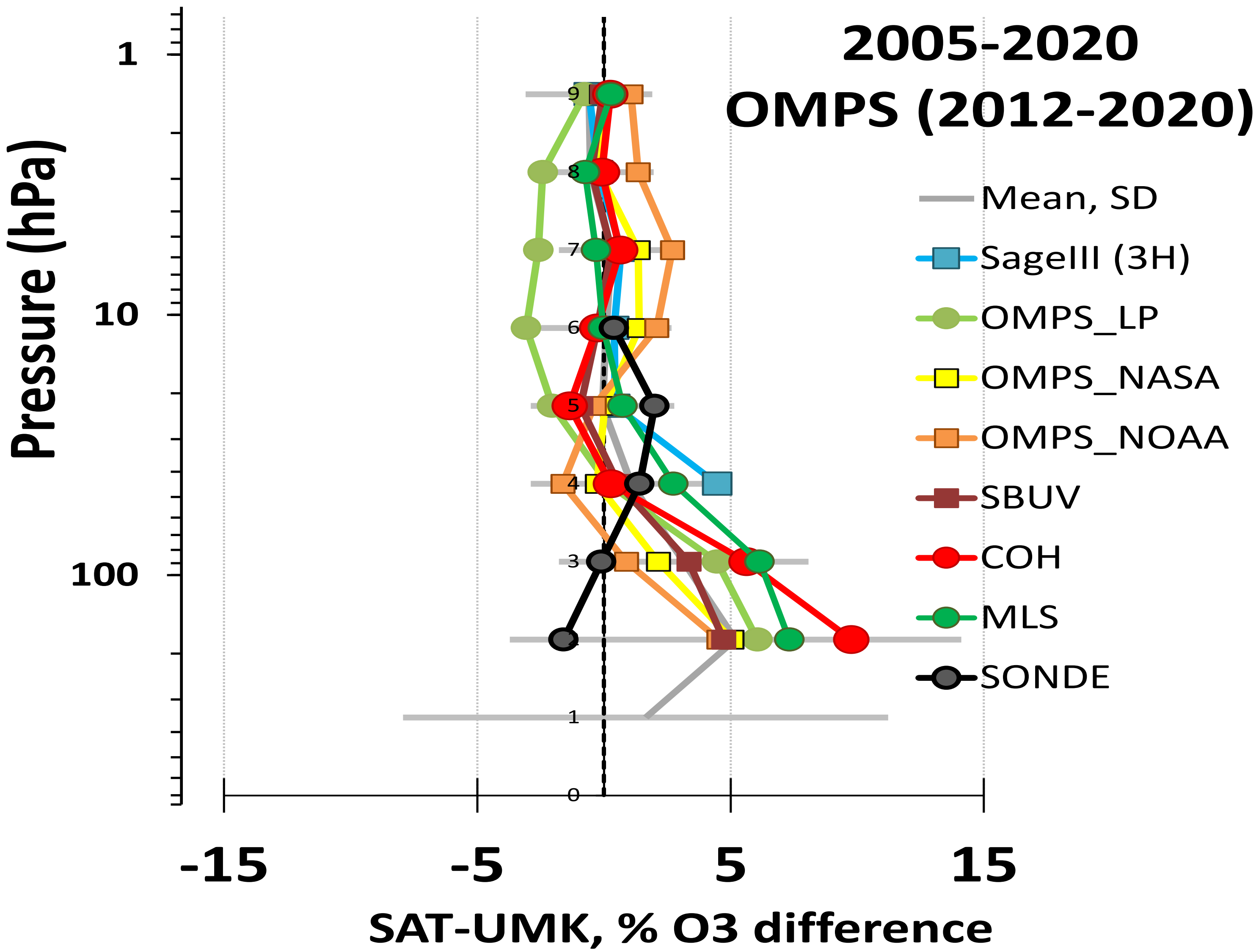
by I. Petropavlovskikh et al., in preparation 5/2021,



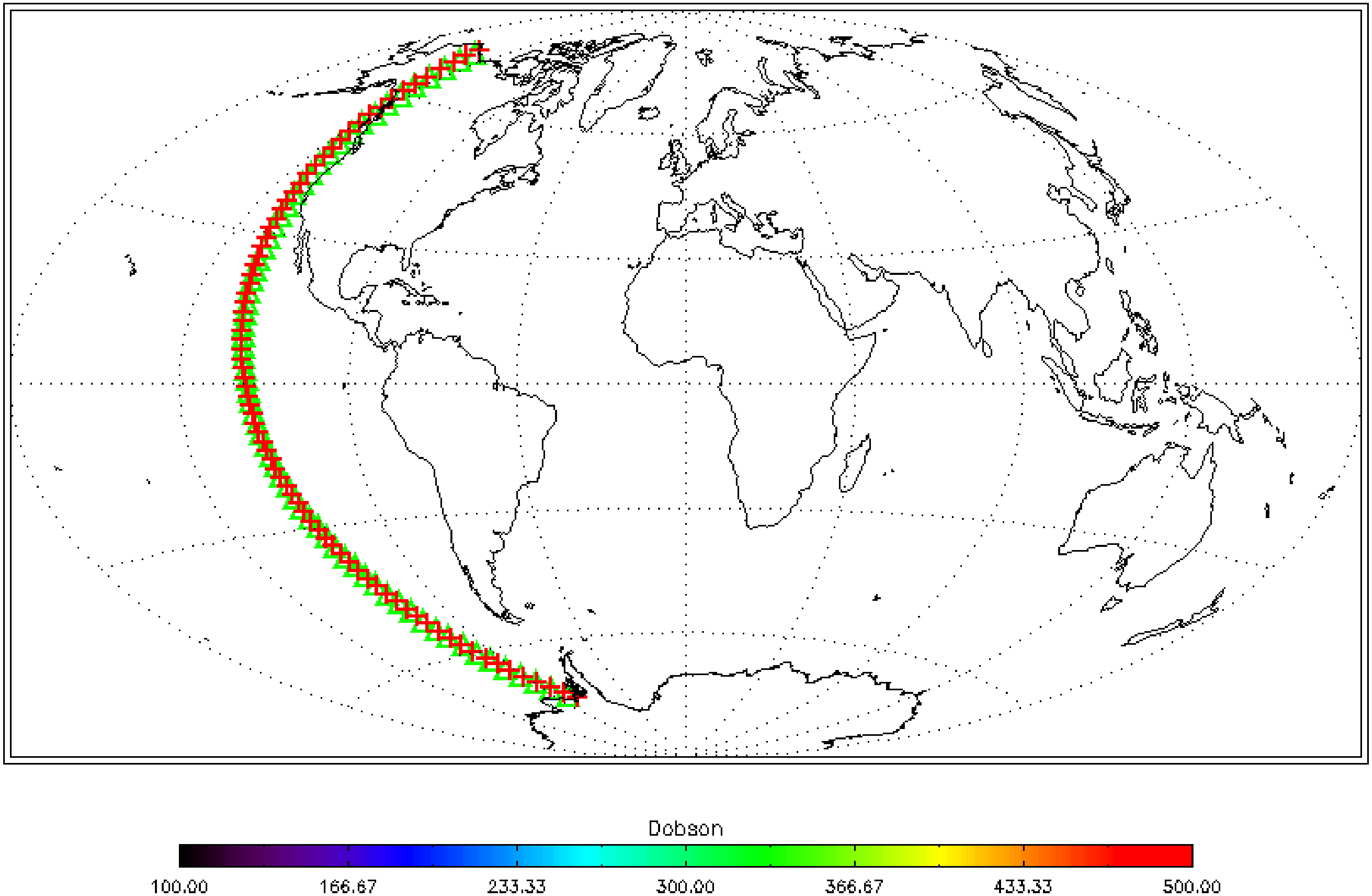
S-NPP V8Pro versus Boulder CO Umkehr



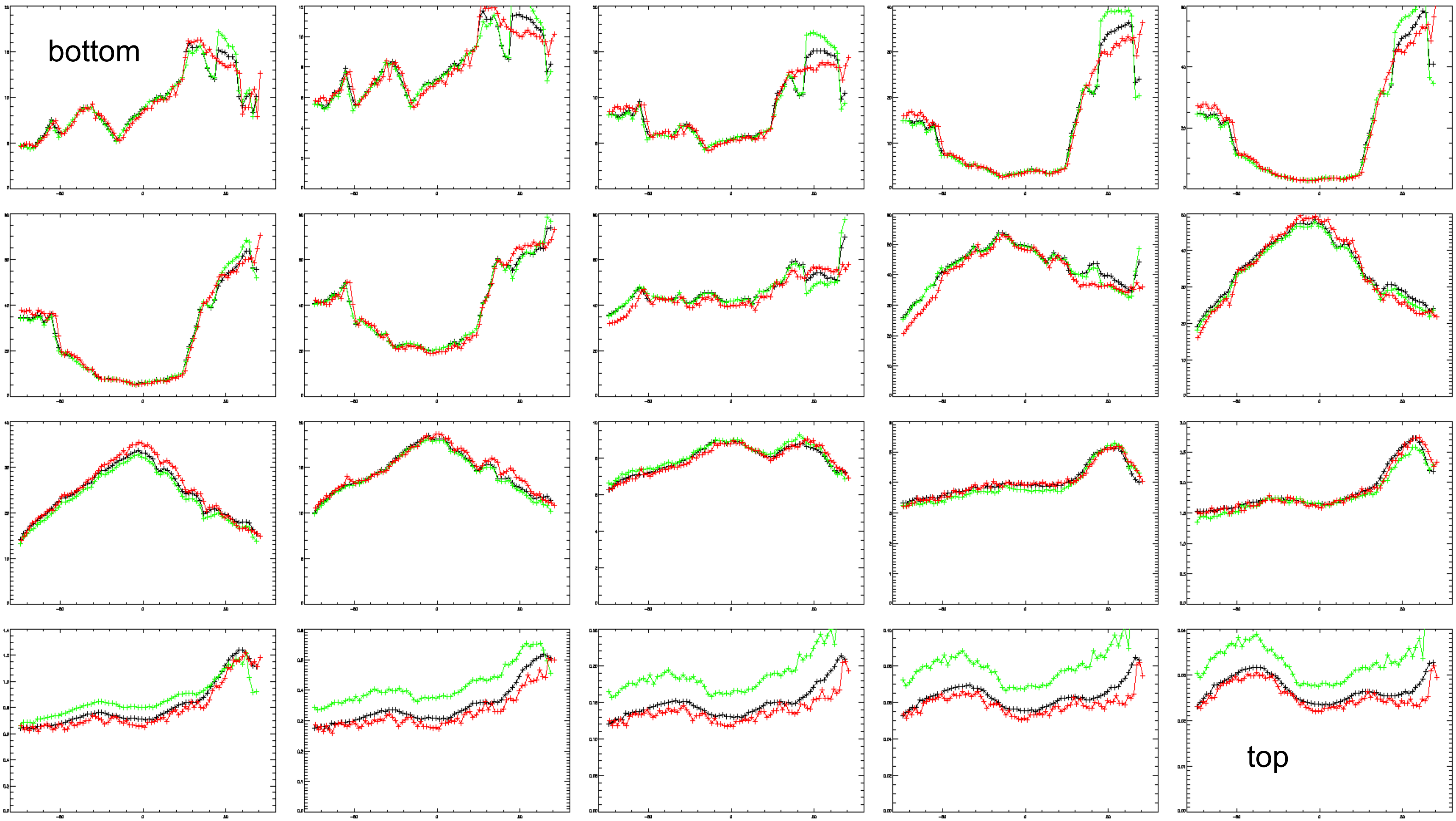
Boulder Umkehr Comparison



NOAA19(red) and OMPS(green) orbits within 1.5 hour and 100km in 20170217



Comparison of OMPS NP (NDE I&T and STAR Adj.) and NOAA-19 SBUV/2 2017/2/17

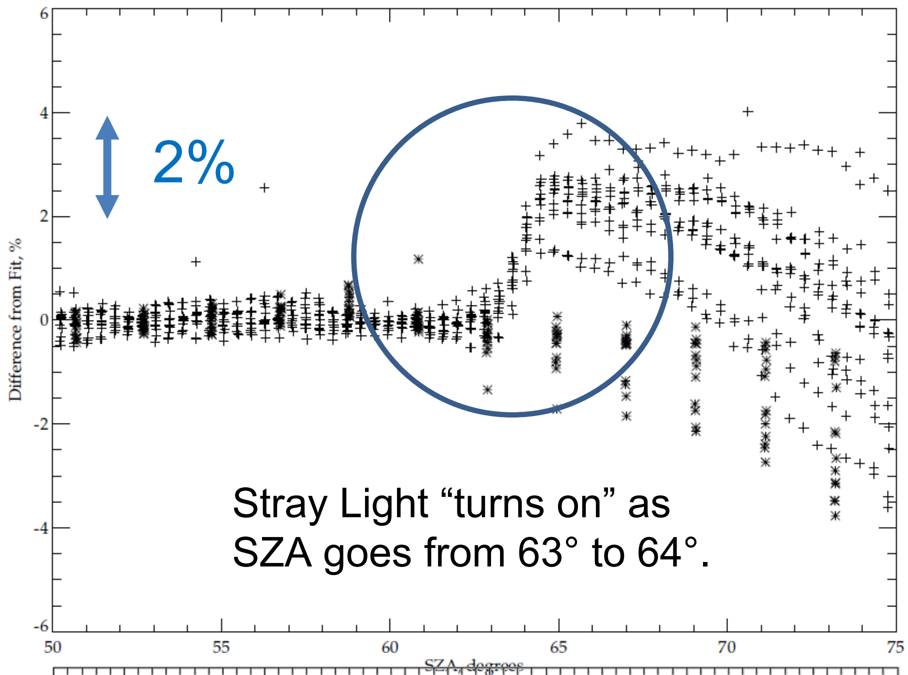


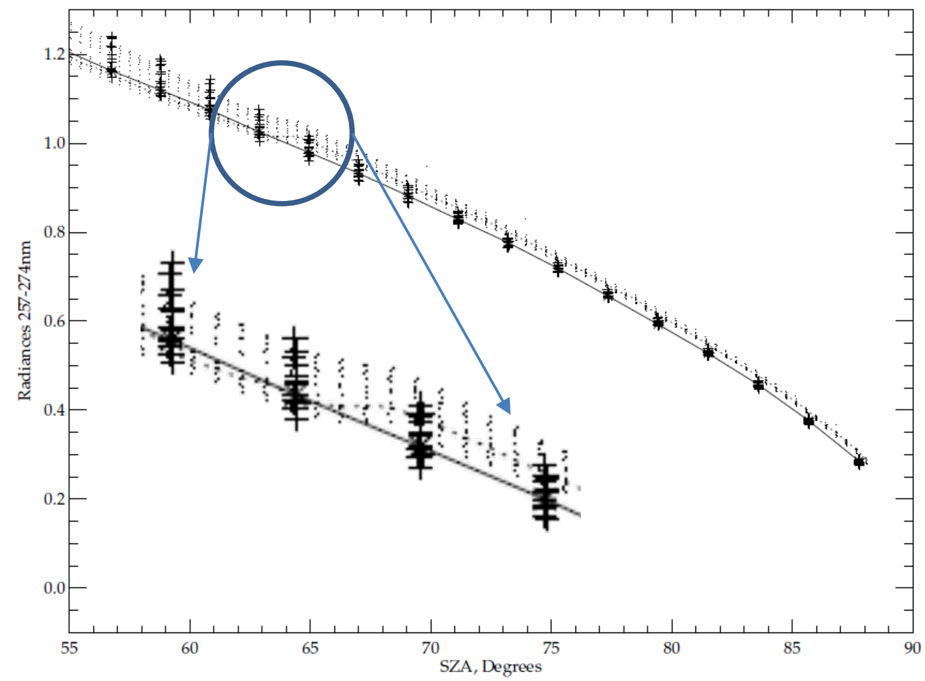
Layer Ozone in DU along orbital tracks for matchup orbits

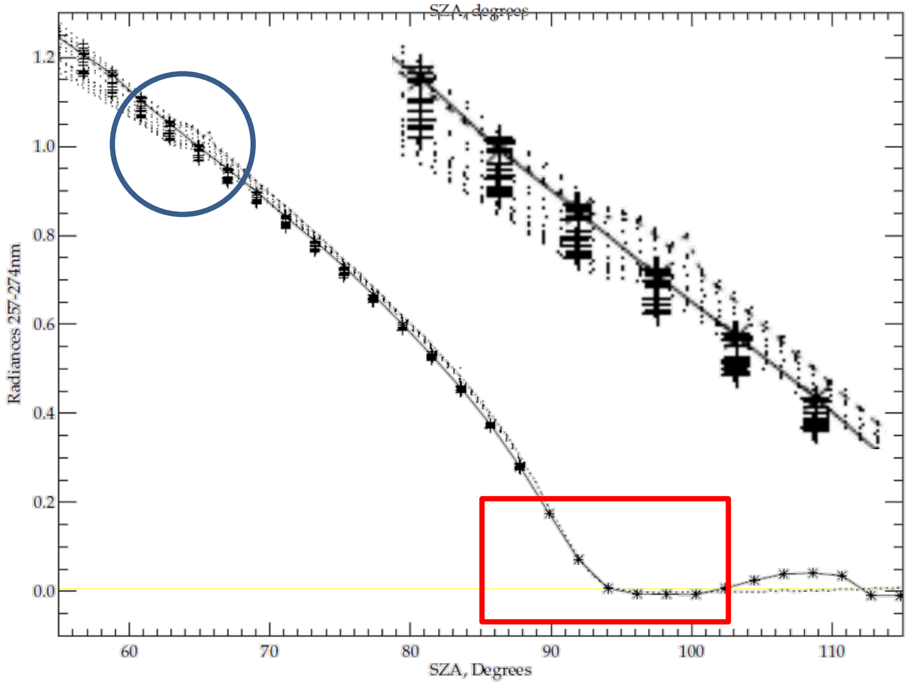
Focused looks at other topics and material from previous presentations

- N20 OMPS NP Solar Intrusion studies – impact and correction
- Forward model channel interpolations errors and path forward
- Intra-orbit wavelength shifts for OMPS NP
- Polarization sensitivity differences for N20 and NPP
- Previous material

Why don't the shorter channels agree?
In-Band Stray Light Discovery



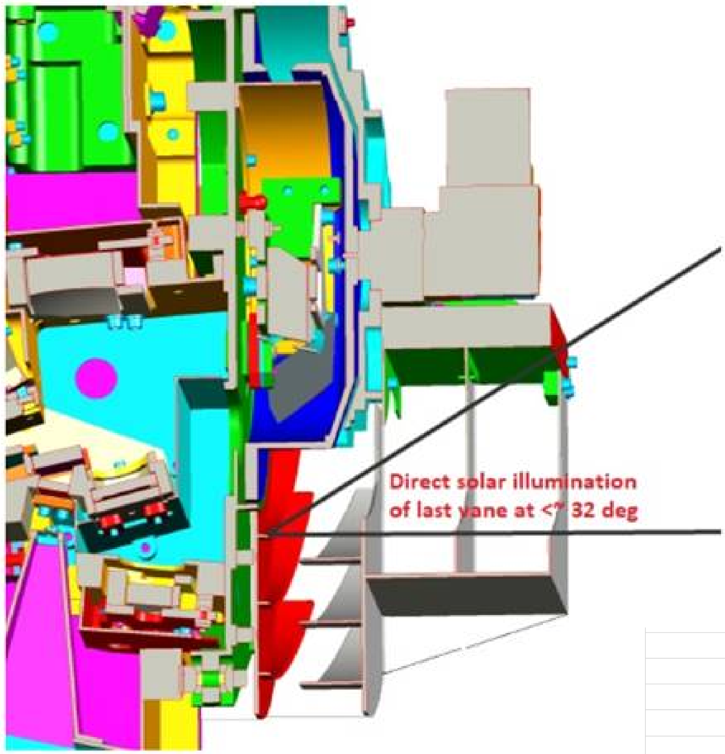


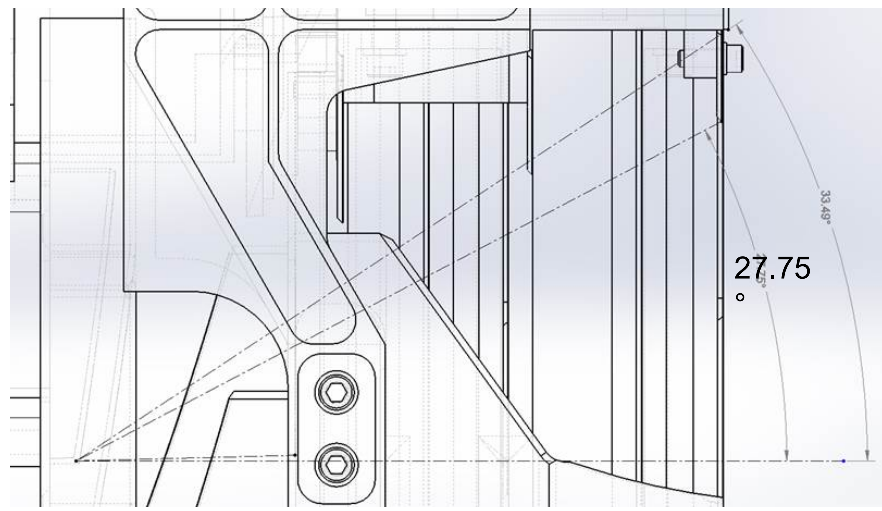


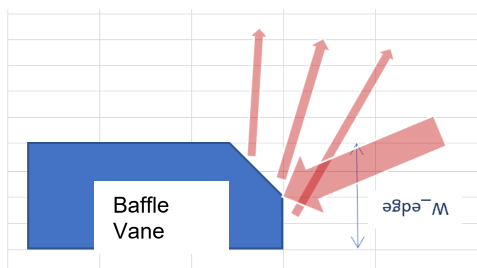
Comparisons of 41-wavelength (257 nm to 274 nm) radiance totals versus Solar Zenith Angles for April 2020 for the Northern Hemisphere.

Top Right: Radiance total versus SZA for April 13th, N20 Dots, NPP +.
Top Left: Differences with linear fits for April 13th N20 +, NPP *. Fit models use 50 < SZA < 63.
Bottom Left: Comparisons of total Radiances for days with EV360. N20 Dots for April 12th, NPP * for April 15th.

Additional path could illuminate baffle directly

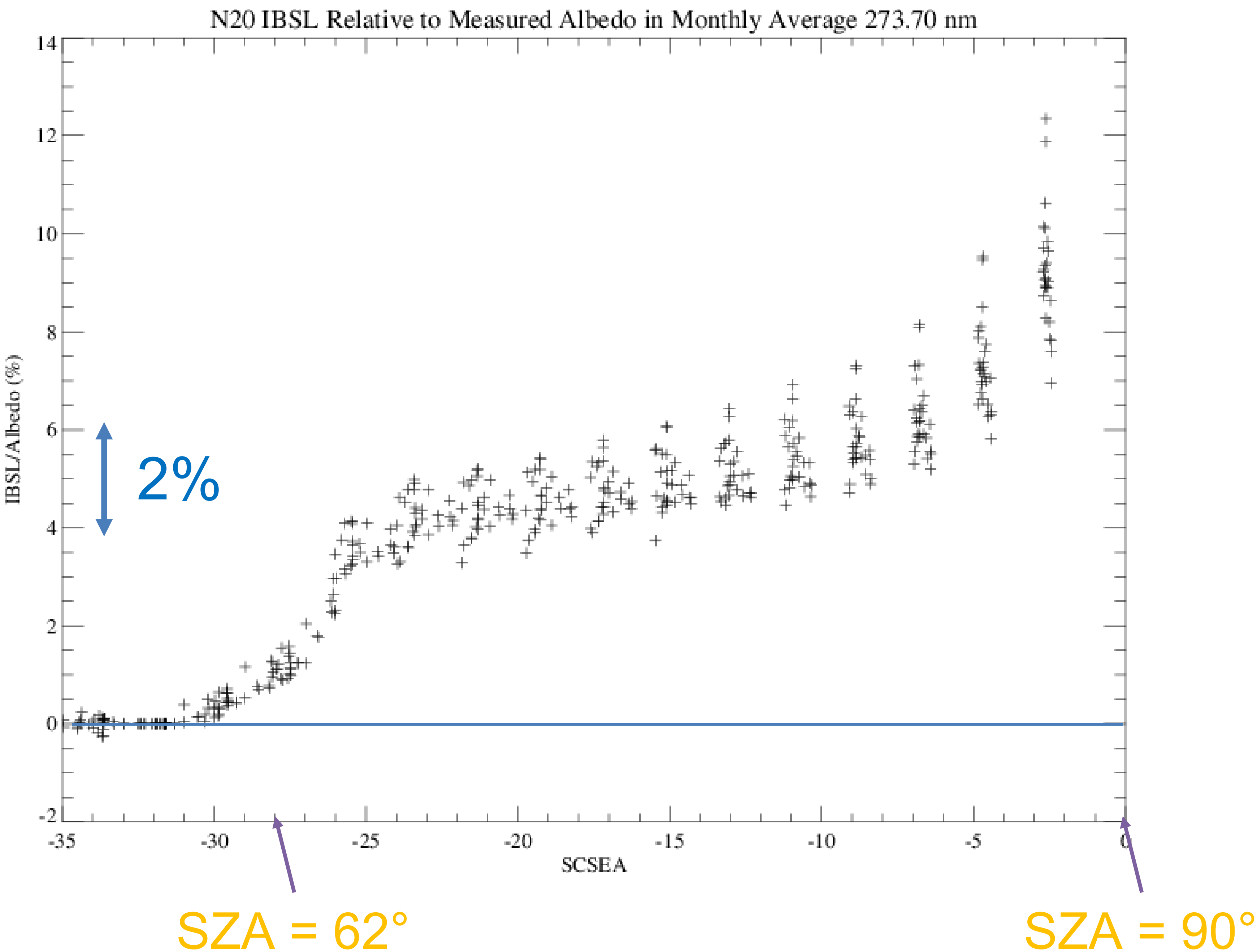






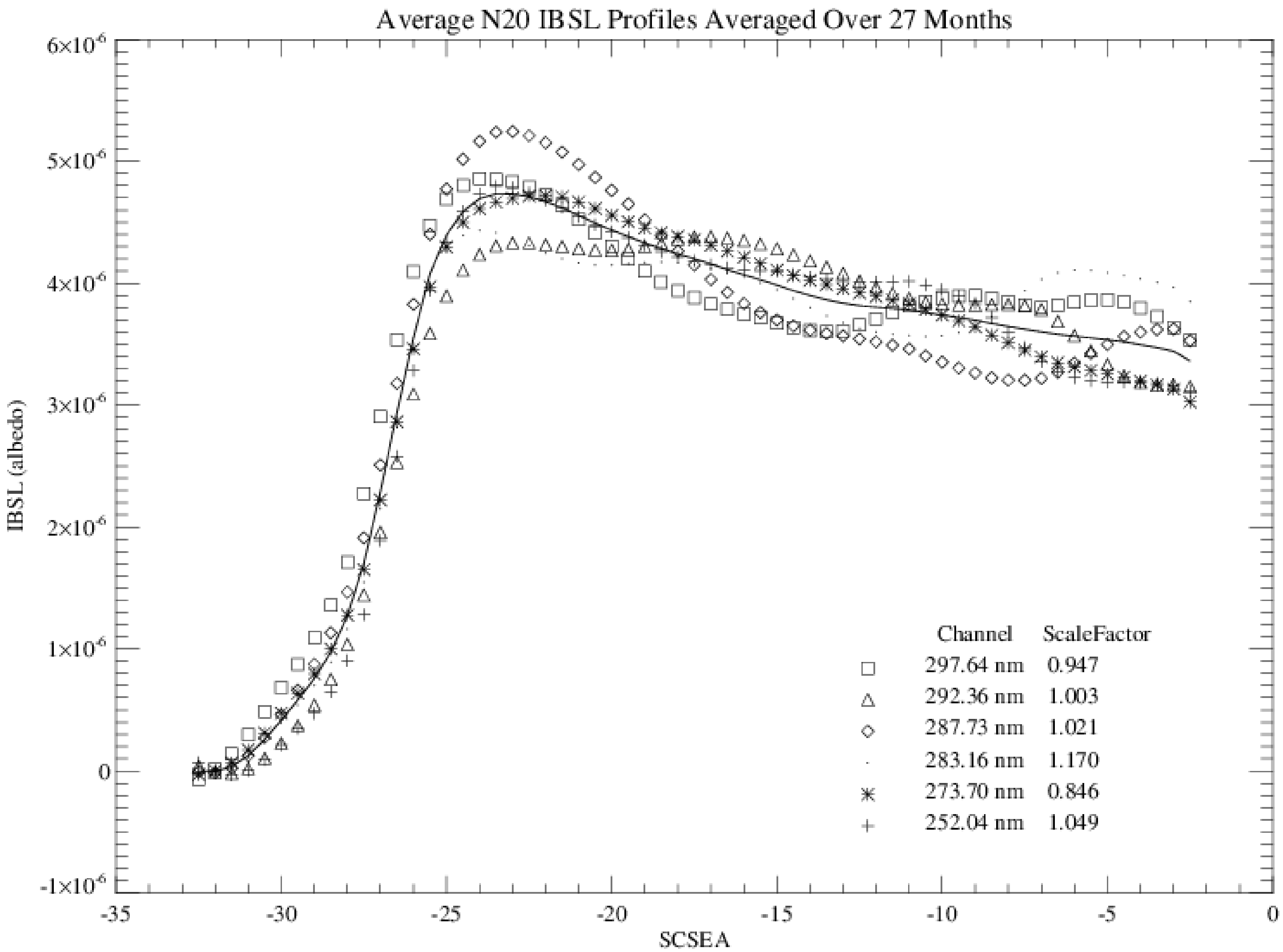
Slide from presentation by G. Jaross NASA-GSFC with analysis by BATC.
Note: Estimates of IBSL for J02 are at ¼ of the level observed for J01 inflight.
Note: One hypothesis is that this out-of-field stray light is produced by ghosts from a gap between the depolarization wedges.

Estimates of IBSL Error for 274 nm



Slide from presentation by L.-K. Huang NASA-GSFC (SSAI).

NOOA-20 OMPS Solar Intrusion IBSL SCSEA Dependence



- ❖ Use average of 6 short wavelength channels for SCSEA dependence profile.
- ❖ It can be scaled to different wavelength channels.
- ❖ Differences with each individual channel in the profile shape are less than 10% of the profile, which contributes less than 1% of albedo calibration.

Model developed by L.-K. Huang (SSAI) for NASA GSFC

Solar Straylight Model & Coefficients

NOAA-20 OMPS Nadir Profiler In-Band Stray LightCharacterized with comparison of a priori profile residues between SNPP and N20IBSL is given in terms of albedo values:

```
IBSL = AvgPrfile(scsea)/{AvgScaleFactor(lamda)*
       [1+DriftRate(lamda)*(YearFrac-y18m2)]*
       [C0+C1*(scsaa-scsaa21)]}
```

where scsea is the Spacecraft Centered Solar Elevation Angle in degrees near the North Pole, scsaa is the spacecraft Centered Solar Azimuth Angle at SCSEA=-2.5 degrees near the North terminator.

Wavelength (nm)	252.04	273.70	283.16	287.73	292.36	297.64
AvgScaleFactor	1.0868	0.7949	1.0940	0.9960	0.9860	0.9232
DriftRate (per year)	-0.0888	0.0860	0.0255	0.0452	0.0169	0.0287

y18m2 2018.1383

SCSAA Dependence coefficients C0 and C1, scsaa21 1.01454 0.0156717 21.0

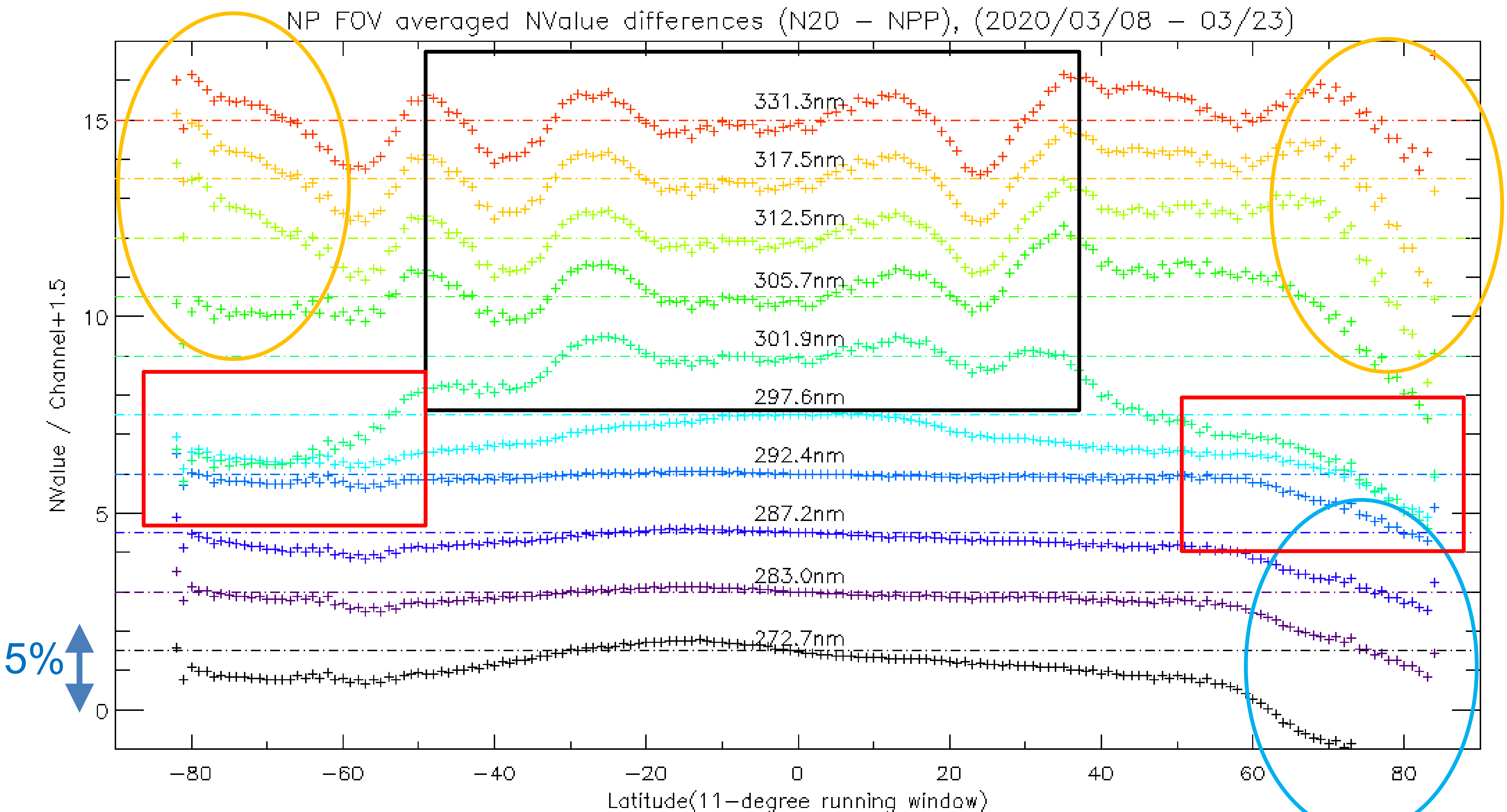
SCSEA	AvgPrfile	SCSEA	AvgPrfile	SCSEA	AvgPrfile	SCSEA	AvgPrfile
-32.5	-3.57012e-10	-32.0	-2.46618e-09	-31.5	3.71044e-08	-31.0	1.25923e-07
-30.5	2.57902e-07	-30.0	4.17625e-07	-29.5	5.83126e-07	-29.0	7.57621e-07
-28.5	9.77070e-07	-28.0	1.27436e-06	-27.5	1.70243e-06	-27.0	2.29045e-06
-26.5	2.93787e-06	-26.0	3.55427e-06	-25.5	4.07955e-06	-25.0	4.39430e-06
-24.5	4.58811e-06	-24.0	4.69329e-06	-23.5	4.73407e-06	-23.0	4.73334e-06
-22.5	4.70880e-06	-22.0	4.66781e-06	-21.5	4.61961e-06	-21.0	4.55450e-06
-20.5	4.49243e-06	-20.0	4.43471e-06	-19.5	4.38297e-06	-19.0	4.32941e-06
-18.5	4.28213e-06	-18.0	4.23993e-06	-17.5	4.20200e-06	-17.0	4.15617e-06
-16.5	4.11063e-06	-16.0	4.06831e-06	-15.5	4.02767e-06	-15.0	3.98455e-06
-14.5	3.93823e-06	-14.0	3.89867e-06	-13.5	3.86421e-06	-13.0	3.83727e-06
-12.5	3.81579e-06	-12.0	3.80310e-06	-11.5	3.79163e-06	-11.0	3.78188e-06
-10.5	3.75885e-06	-10.0	3.73905e-06	-9.50	3.71801e-06	-9.00	3.69786e-06
-8.50	3.66910e-06	-8.00	3.64524e-06	-7.50	3.62236e-06	-7.00	3.60143e-06
-6.50	3.58109e-06	-6.00	3.56617e-06	-5.50	3.55148e-06	-5.00	3.53569e-06
-4.50	3.51905e-06	-4.00	3.49583e-06	-3.50	3.47206e-06	-3.00	3.44312e-06
-2.50	3.36228e-06						

Model developed by L.-K. Huang (SSAI) for NASA GSFC

Questions from Alisa

- Here is what I'd like to review and hope you can give a status update so that we'll know how to proceed with our planning.
- In one of your recent OMPS EDR Science Team Meetings for the slide deck, Compare_effects202003.ppt, you mentioned that your team had found a one-line code error responsible for much of the remaining differences between the NPP and N20 N-values for the middle channels and expected that the error would account for 70% of the remaining differences. I'm curious on how much time you'll need to demonstrate this update when comparing NPP and NOAA-20 for ~1 year of data.
- On slide #9 of your Validated Review Dry Run, you show that NOAA-20 measurement accuracy was greater than 10% versus SNPP, what is this accuracy now (based on correcting the errors you've discovered and implementing all the other updates listed on slide #2 of the Compare_effects202003.ppt)?
- At the time of the dry run ADR9308: Inconsistencies between S-NPP and NOAA-20 OMPS SDRs was open/in analysis. Has this been concluded or is it still open? If it is still opened, is it critical to get it resolved prior to pursuing the validated maturity review?
- For slide #16 of your validated maturity review dry run slides, the following features remained: S-NPP / NOAA-20 differences in the V8Pro channel radiance/irradiance ratios for 1) Differences in the shorter wavelength channels in the Northern Hemisphere. 2) Differences in the longer wavelength channels (302 nm and 306 nm from the NP and 313 nm, 318 nm and 331 nm from the NM) 3) Differences with latitude for the mid-ranges wavelengths. (I assume that item #3 is mostly resolved based on the code error addressed in bullet #1. However, I'm not sure if this is completely resolved) Please let me know what aspects of these 3 differences still remain or if they've been minimized enough to improve the measurement accuracy to within the requirements.
- Do you expect that you would have improved results for slide #54 of your dry run slides which showed that N-values between S-NPP and NOAA-20 disagreed over middle/high latitude region following adjustments to force agreement in the Equatorial zone (based on soft calibration).
- If we have good outcomes on these issues whereby SNPP and NOAA-20 comparisons demonstrate that NOAA-20 is within specs/requirements, I think we can bypass the ground station comparison. Also, if any of this work is not complete but forthcoming, please let me know when you could have these items completed. We'd like to confirm that the product is within specs either based on SNPP and NOAA-20 evaluation or NOAA-20 and ground station evaluation prior to scheduling dry run and validated maturity review.

11-degree running means of N-Value Differences for N20 – NPP Versus Latitude for V8Pro Channels Channels are offset by 1.5*(channel #)

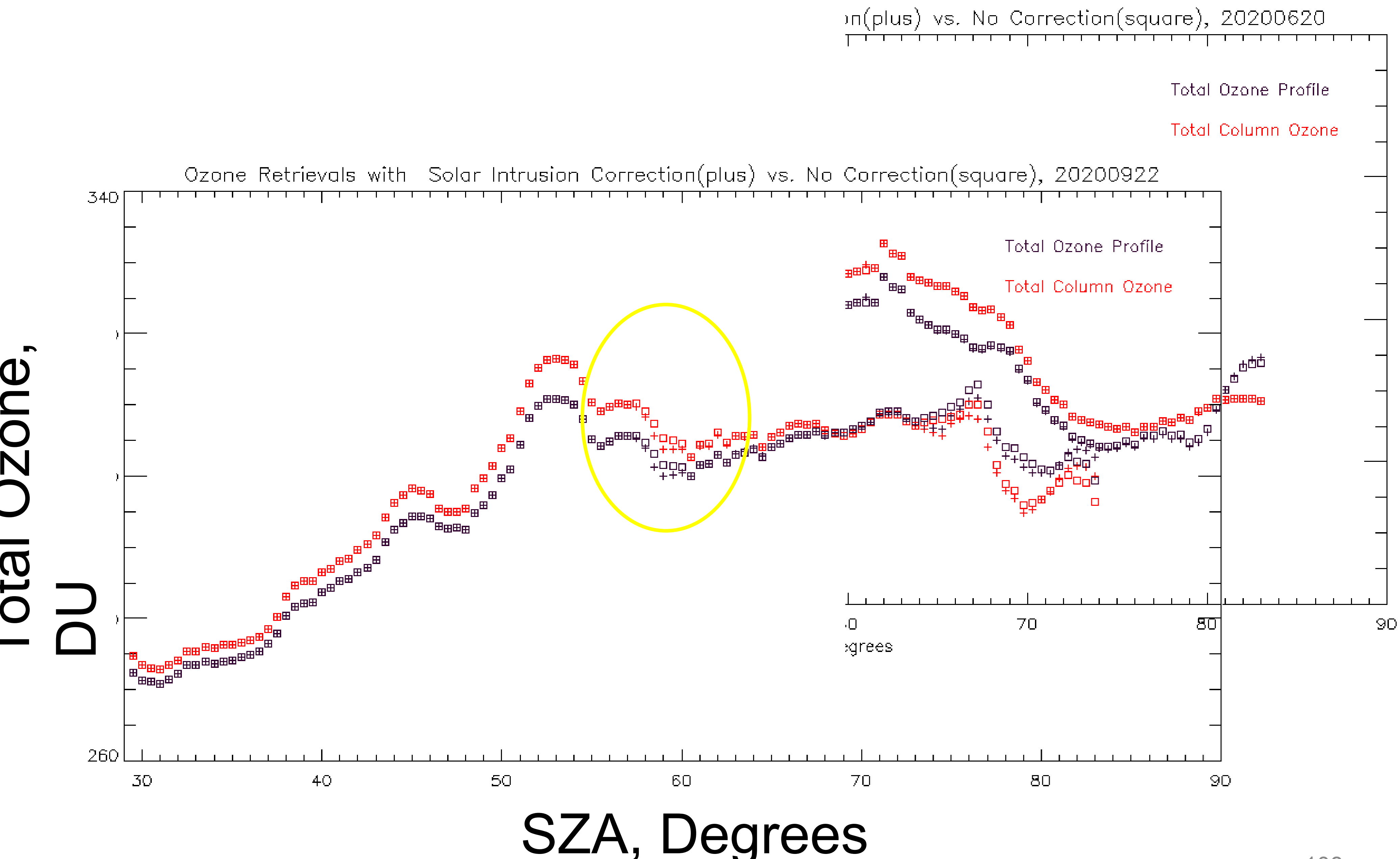


Latitude, Degrees North

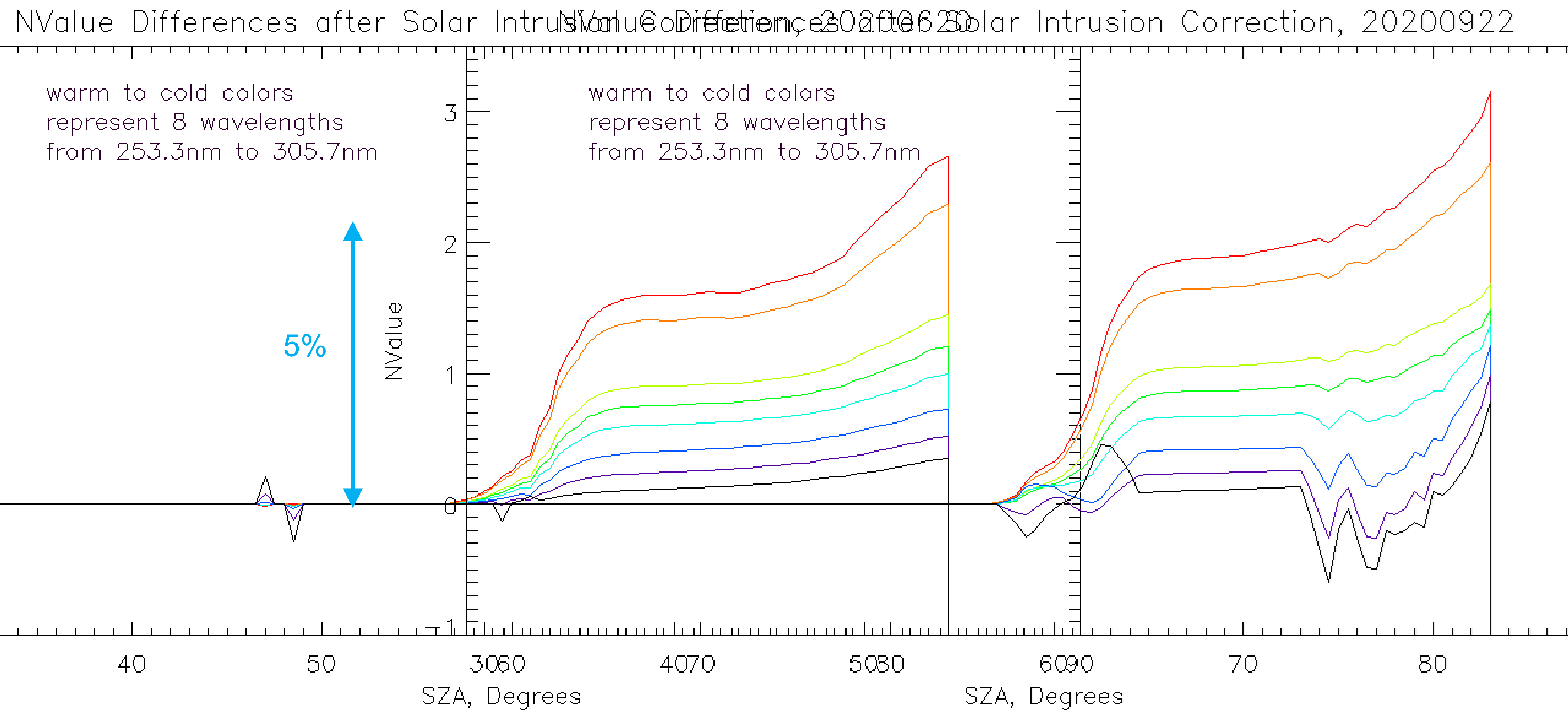
Case Study Solar Intrusion Correction

Z. Zhang

Total Ozone check on the matchup success

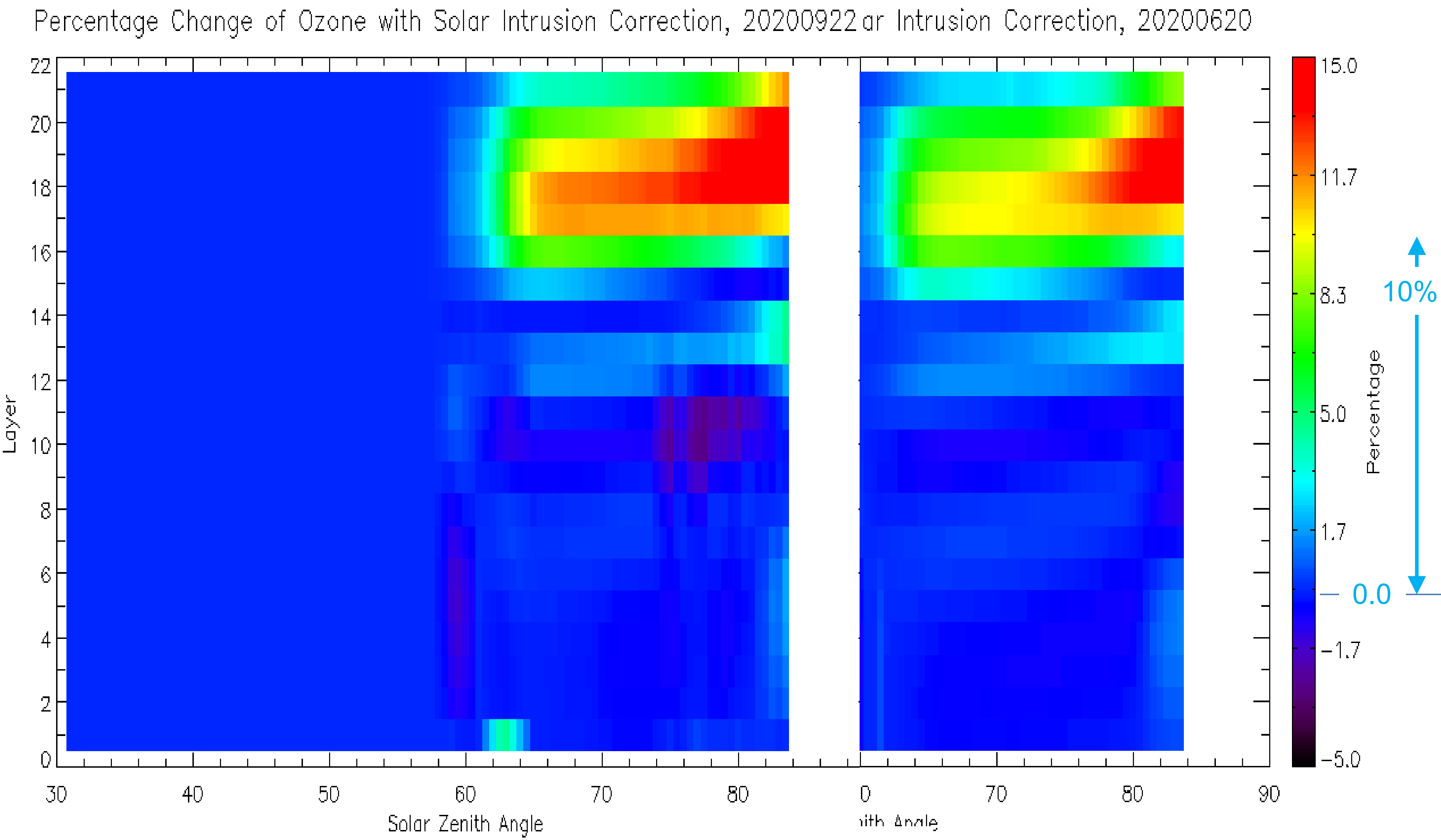


Changes in N-values for OMPS NP V8Pro Chann



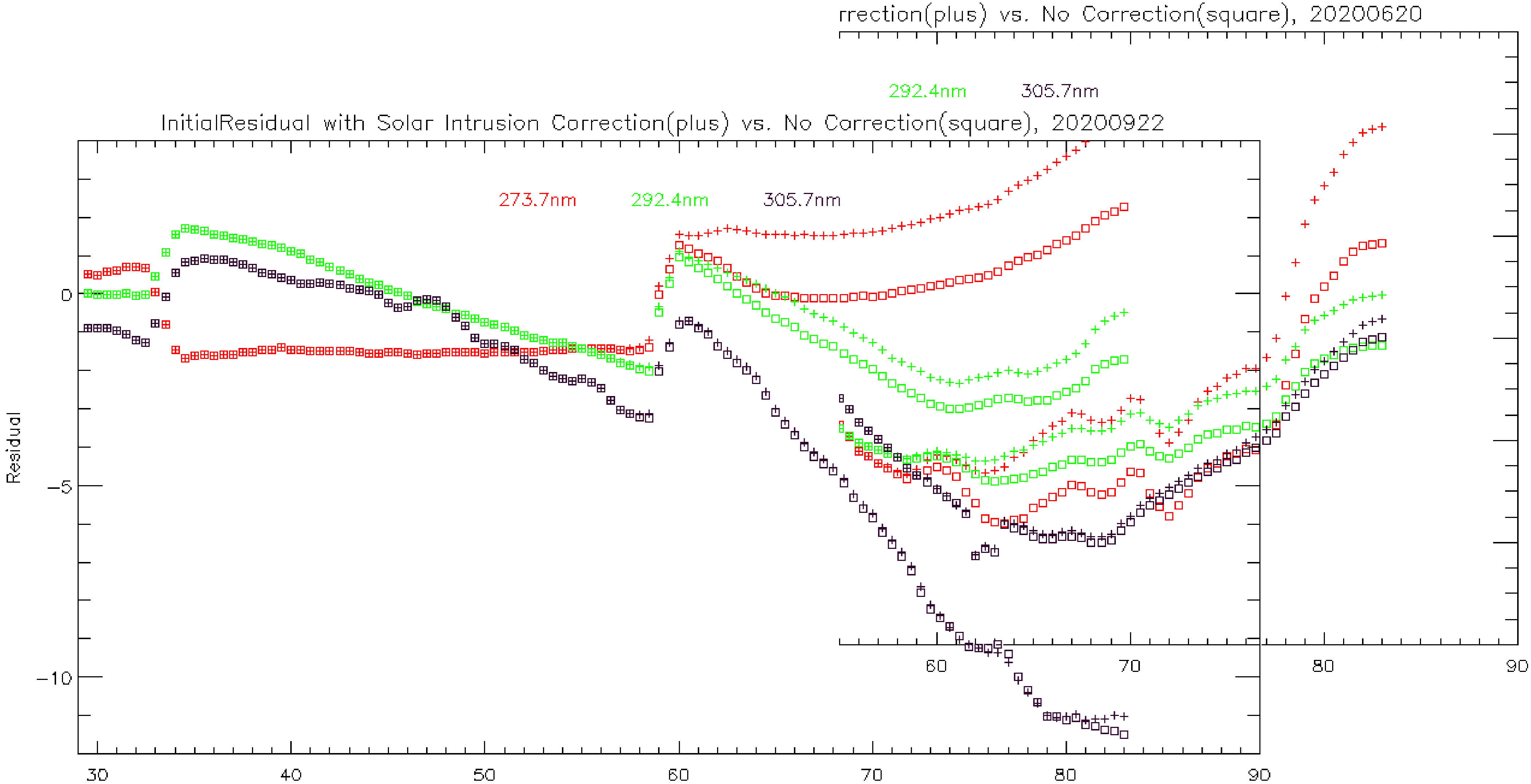
SZA, Degrees

Changes in the Northern Hemisphere Layer Ozone from the Correction



SZA, Degrees

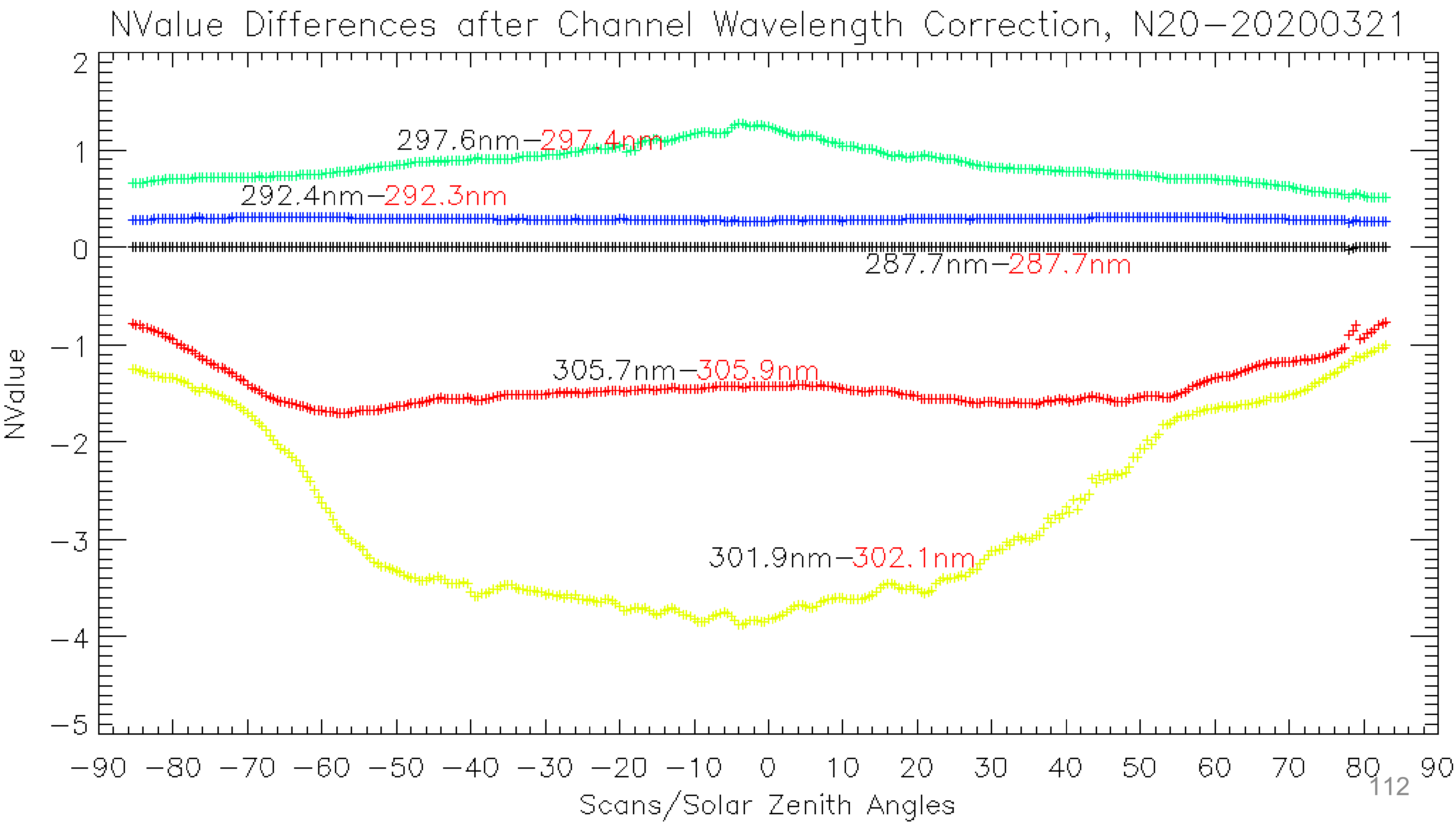
Changes in the Initial Residuals



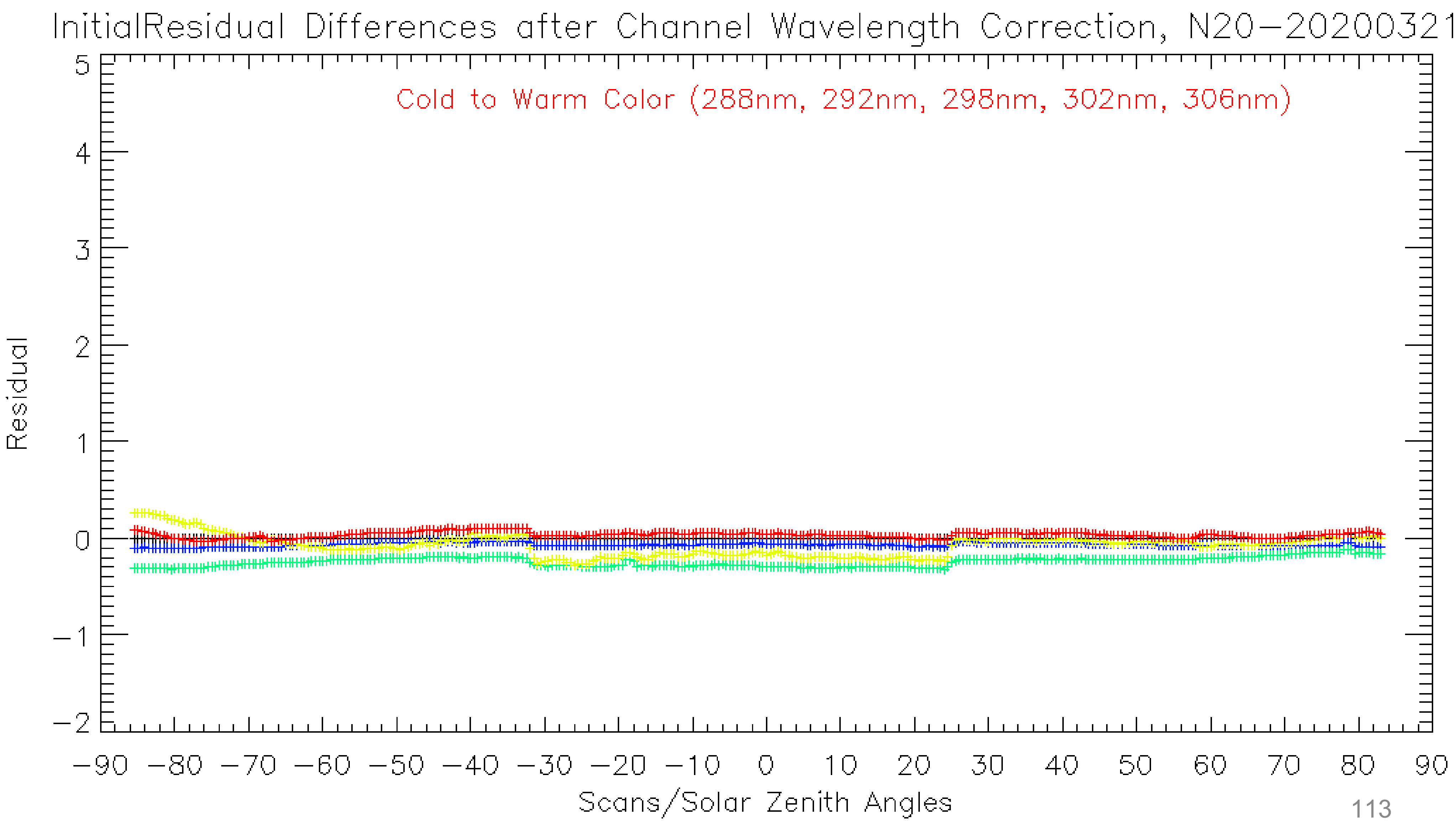
SZA, Degrees

Case study of effects of the channel interpolation & wavelength shift for V8PRO (1/4)

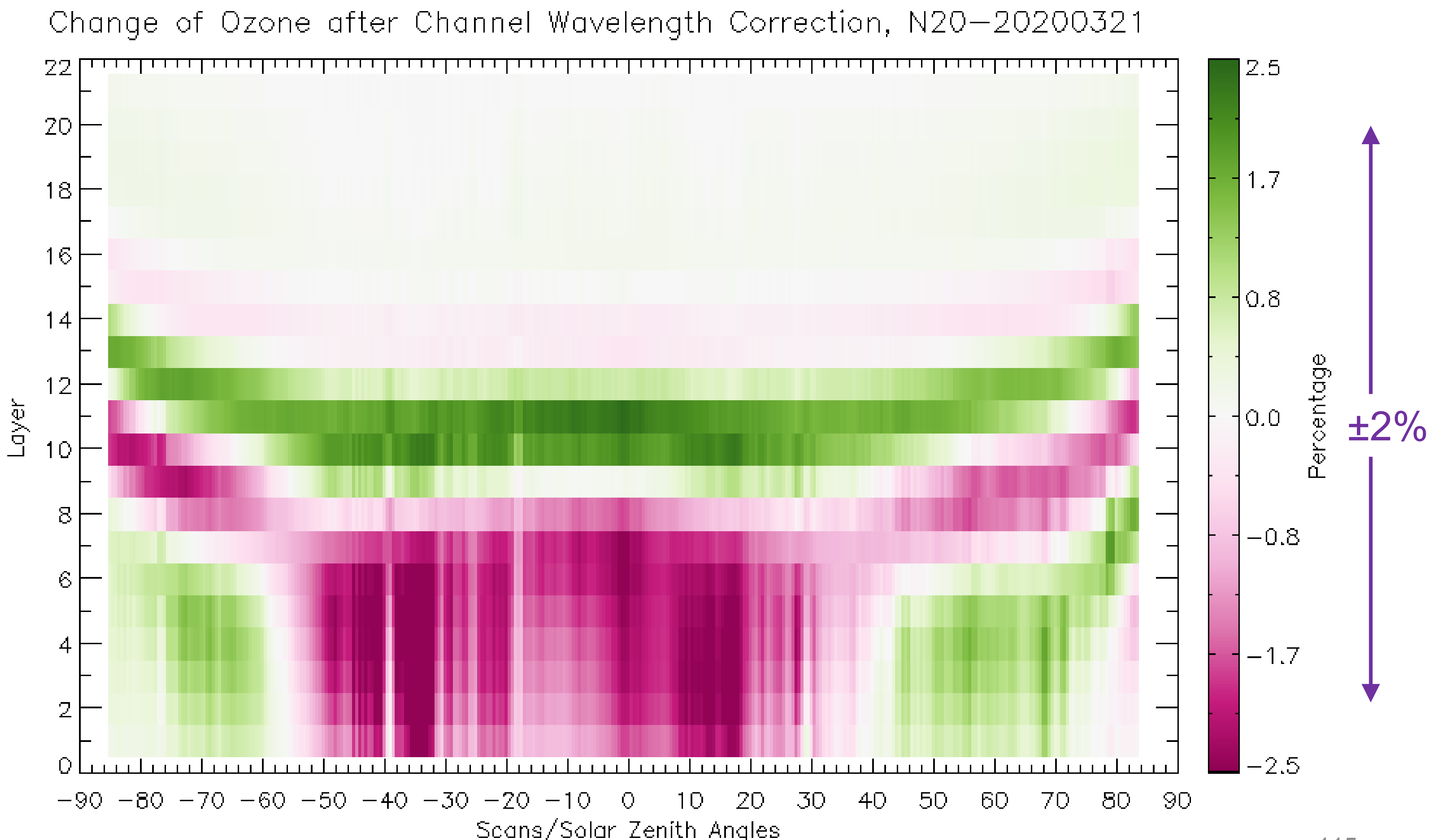
Effects of moving V8Pro channels to the nearest N20 center wavelengths where no interpolation is required.



Case study of effects of the channel interpolation & wavelength shift for V8PRO (2/4)



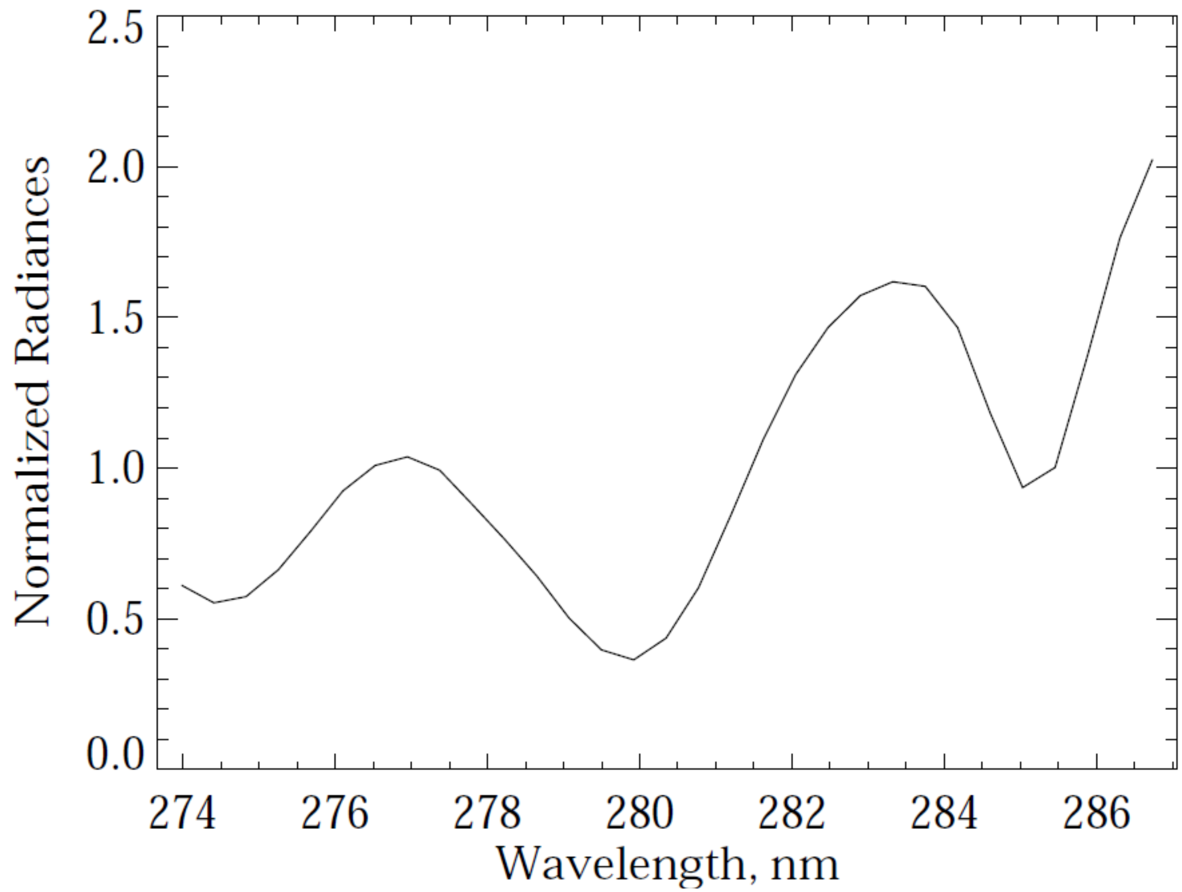
We will correct most of this interpolation error with the next table deliveries. The tables will adjust the bandpasses for the as-interpolated effective bandpasses. (4/4)



Shifts using Mg I & II Features in Earth Radiances

- Create 8-day averages of SDR radiance spectra for 10-degree latitude bands for 3/2019, 9/2019, 3/2020 and 9/2020.
- Fit four features (at 277, 280, 283 & 285.5 nm) with local 7-point quadratics.
- Compute vertices locations for all 16 latitude bands.
- Large differences in results for peaks and valleys for Earth vs Solar

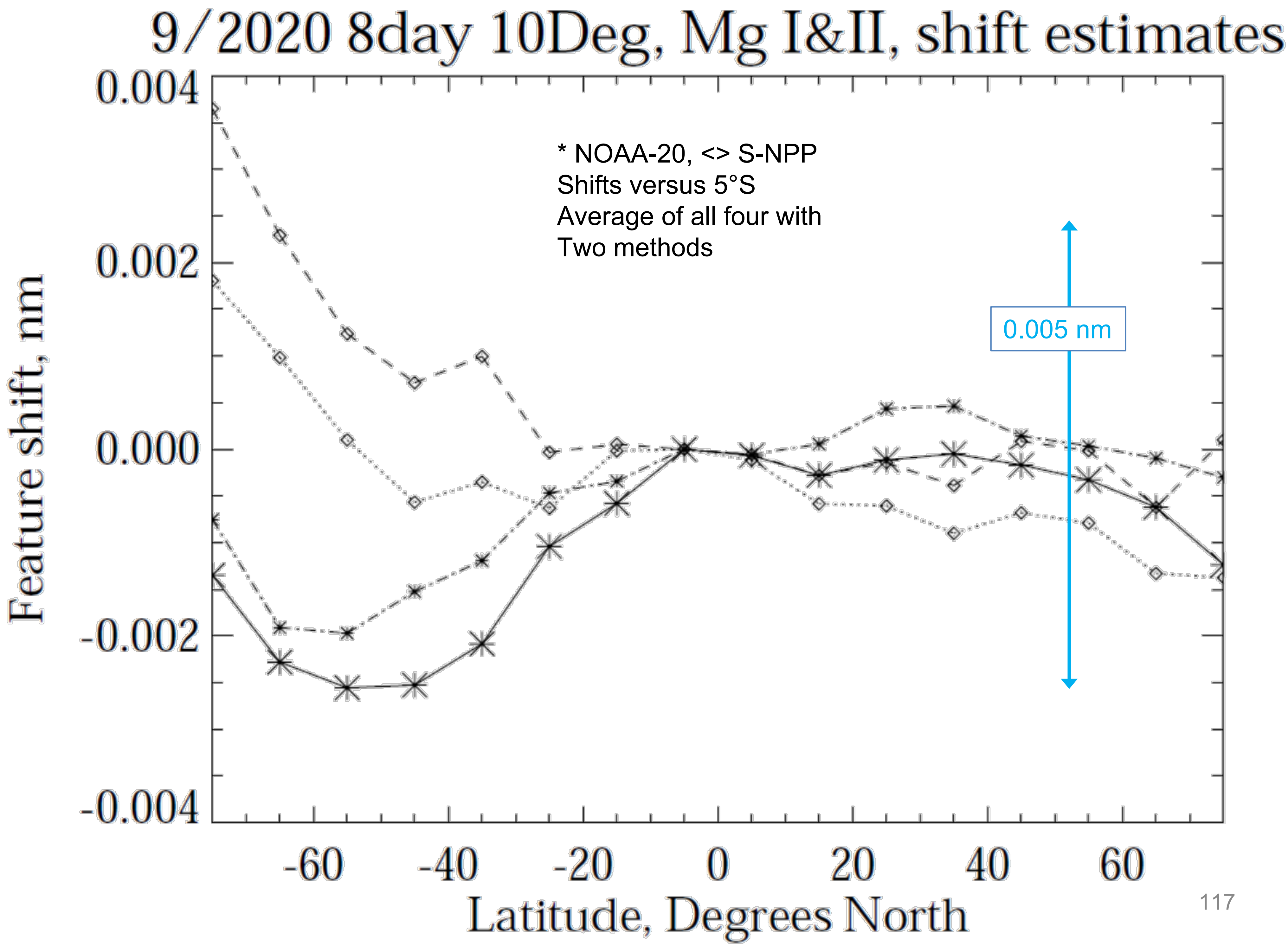
0.06 -0.06 0.09 -0.09 nm



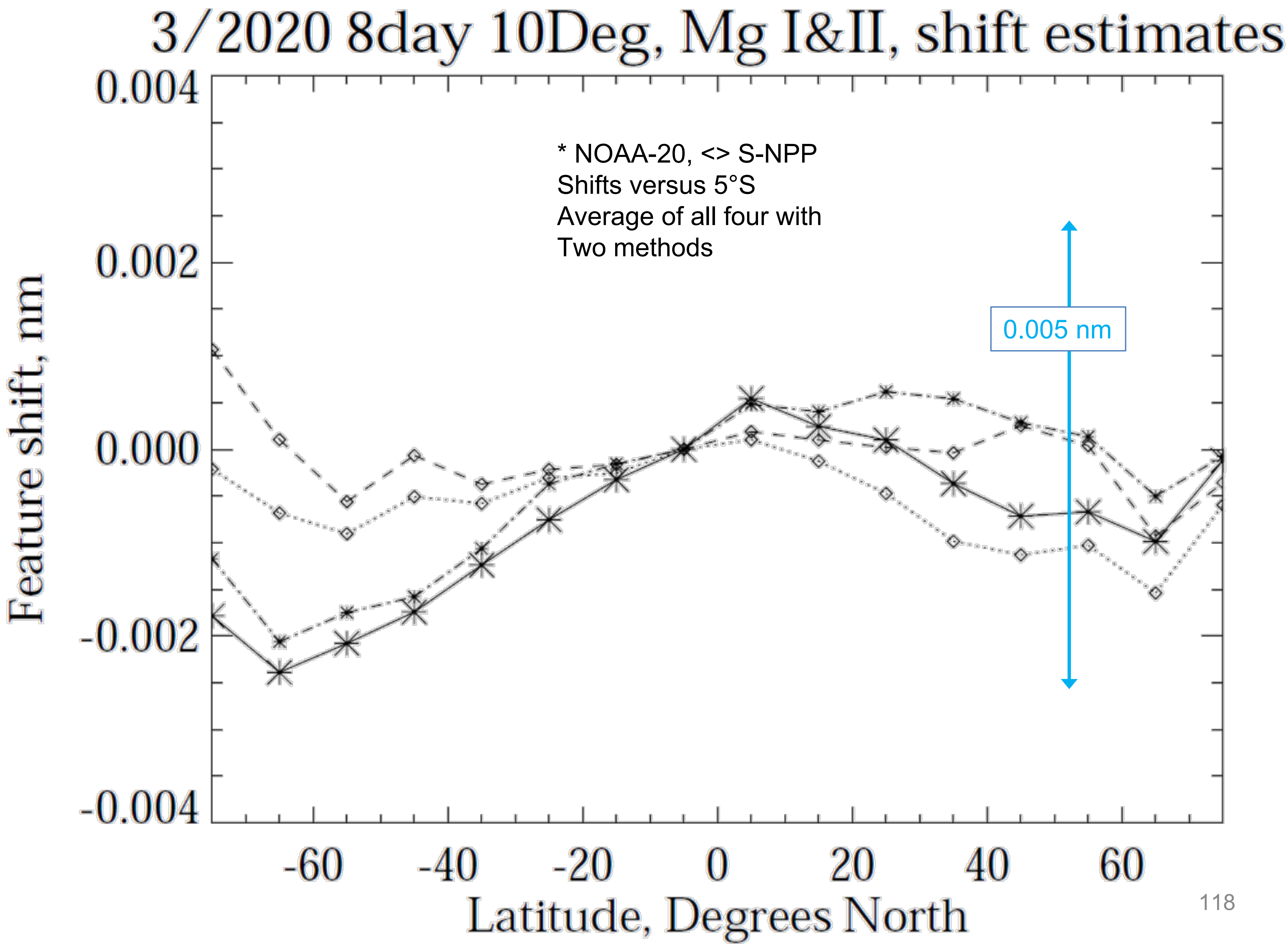
- Ozone absorption creates opposite sign “wavelength shifts” for peaks as opposed to valleys. Shift estimate sensitivities to 10% gradient in radiances over these 31 wavelengths for S-NPP are:

0.041 -0.021 0.041 -0.025 nm

Along-Orbit OMPS NP Shifts



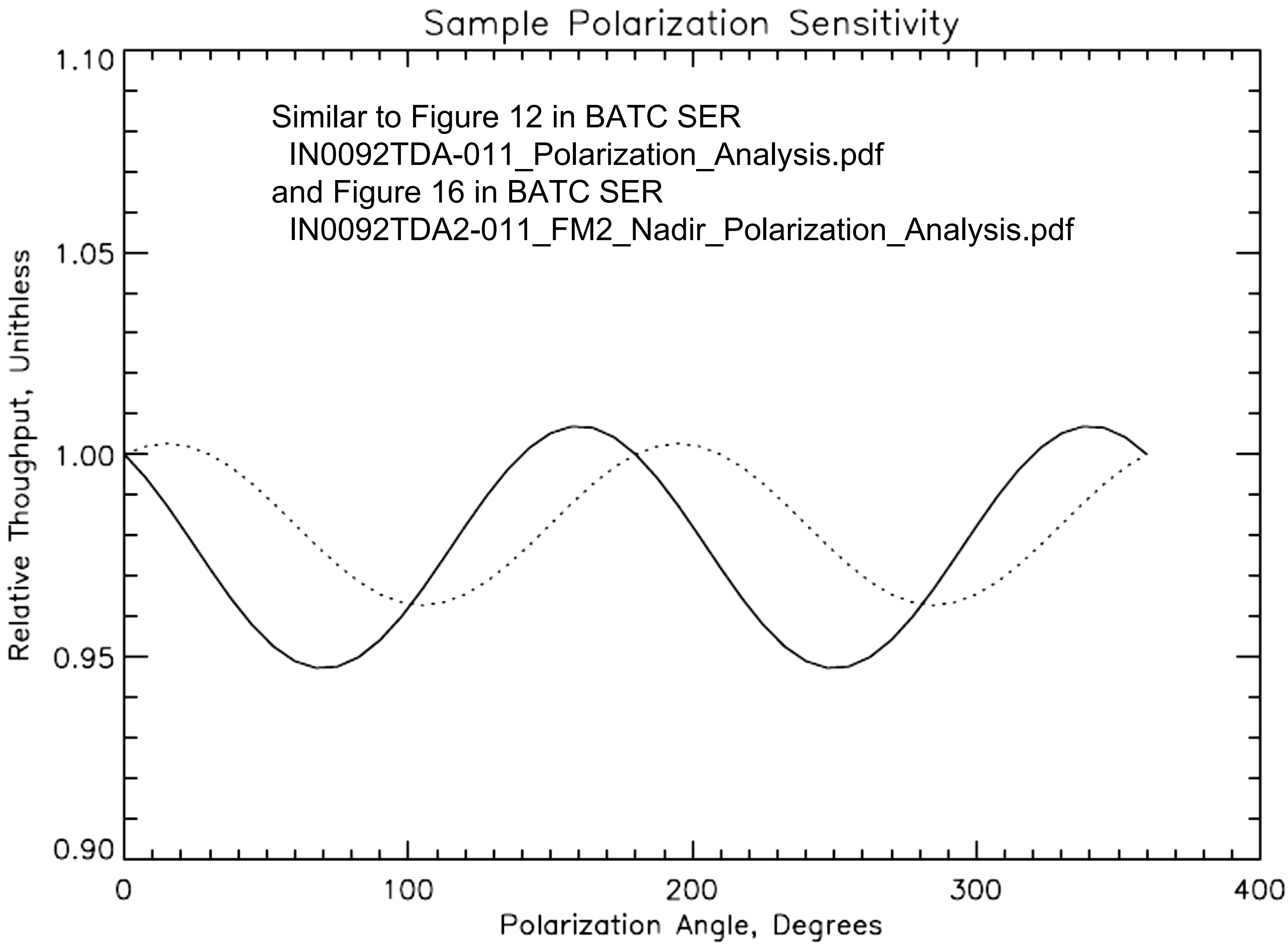
Along-Orbit OMPS NP Shifts



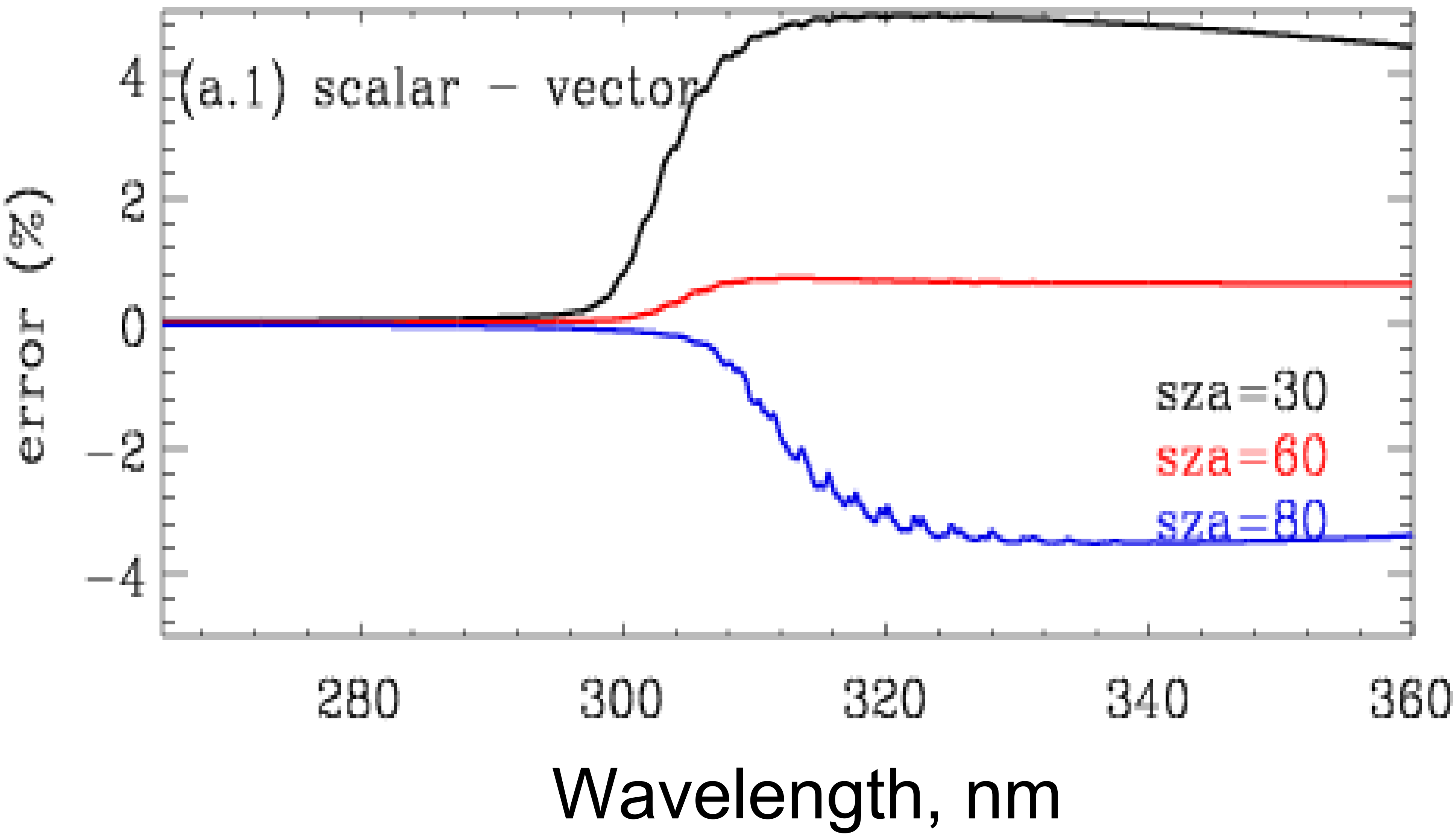
Is there a potential source for the longer wavelength differences?

- Laboratory testing to verify polarization insensitivity levels suggest that there are differences for these between S-NPP and NOAA-20.
- The shorter channels are primarily from single scattering and have very small contributions from surface or cloud reflectivity.
- The longer channels have significant contributions from multiple scattering and cloud and surface reflectivity variations.
- The middle channel change have less multiple scattering and reflectivity sensitivity as the SZAs increase.

Generic figure showing the magnitude of polarization sensitivity differences between S-NPP and NOAA-20.

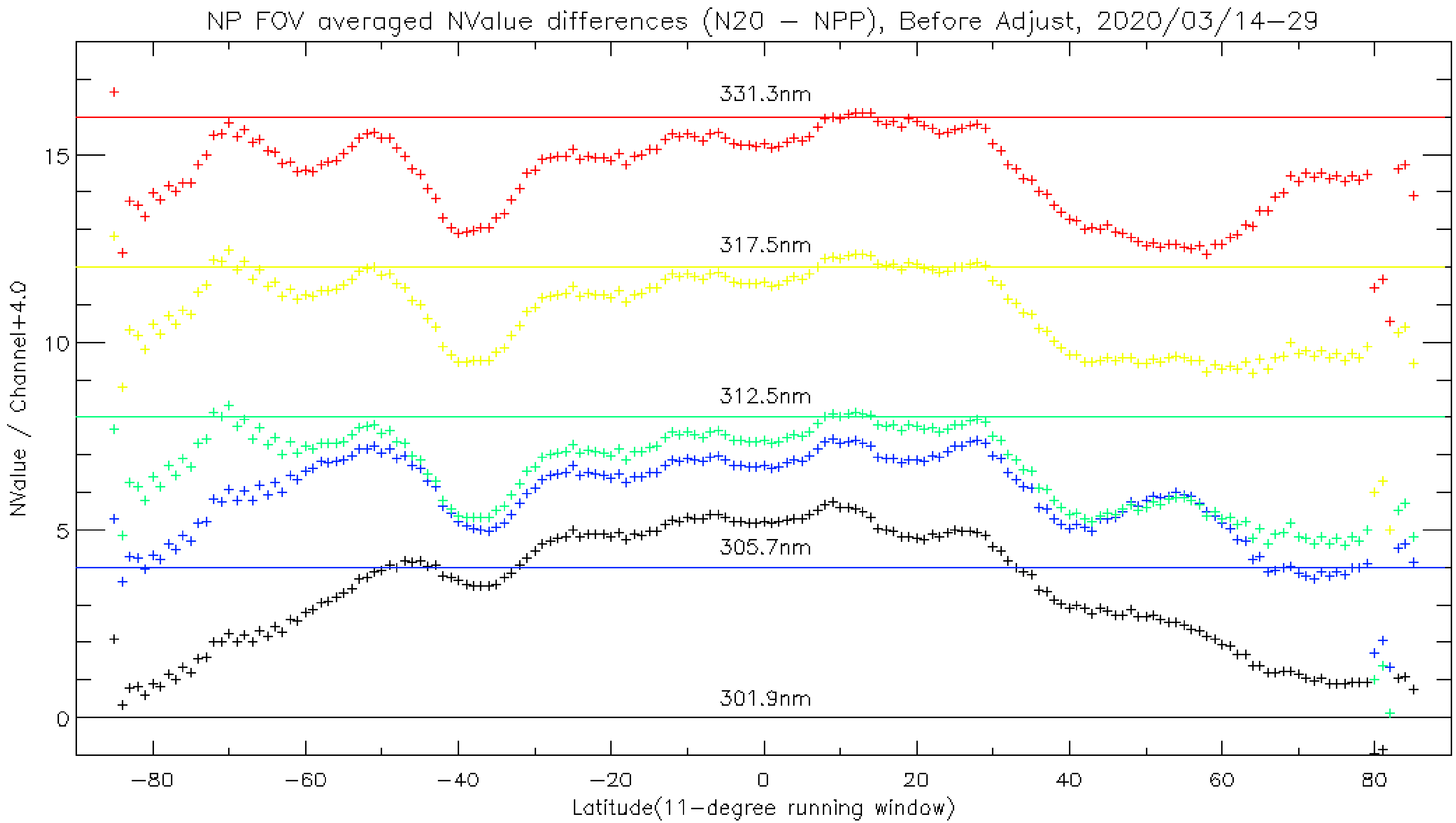


Radiance differences due to neglecting polarization in an RT model

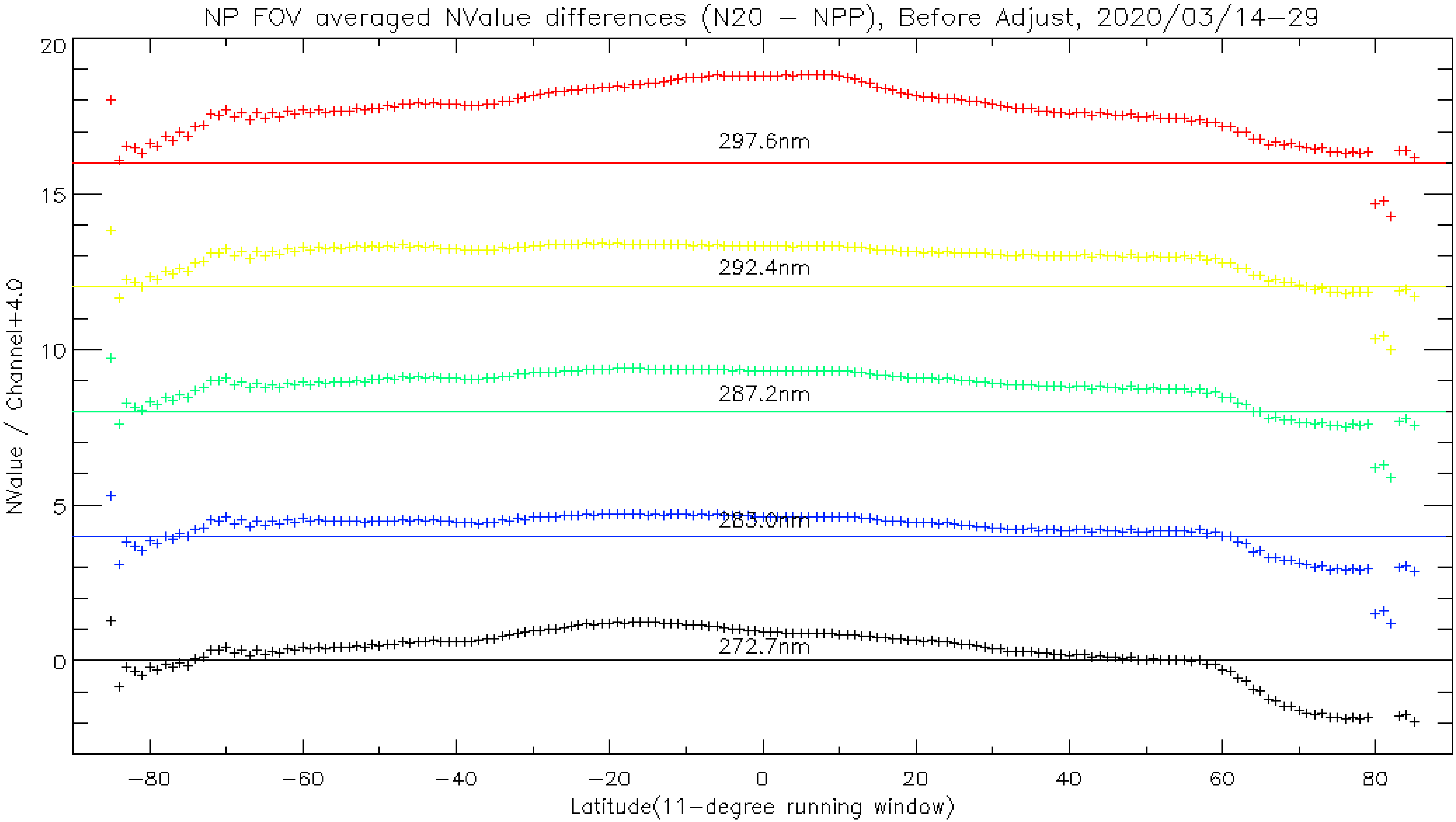


***Fr**om a presentation at the NASA OMI/OMPS meeting on 09/10/2020 by Juseon Bak (Harvard Smithsonian), with contributions from Xiong Liu, Robert Spurr, Kai Yang, Caroline R. Nowlan, Christopher Chan Miller, Gonzalo Gonzalez Abad and Kelly Chance*

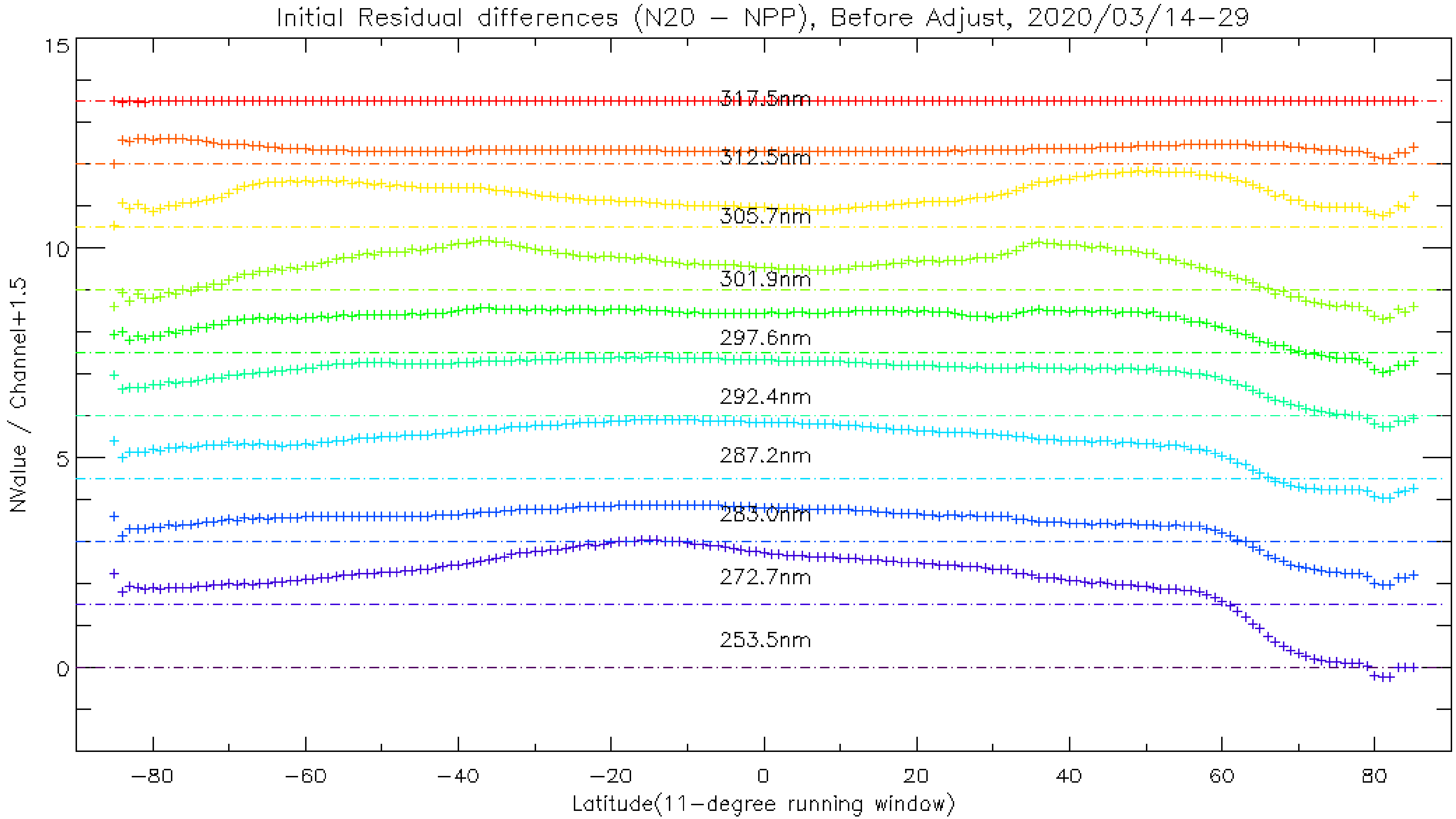
11-degree zonal mean differences N-Value [-100*log10(Rad/Irrad)] for the six longer channels



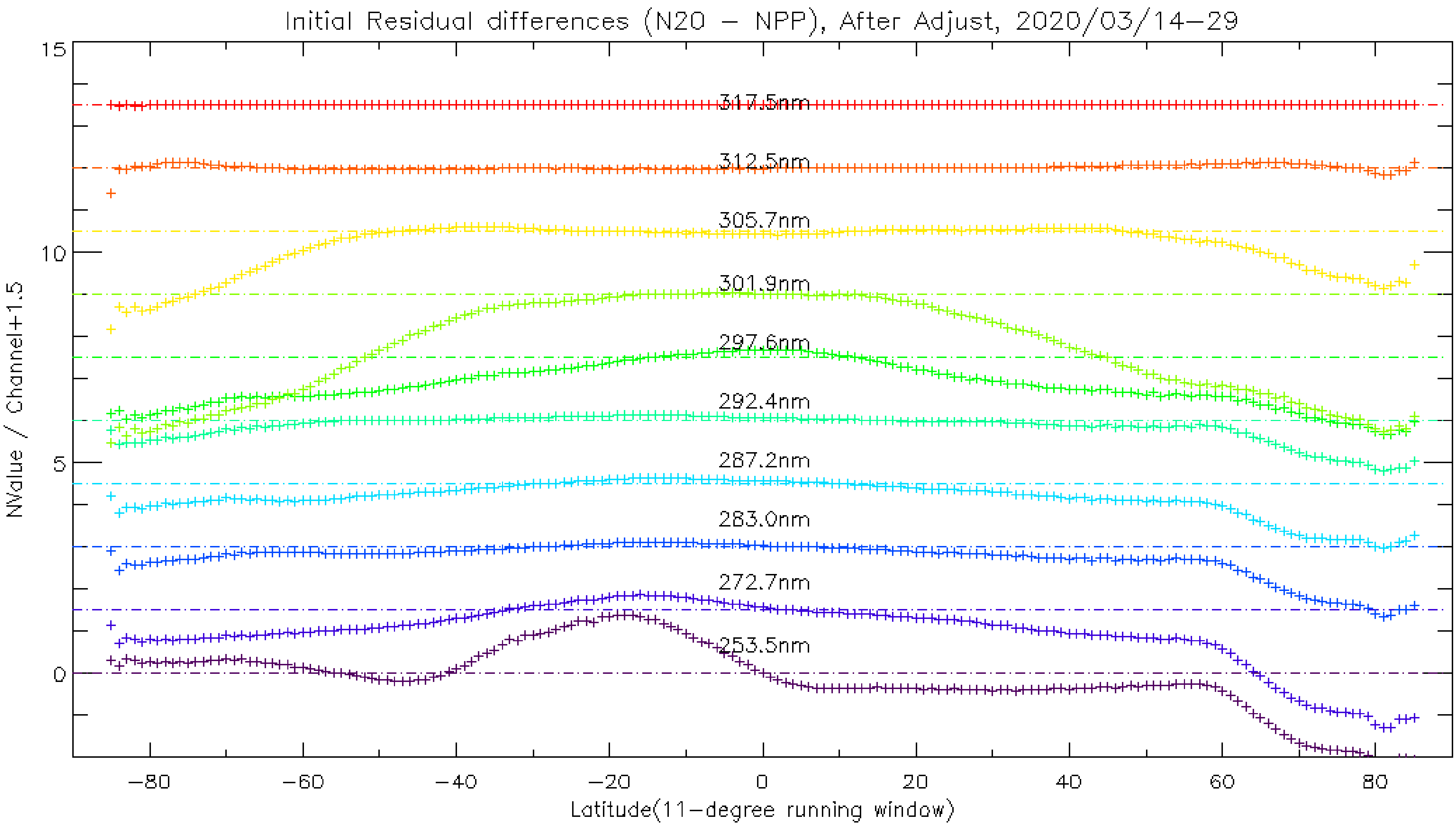
11-degree zonal mean differences N-Value [-100*log10(Rad/Irrad)] for the six shorter channels



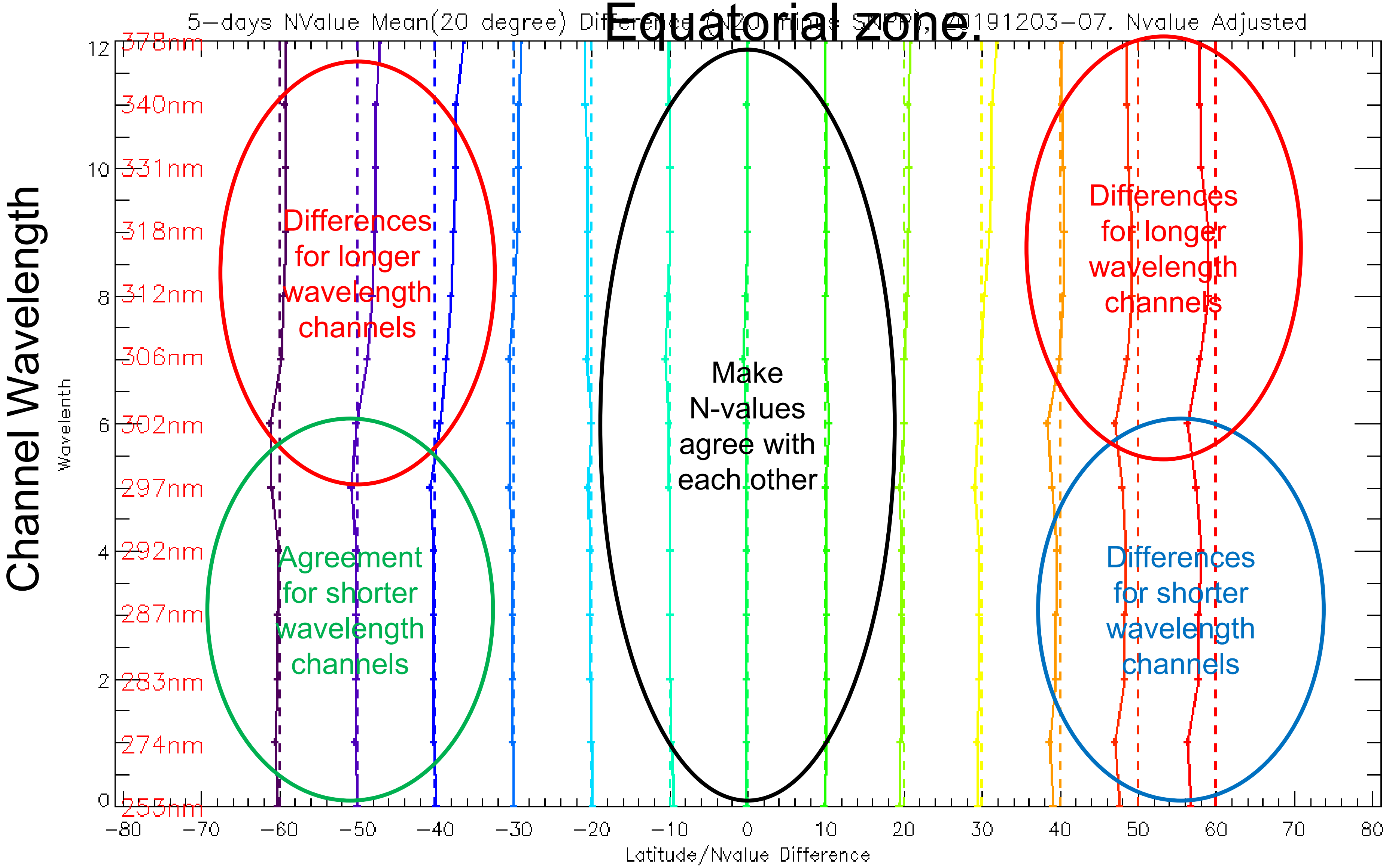
11-degree zonal mean differences Unadjusted Initial Residuals for all channels



11-degree zonal mean differences Adjusted Initial Measurement Residuals for all channels

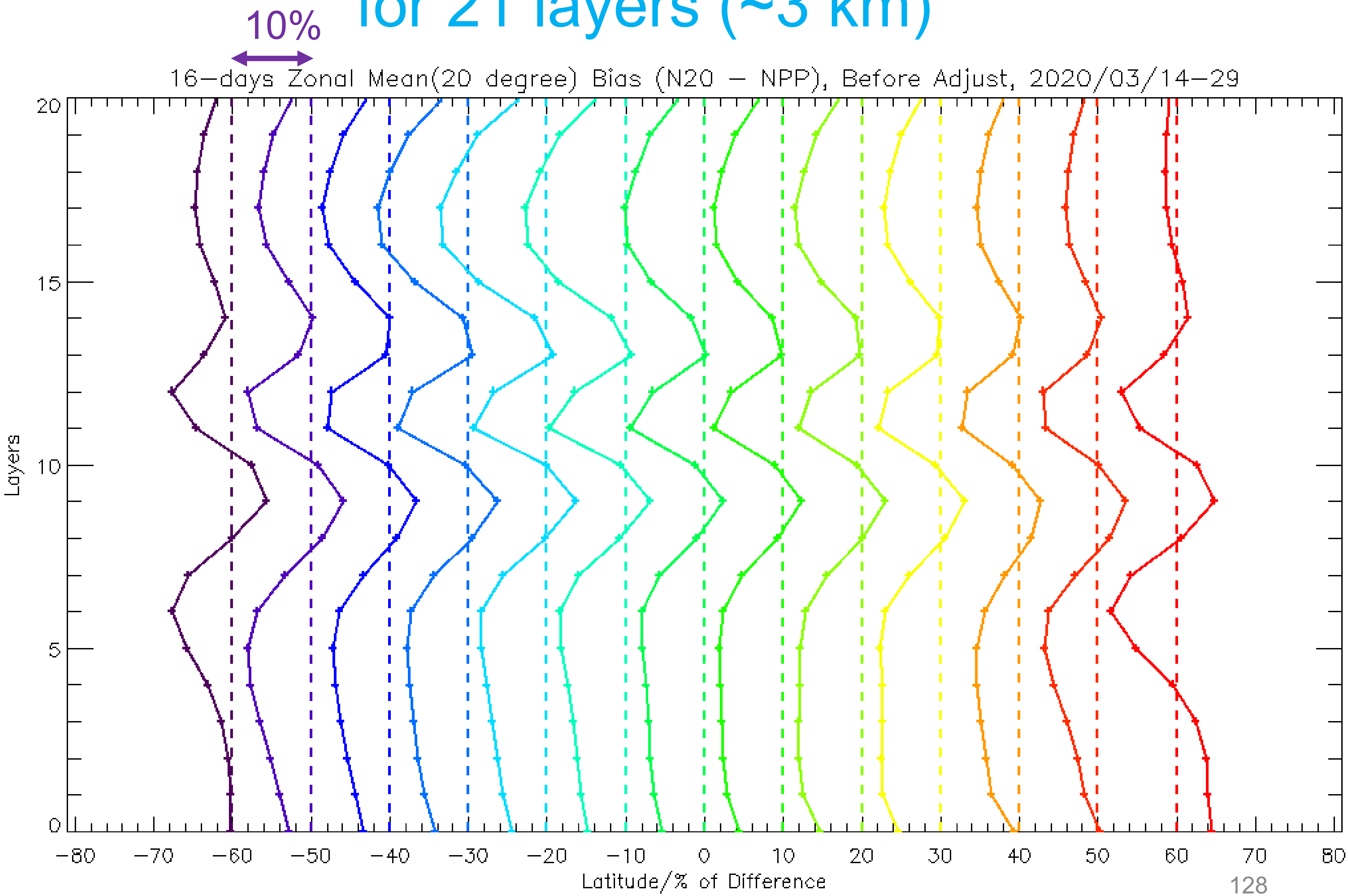


Disagreement in N-values between S-NPP and NOAA-20 still exist over middle/high latitude region after making adjustments to force agreement in the Equatorial zone.

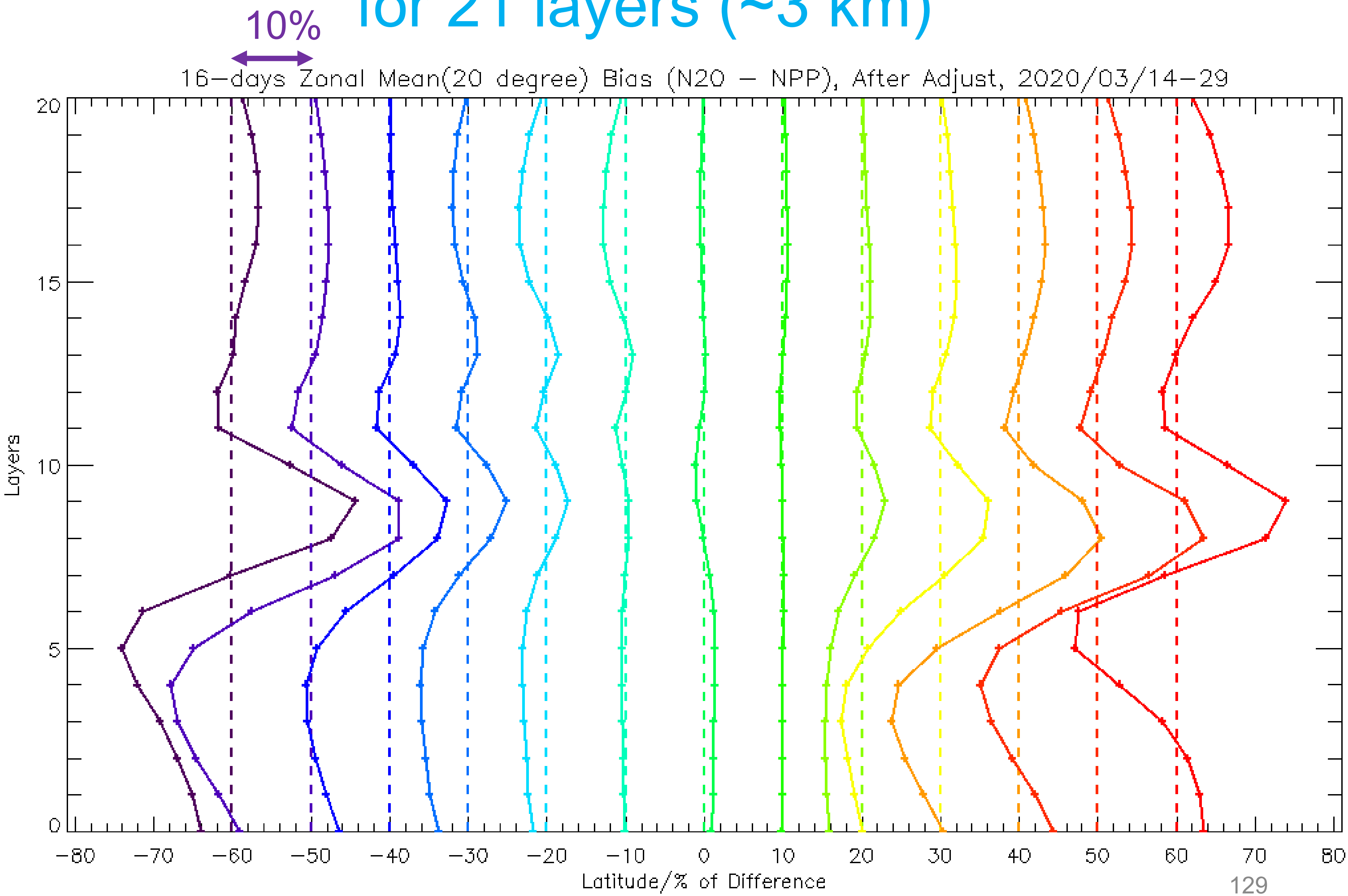


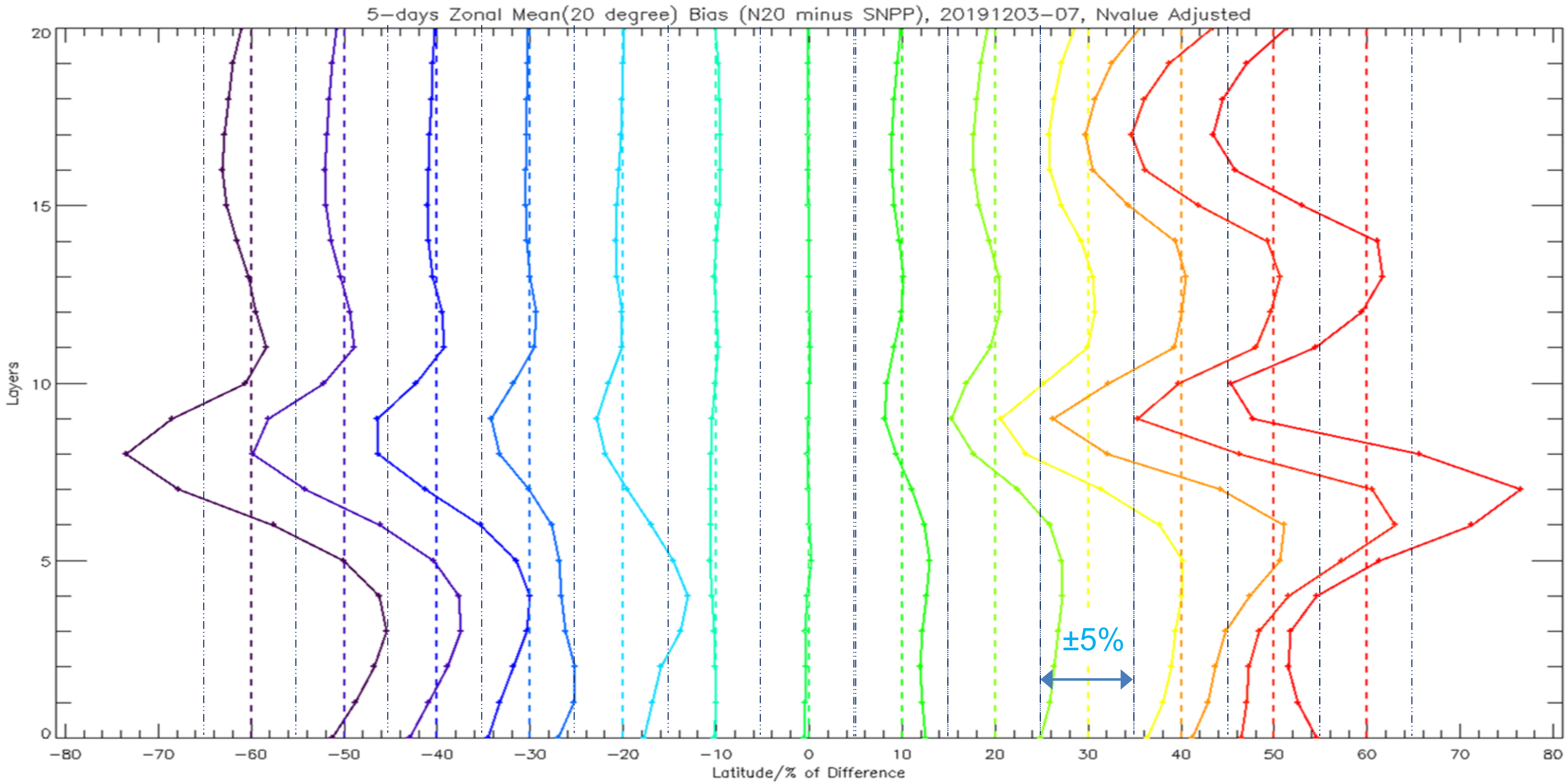
Latitude, Degrees North or N-Value Differences

20-degree zonal mean differences Unadjusted Retrieved Ozone Profiles for 21 layers (~3 km)



20-degree zonal mean differences Adjusted Retrieved Ozone Profiles for 21 layers (~3 km)

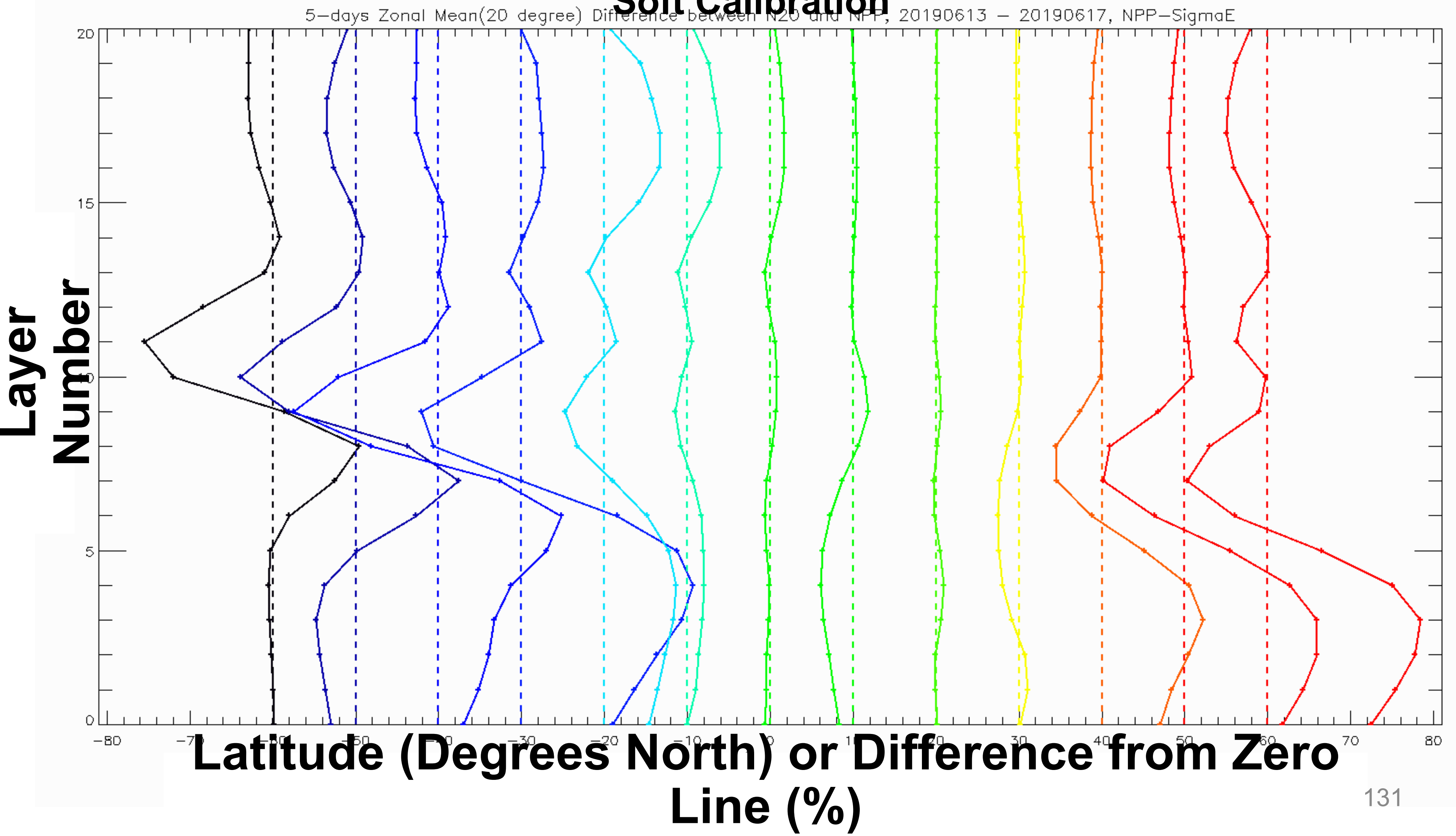




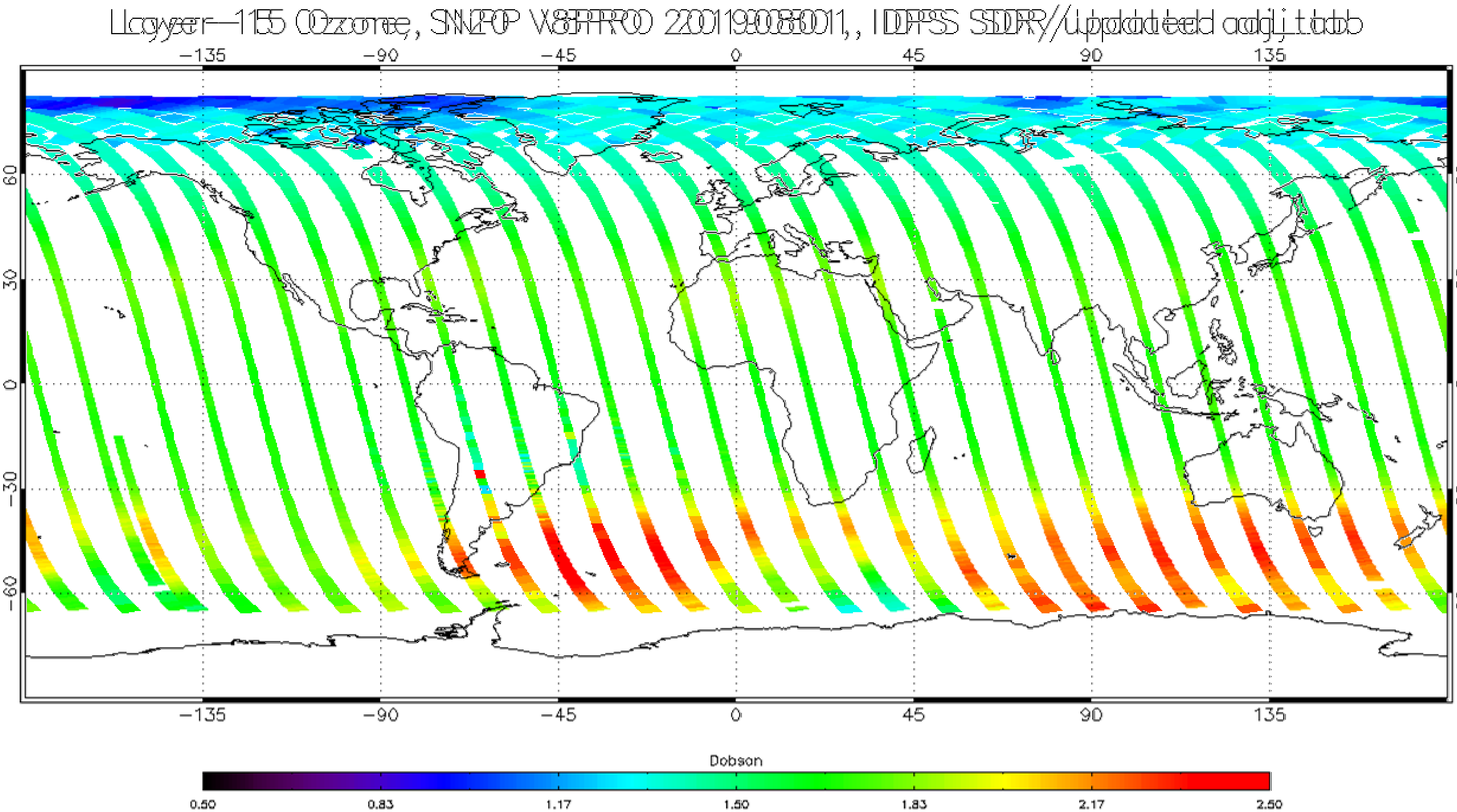
5-days Zonal Mean(20 degree) Bias (N20 minus SNPP), 20191203-07, Nvalue Adjusted
Layers
Latitude/% of Difference
±5%

Failure to Force Agreement between NOAA-20 V8Pro and S-NPP V8Pro with Soft Calibration Adjustments

Profile shape differences for S-NPP and NOAA-20 V8Pro Zonal Means after Soft Calibration



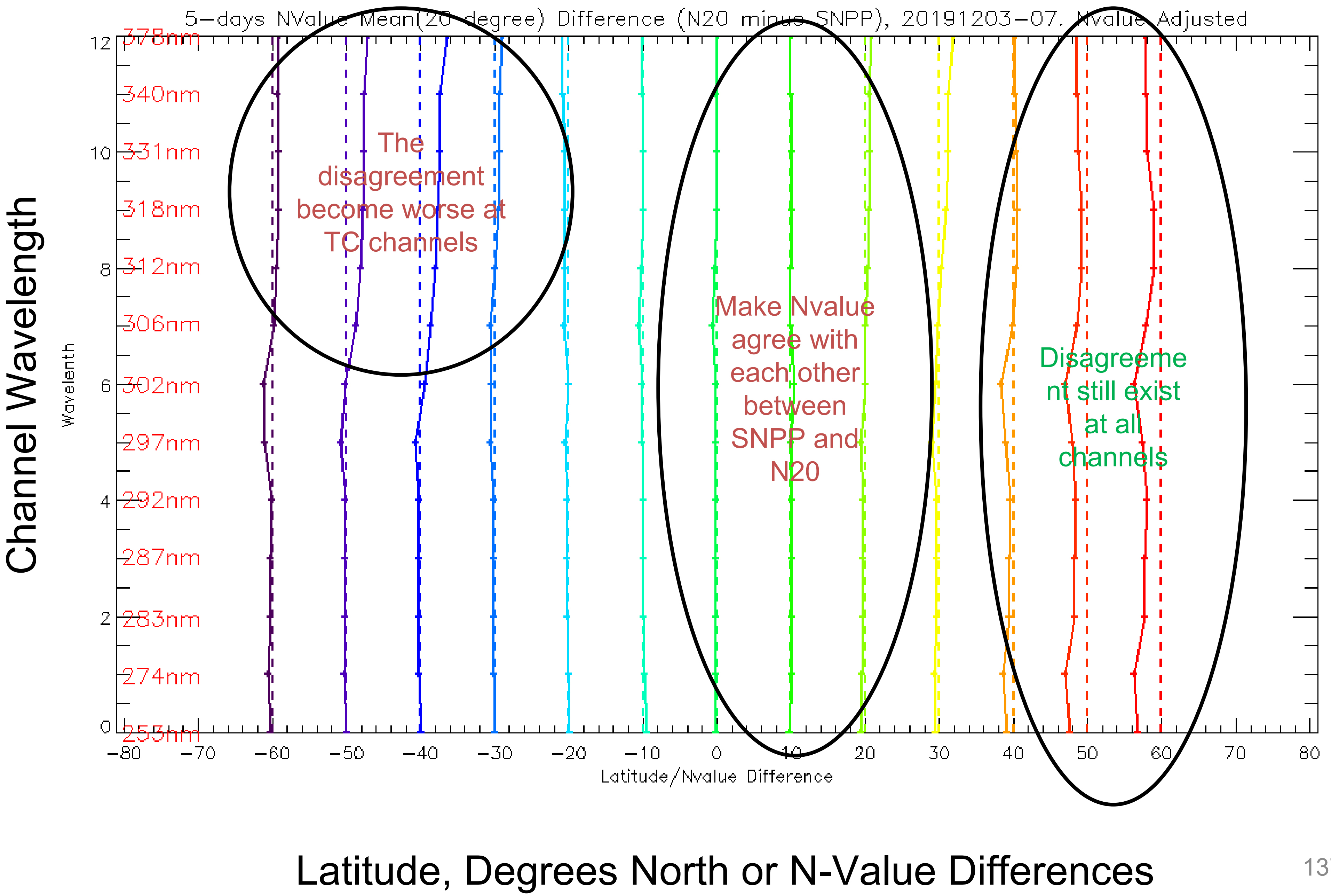
Layer 15 STAR Offline N20 versus NPP



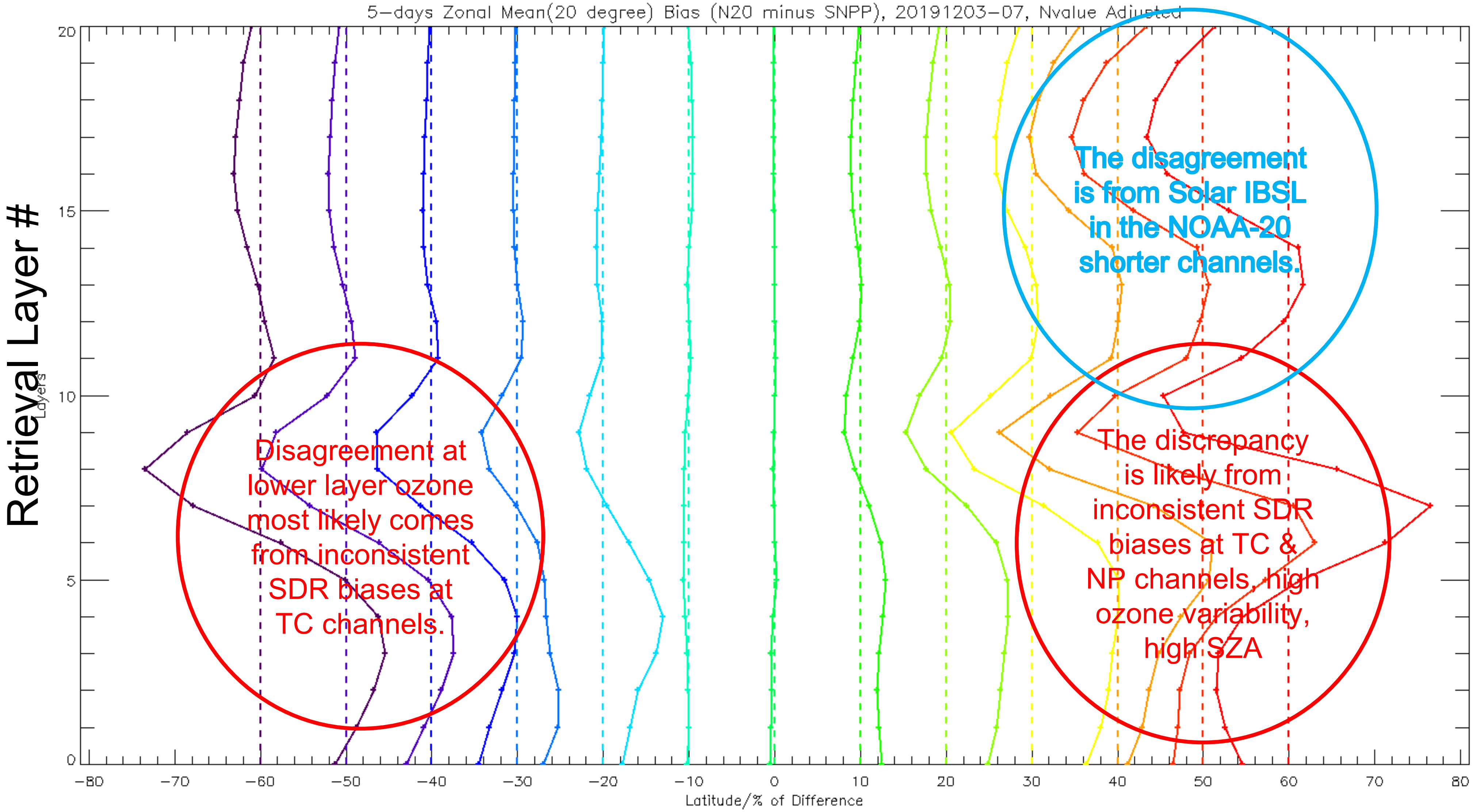
Notes on Selected Areas of the Figure on the Previous Slide

- The variations in the Black Rectangle are shared for wavelengths from 302 nm to 331 nm. They are present for channels from both the Nadir Mapper and Nadir Profiler.
- The deviations in the Red Rectangles are at higher latitudes for 302 nm and 298 nm channels. Some portion of these differences are due to bandpass and wavelength differences between the instruments.
- The differences in the Blue Oval are for shorter wavelength channels in the Northern Hemisphere. They are the of result of solar in-band stray light in the NOAA-20 OMPS NP.

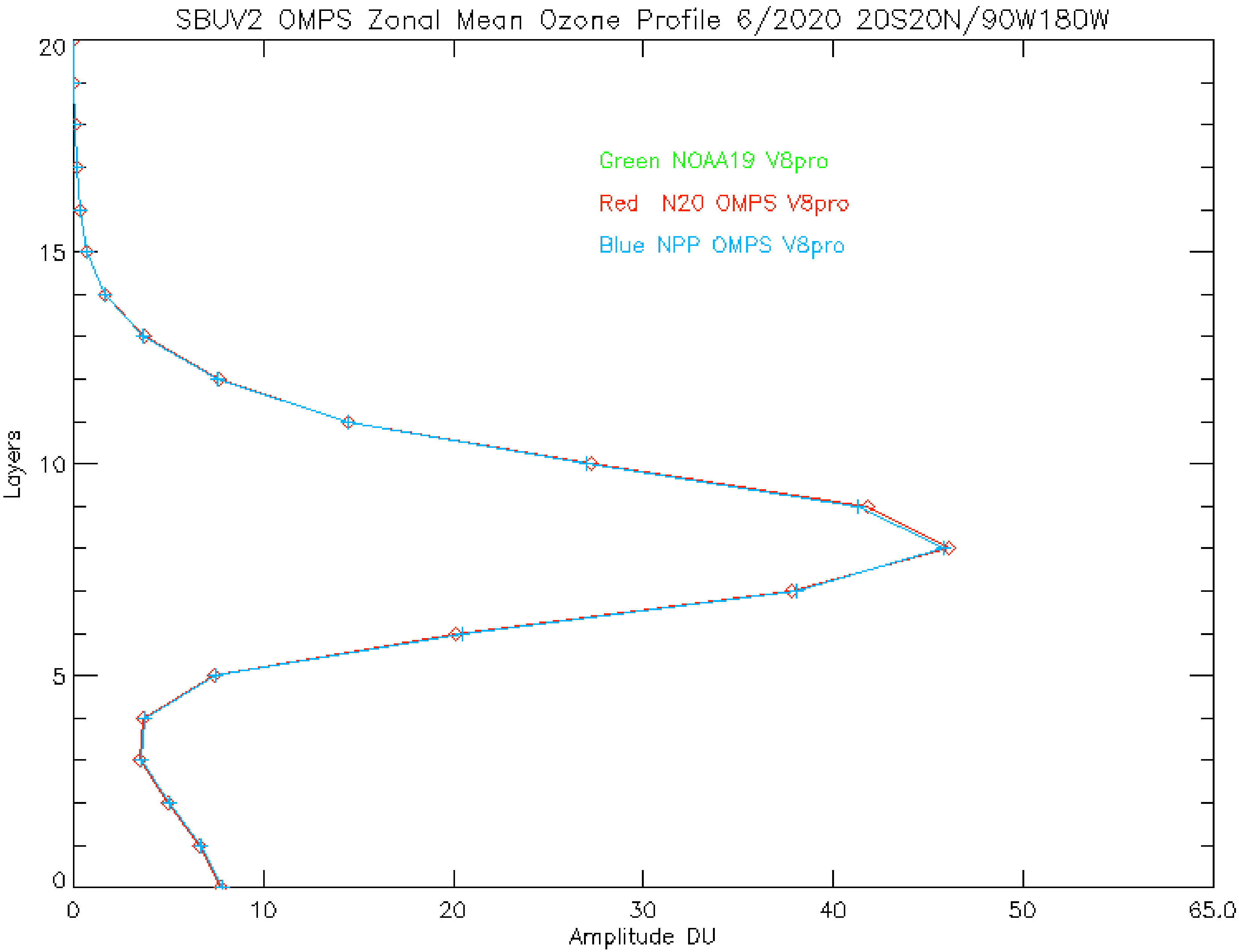
Disagreement in Nvalues between SNPP and N20 still exist over middle/high latitude region after making the SDR agree in the Equator
December 2019 Test Data

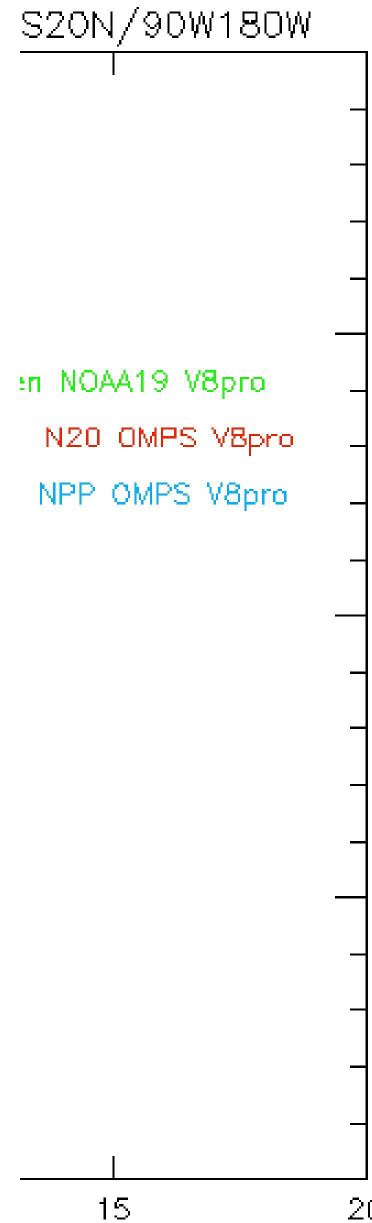


Discrepancy of ozone profile retrieval between SNPP and N20 still exist after soft-calibration based on equator statistics
December 2019 Test Data



Latitude, Degrees North or % Layer Differences


SBUV2 OMPS Zonal Mean Ozone Profile 6/2020 20S20N/90W180W
Green NOAA19 V8pro
Red N20 OMPS V8pro
Blue NPP OMPS V8pro
Layers
0
5
10
15
20
0
10
20
30
40
50
65.0
Amplitude DU


S20N/90W180W
NOAA19 V8pro
N20 OMPS V8pro
NPP OMPS V8pro
15

Key Issue for Path Forward from Beta Updates

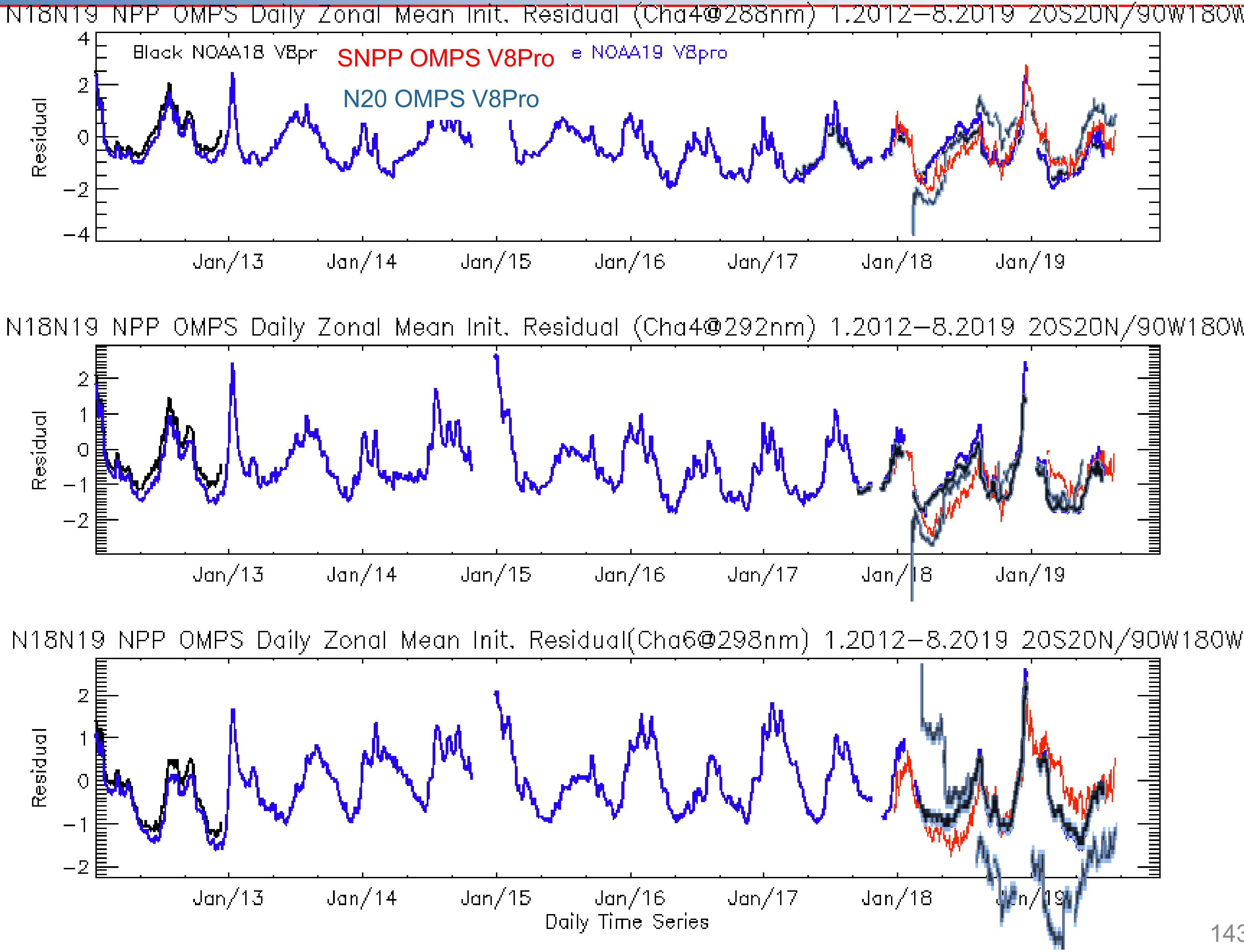
- ADR 8730 New DR. Counts not uniformly distributed for NOAA-20 OMPS NP. This has been traced to discretization errors from the non-linearity correction. A new flight non-linearity was loaded October 19, 2018, and adjustments to the calibration coefficients were implemented at IDPS on December 4, 2018.
- Test data was taken with NOAA-20 OMPS using the new sample tables -- 140 5-pixel for NM and rectangular NP. Tables are under development to make operational 103x15 granule NM SDRs. The SDR team will be requesting that the instrument be switched to the 140 5-pixel mode. We adjusted (v3r3) the V8Pro Glueware to handle the NMmacropixels with

[10,10,10,10,5,10,5,10,10,10,10] pixels

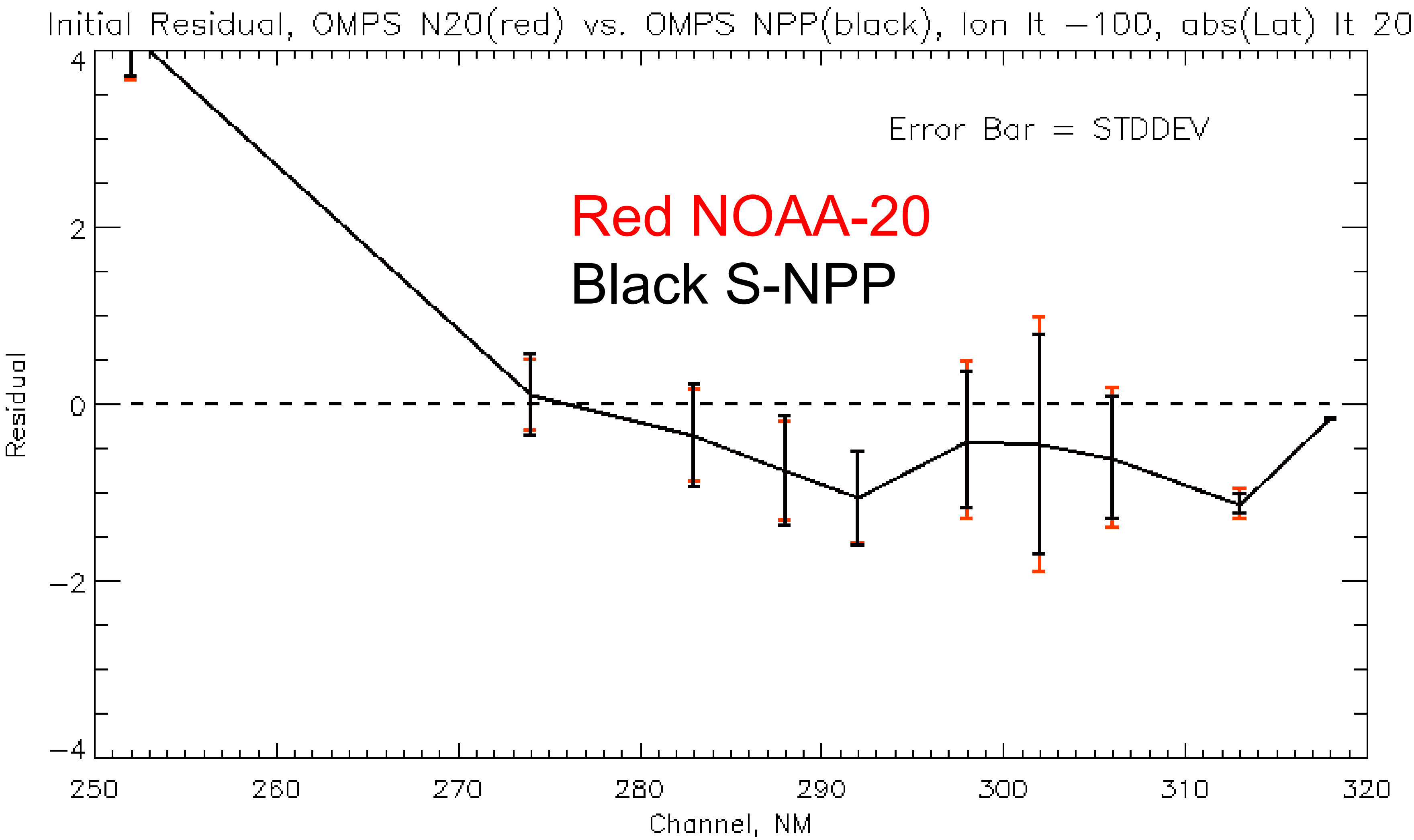
Outline

- Show SDRs are stable away from updates with allowance for degradation as estimated by reference diffuser.
- Show S-NPP and NOAA-20 Diffs for V3SDR with no adjustments and with adjustments for force agreement at the Equator
- Show S-NPP comparisons to Umkehr and Sondes.
- Show bandpass differences.

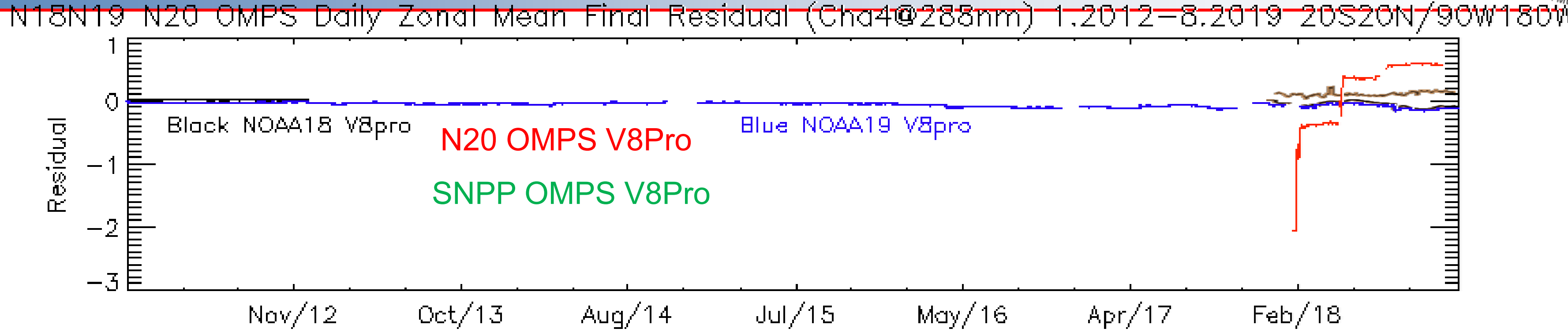
Initial Residuals from NDE V8Pro

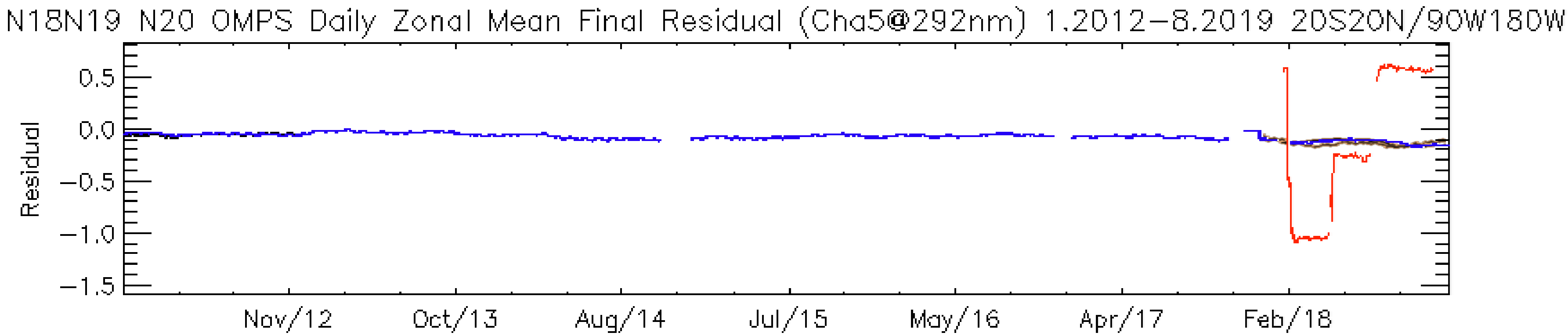


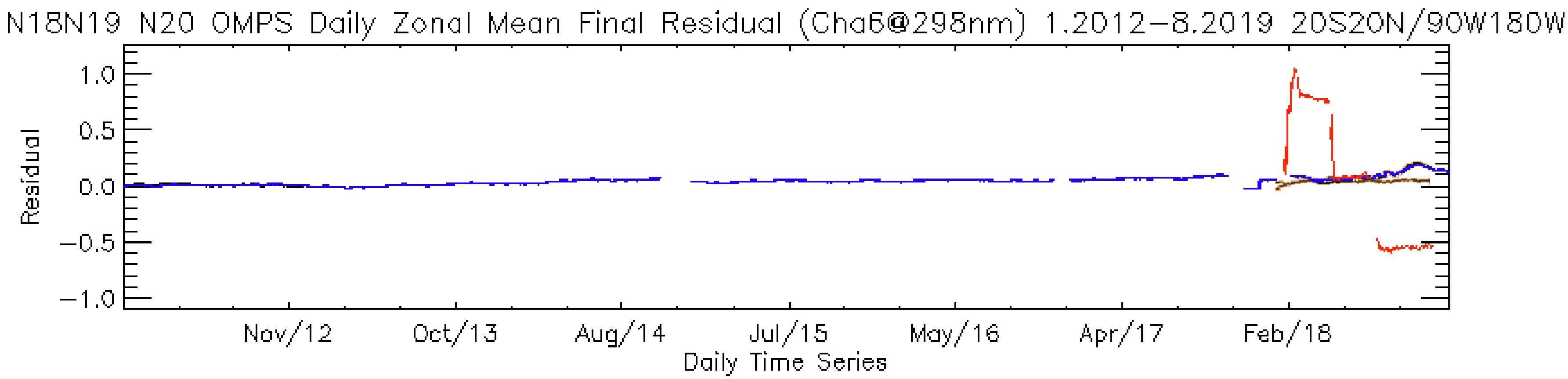
Initial Residuals After Adjustment V8Pro



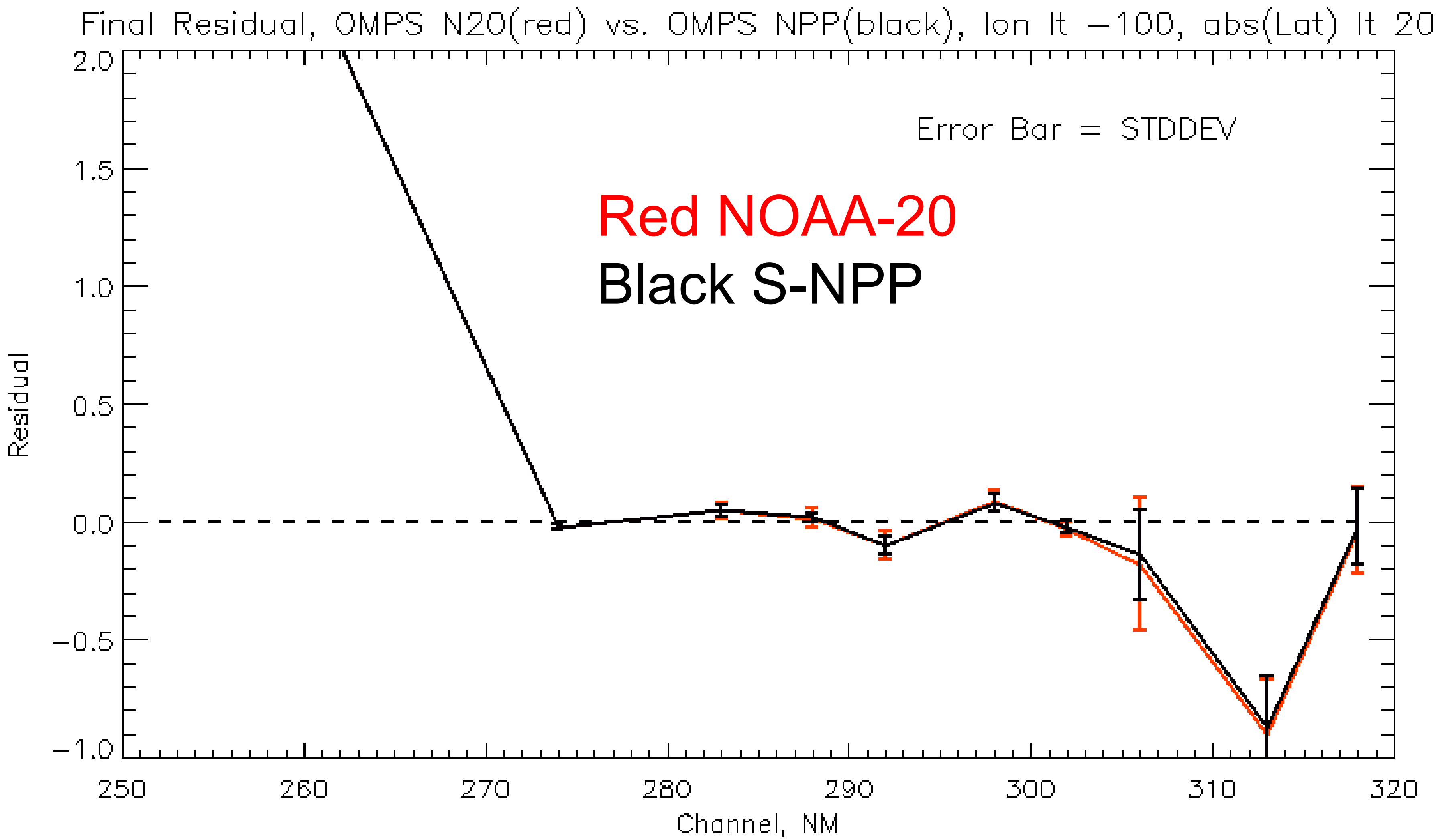
Final residuals from NDE V8Pro



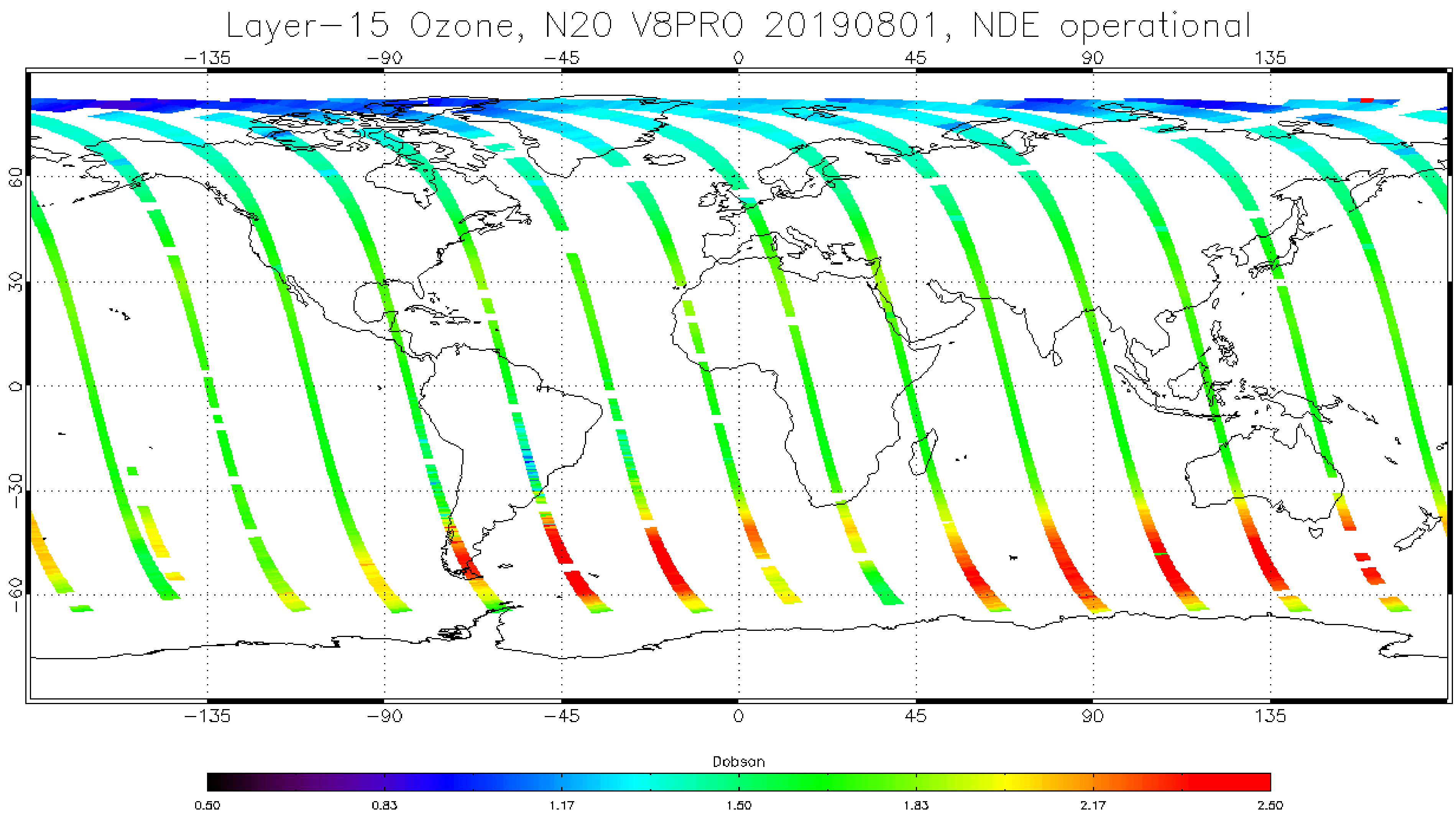




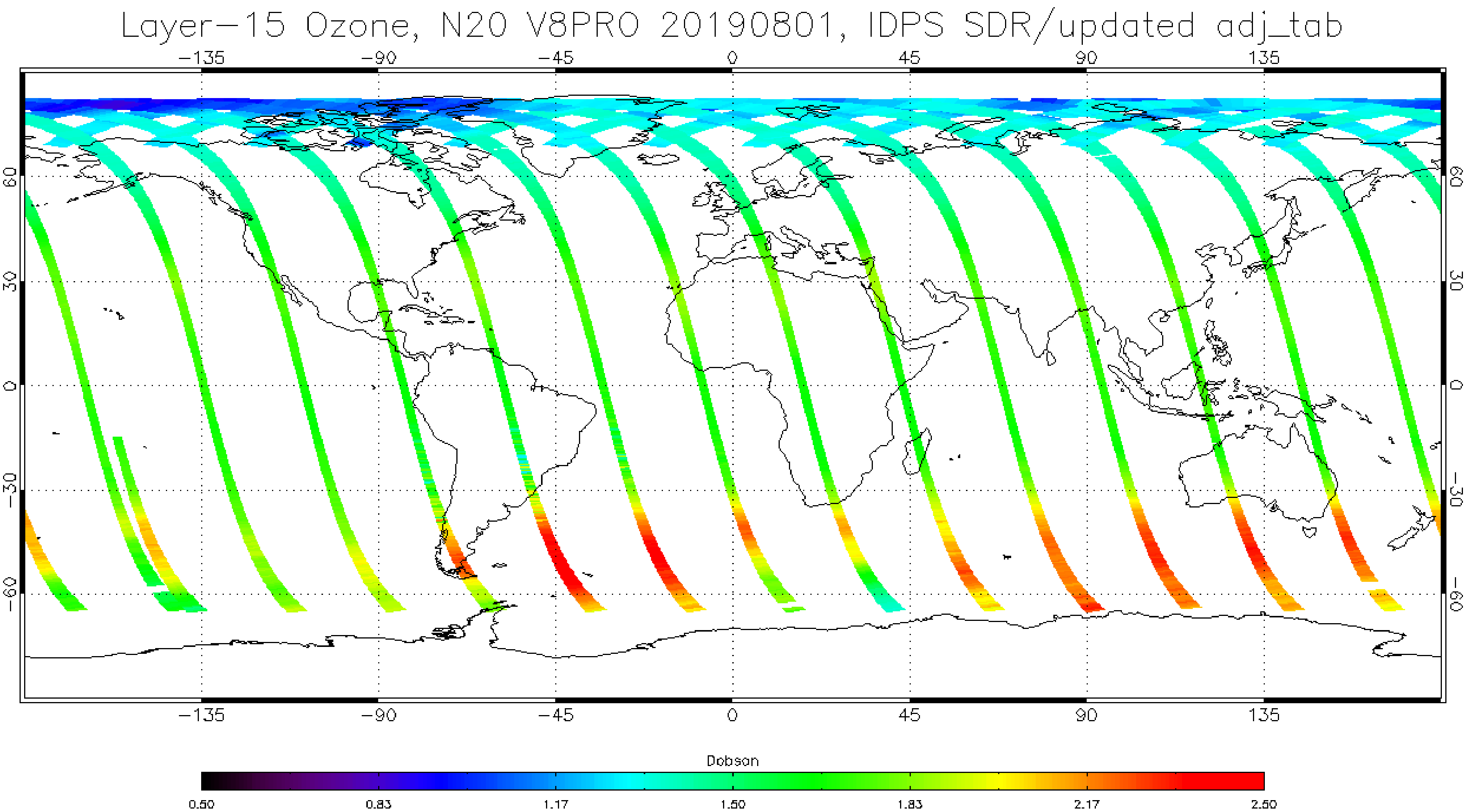
Final Residuals After Adjustment V8Pro



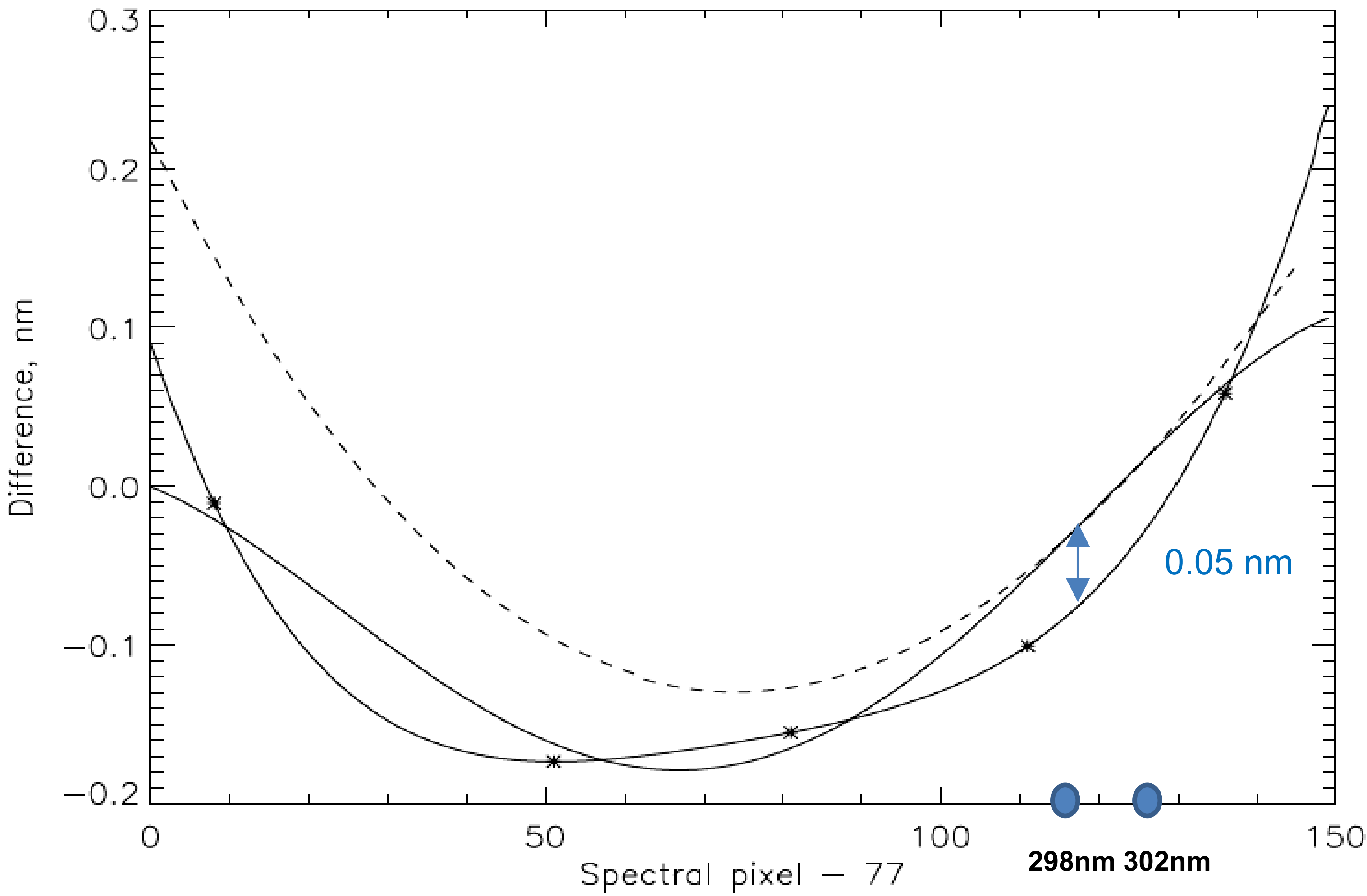
Layer 15 NDE I&T



Layer 15 STAR Offline

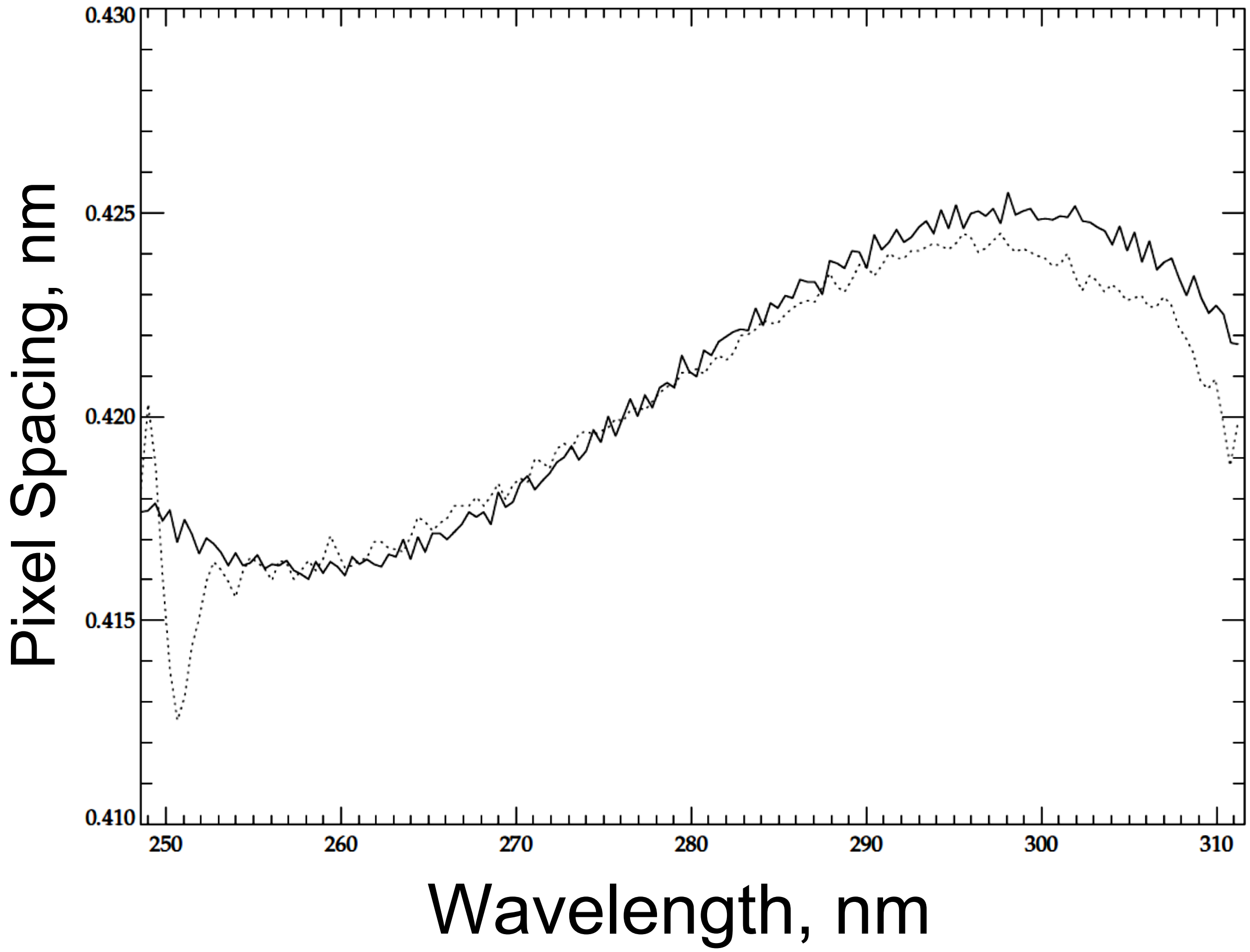


Wavelength Scales versus Linear

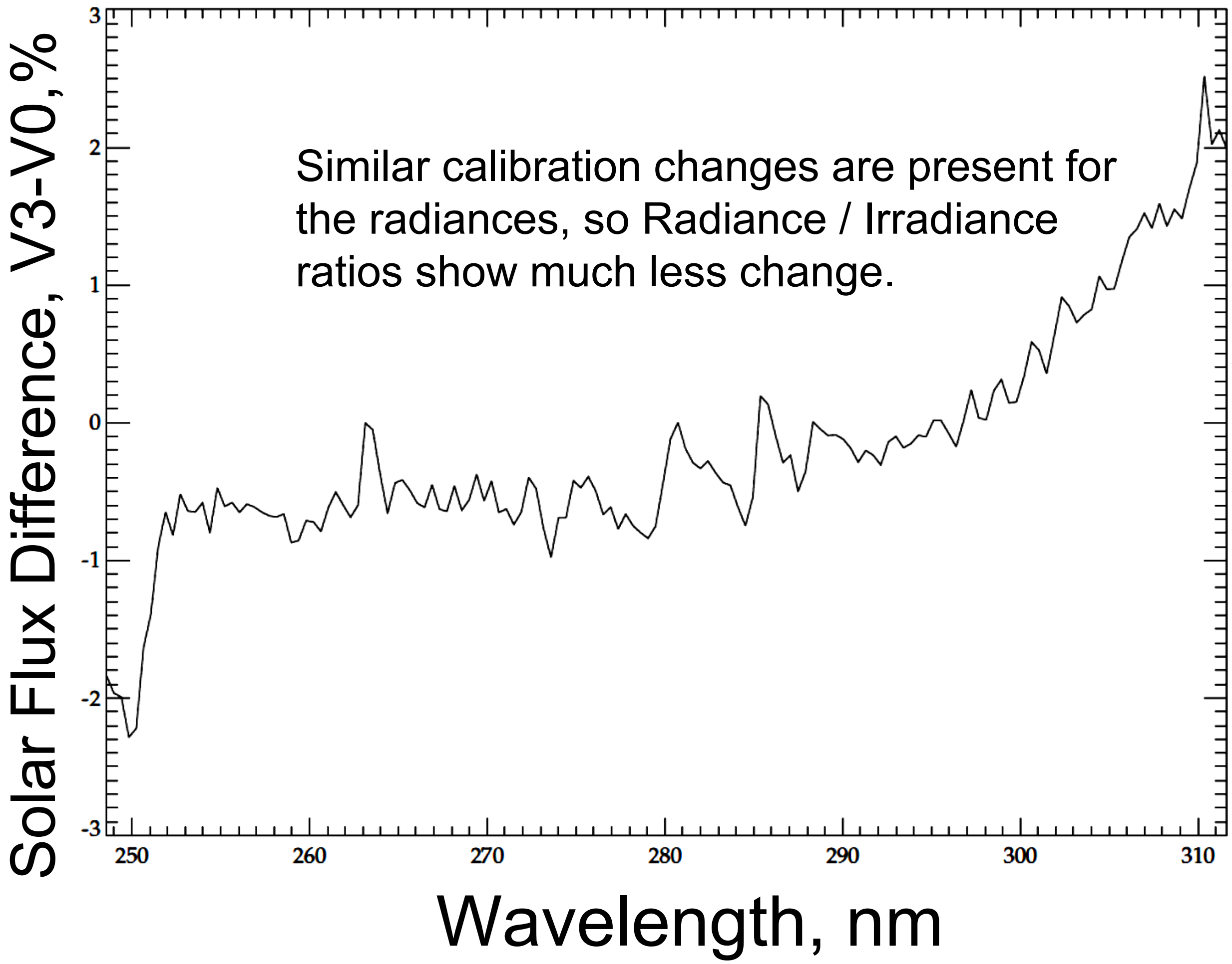


The S-NPP (dashed) show a close to quadratic wavelength scale. The NOAA-20 (solid) follow a quartic wavelength scale. The solid line without symbols are the NOAA-20 CBC data. **The solid line with symbols (*) are the NOAA-20 CBC data adjusted by the bandpass-weighted average wavelengths**. The symbols in the figure show the locations of the five NOAA-20 pre-launch spectral measurement sets.

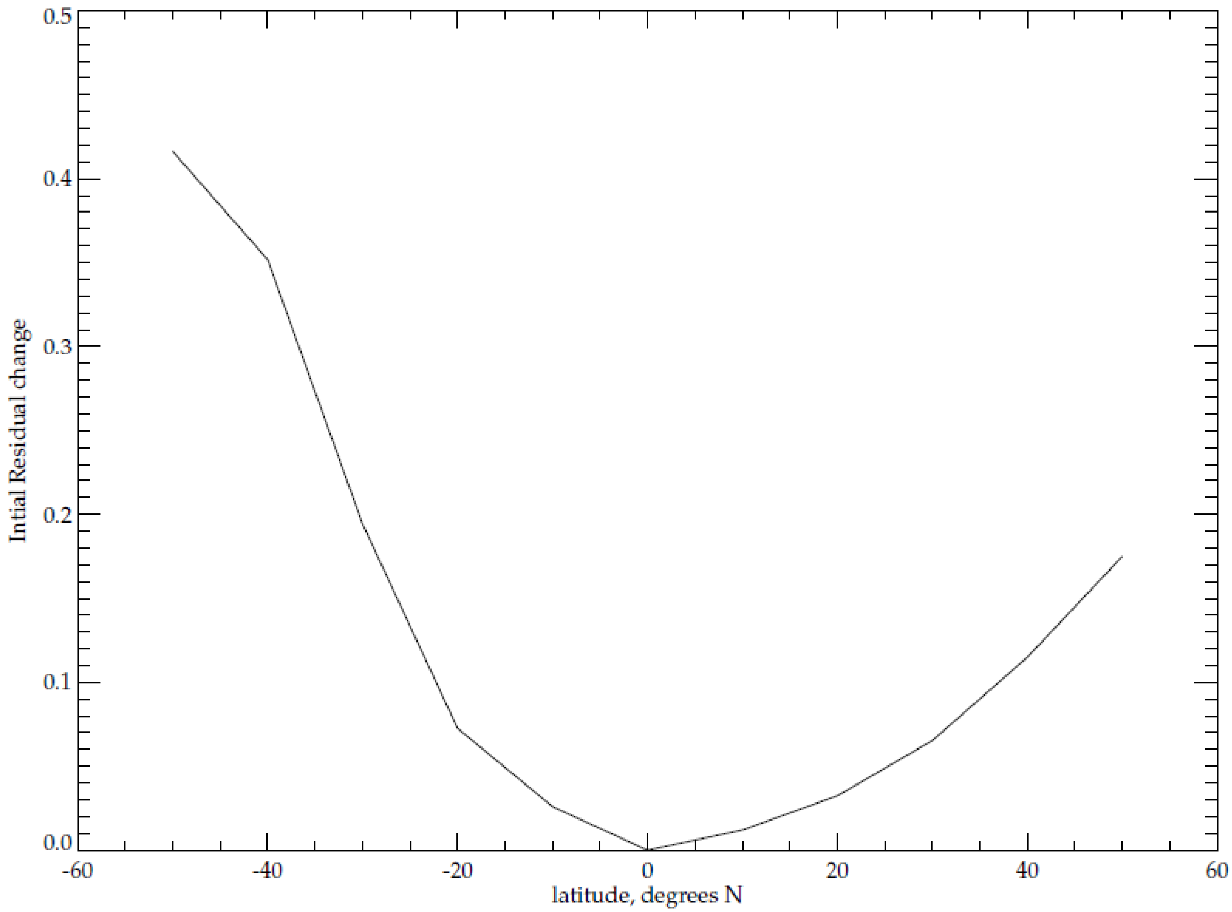
Wavelength Scale Spacing
Solid Old, Dot New



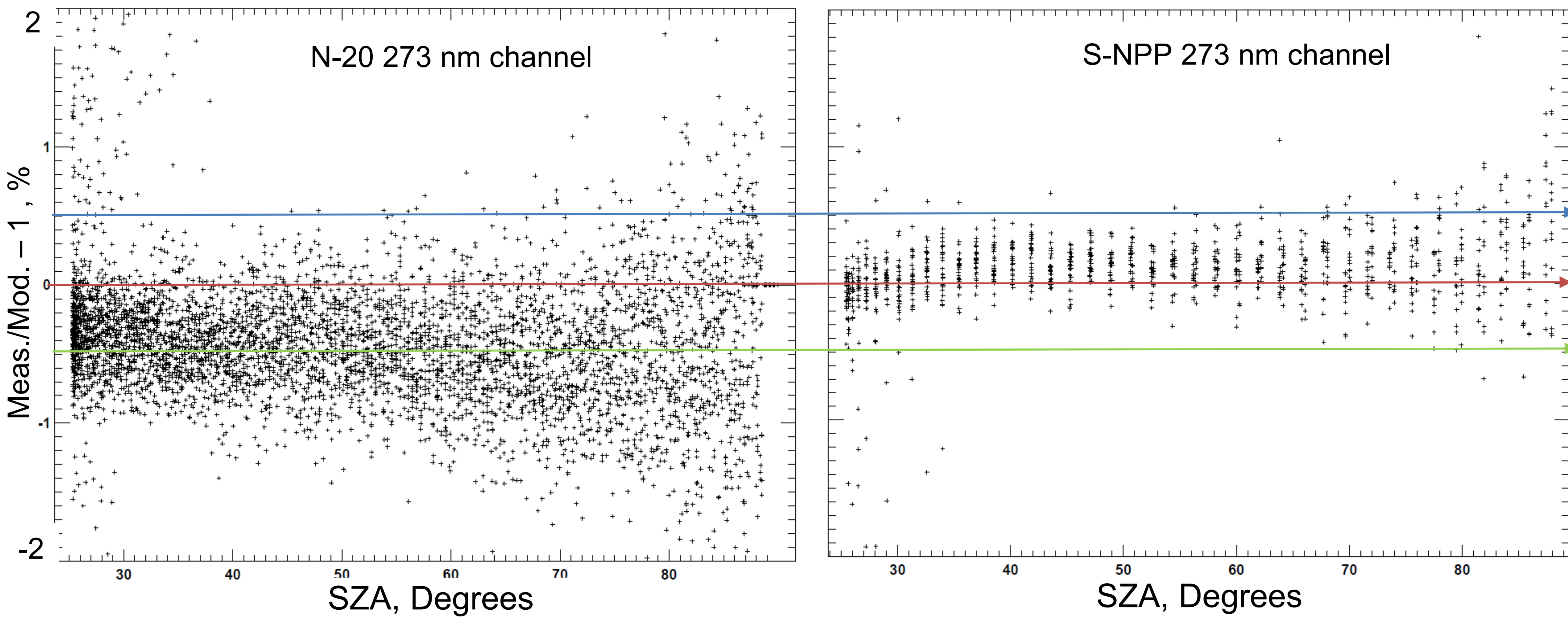
Solar Flux Change
New SDR versus Operations



Sensitivity to 0.04-nm shifts for 302 nm channel Initial Residuals compared to Equatorial change



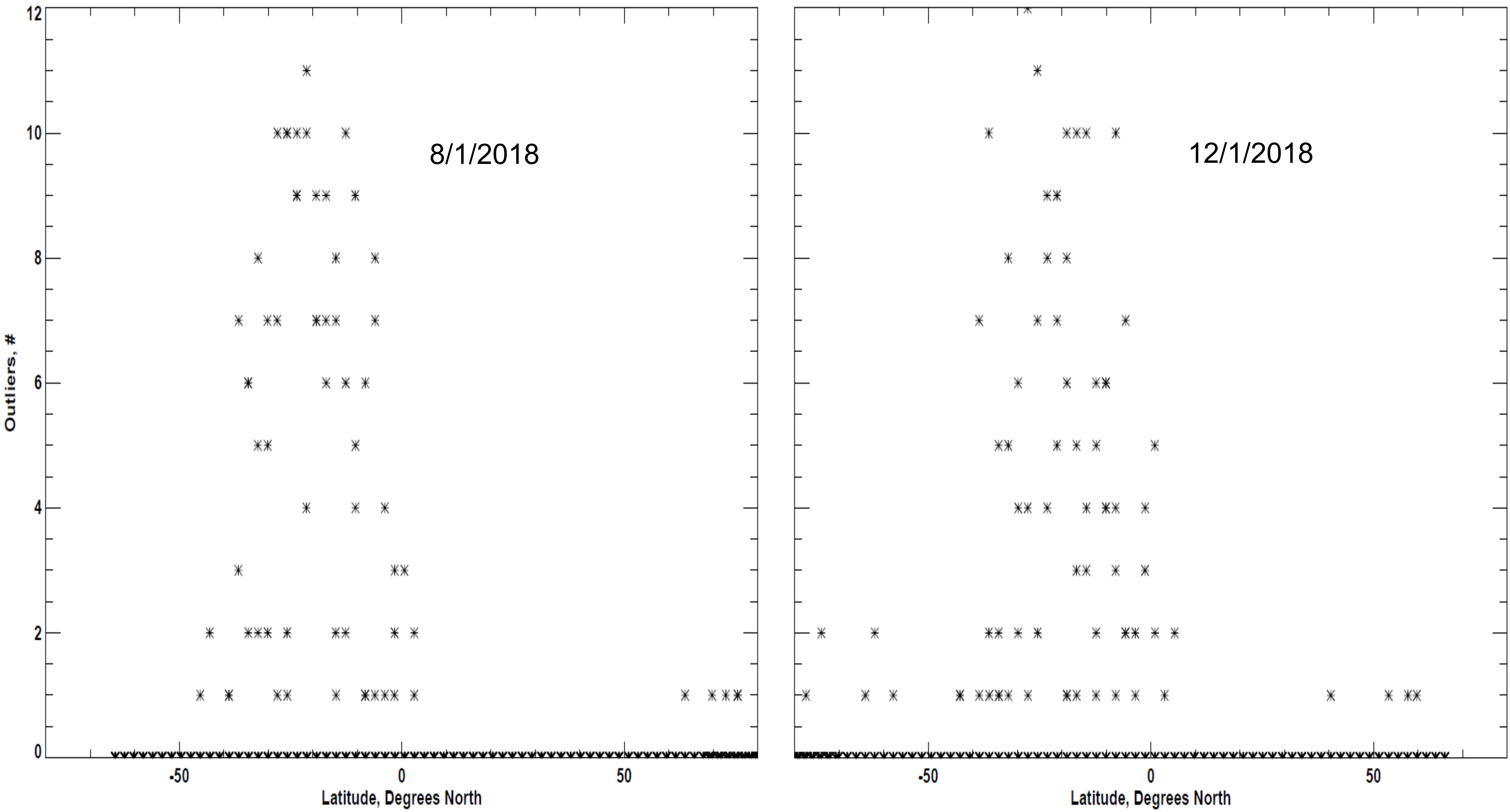
Measured minus Model "Bias" with SZA



Comparison of measured and modelled values for 273 nm channel for December 1, 2018. The figure on the left is NOAA-20 OMPS NP and the figure on the right is S-NPP OMPS NP.

F&IC Summary & Conclusions

- A simple model can be used to identify outliers from charged particle events.
- The single channel albedo values used in the V8Pro can be replaced by values from a fit over a local wavelength interval.
- This method will work well for small numbers of outliers.
- It will provide reduced noise estimates of the values even if no outliers are present.
- The method can also identify the presence of PMCs for the medium resolution NOAA-20 OMPS NP SDRs. Studies could be conducted comparing the aggregated FOVs to the individual ones to estimate the contamination of S-NPP OMPS NP SDRs and EDRs from PMC signals to add to the findings in [2] Thomas et al. 1991 and [3] Bak et al. 2016.



8/1/2018
12/1/2018
Outliers, #
Latitude, Degrees North
Latitude, Degrees North
0
2
4
6
8
10
12
-50
0
50

WHAT I KNOW (AND DON'T KNOW*) ABOUT WAVELENGTH SCALES, BANDPASSES AND DICHROICS

STUDY USING S-NPP OMPS AND NOAA-20 OMPS

L. Flynn, NOAA

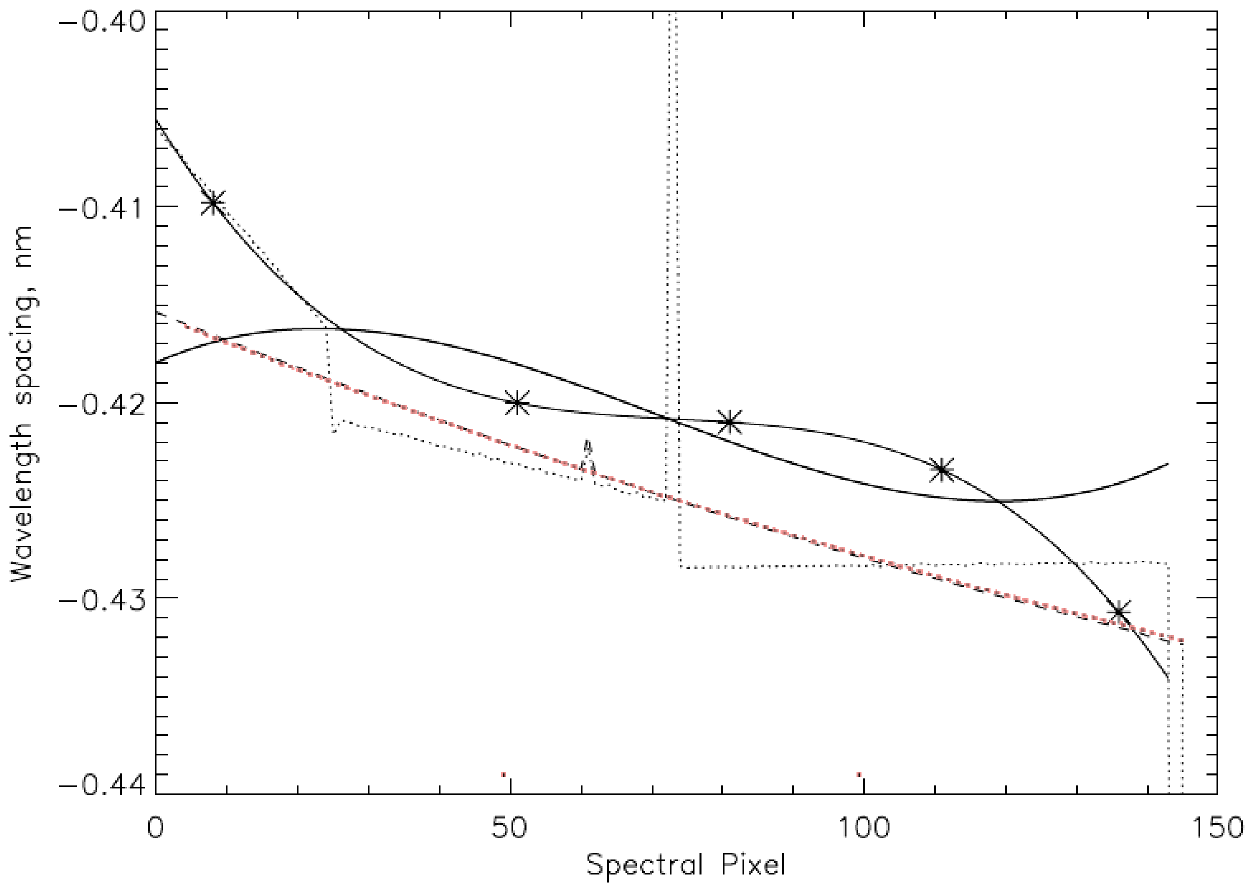
* Not an exhaustive list.

Wavelength Scales (Pixel Centers)

- The response of the instrument to a monochromatic input (e.g., Tunable Laser) at a range of spectral wavelengths, λ_m, and spatial locations, row j, is obtained.
- For each spatial row (or perhaps collection of adjacent spatial rows) above a threshold signal, the corrected (Dark, Offset and Pixel Response) counts are used to find the weighted-average spectral pixel, p_m, for each input wavelength, λ_m. Notice that this does not take into account any wavelength dependent throughput variations as each monochromatic data set is normalized relative to its total corrected counts.
- This gives a two dimensional data set of the form,

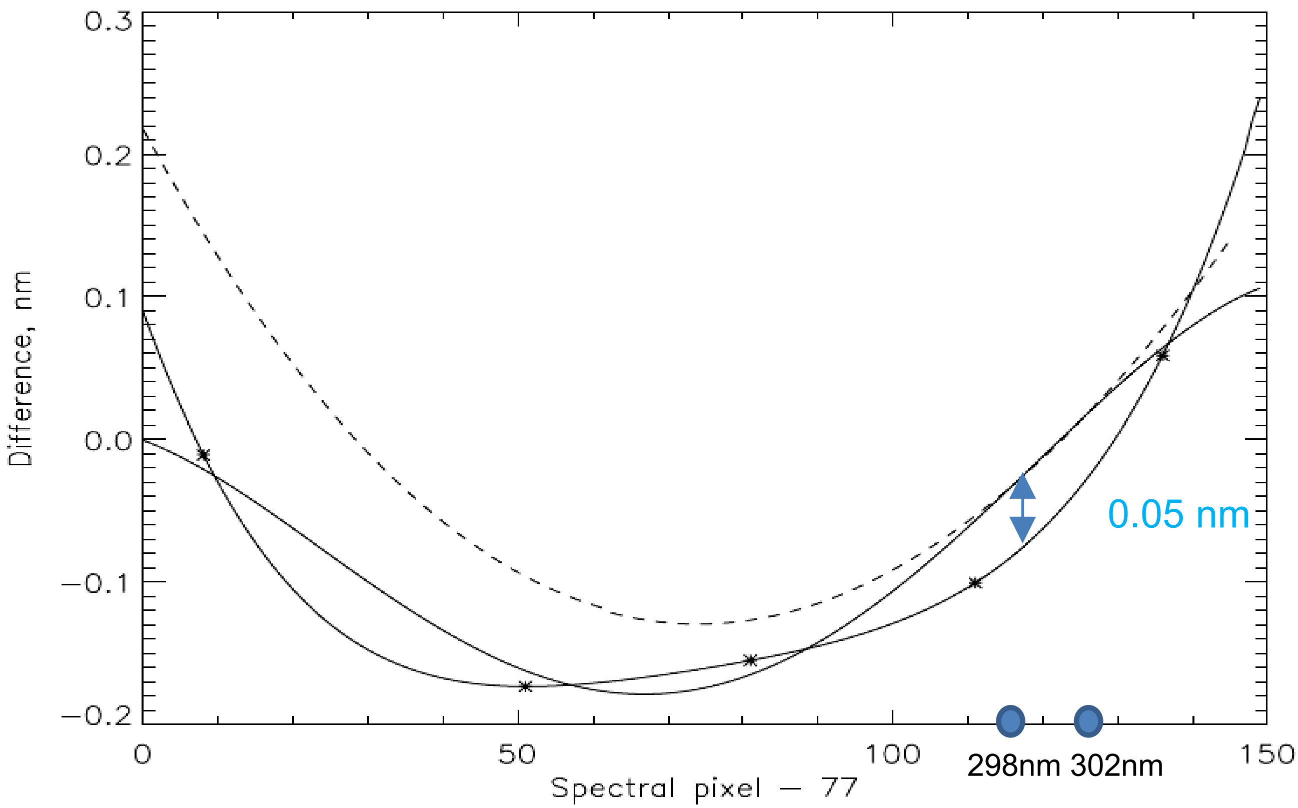
  $$\{(\lambda_m, p_m)_j\}$$

  for input wavelength λ_m and spatial row j.
- Inverting this, by considering wavelength as a function of pixel instead of pixel as a function of wavelength, and fitting with a two-dimensional model provides a way to assign wavelengths to pixels over the full active region. These are used to produce the Band Center data sets.
- The figures on the following slide compare the wavelength scales for OMPS NP for S-NPP and JPSS-1 (NOAA-20) to a simple linear model by examining their spacing. That is, the plots show the differences in the band centers of adjacent pixels (or macropixels). for spatial rows. If the wavelength scales were linear, these curves would be constants. The figure on the slide after the next one shows the differences of the wavelength scales with linear ones.



The S-NPP steps (dashed) are close to linear meaning that the wavelength scale is quadratic while the NOAA-20 steps (solid) follow a cubic meaning that its wavelength scale is quartic. The solid line without symbols are the NOAA-20 CBC data. The solid line with symbols are the NOAA-20 CBC data adjusted by the bandpass-weighted average wavelengths. The symbols in the figure show the locations of the five NOAA-20 spectral measurement sets. The red line is the S-NPP data adjusted by its bandpass-weighted average offsets.

Wavelength Scale versus Linear



The S-NPP (dashed) show the close to quadratic wavelength scale. The NOAA-20 (solid) follow a quartic wavelength scale. The solid line without symbols are the NOAA-20 CBC data. **The solid line with symbols (*) are the NOAA-20 CBC data adjusted by the bandpass-weighted average wavelengths**. The symbols in the figure show the locations of the five NOAA-20 spectral measurement sets.

Wavelength Scale Notes

- The CBC data set from the monochromatic laser analysis is good in that it should provide an accurate estimate of the wavelength that would have a weighted average response at a selected pixel's center.
- The analysis* method is insensitive to throughput variations with wavelength. For example, the results would be the same with or without a dichroic in the system in terms of throughput – the dichroic might also act as a broadening or scattering optical component which would be captured.
- The CBC data does not give the wavelength that would represent a pixel's weighted-average response wavelength (its bandpass-weighted wavelength centroid).

* This assumes that the analysis works with corrected counts (or counts converted to radiance by using the instrument's throughput for the input wavelength, not by using each pixel's average calibration coefficient).

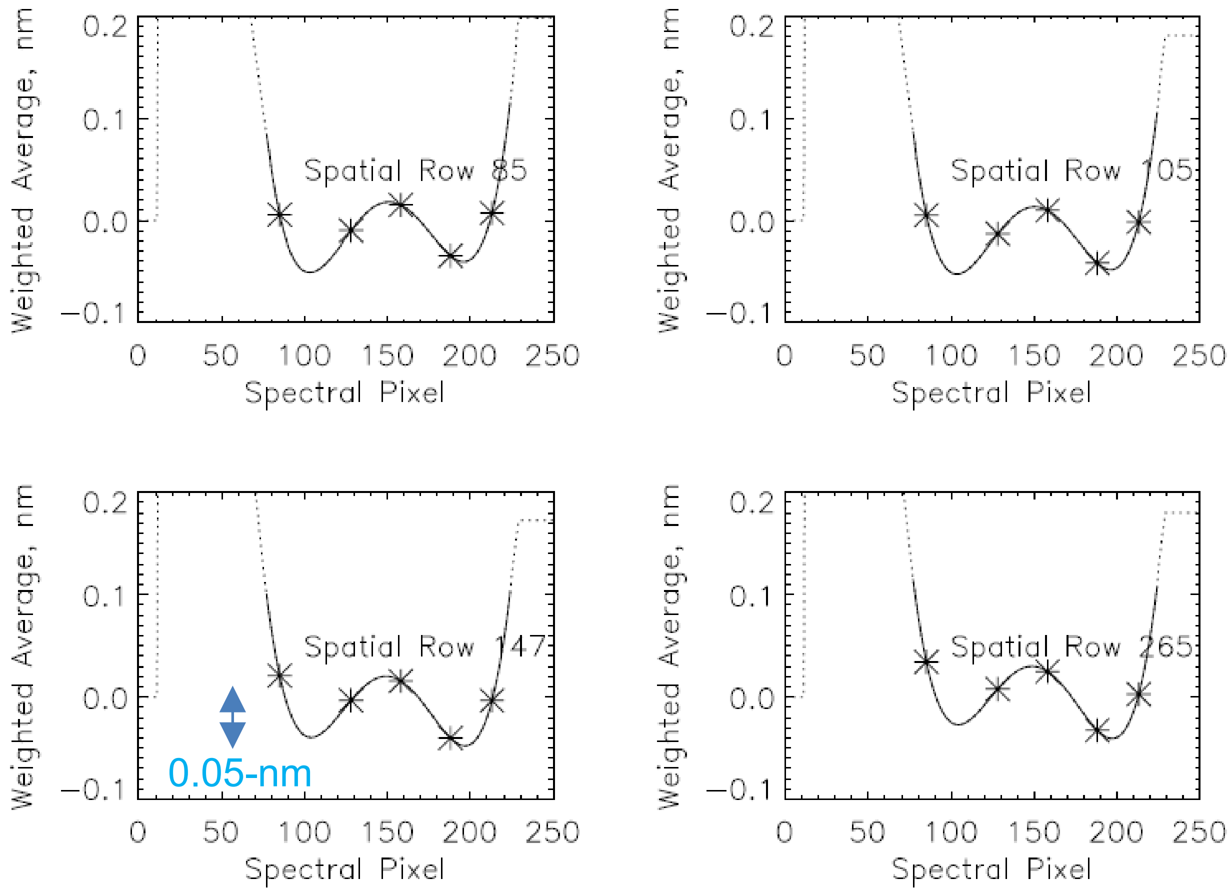
Bandpass offsets

- The bandpass-weighted average wavelength offsets in nm are computed as

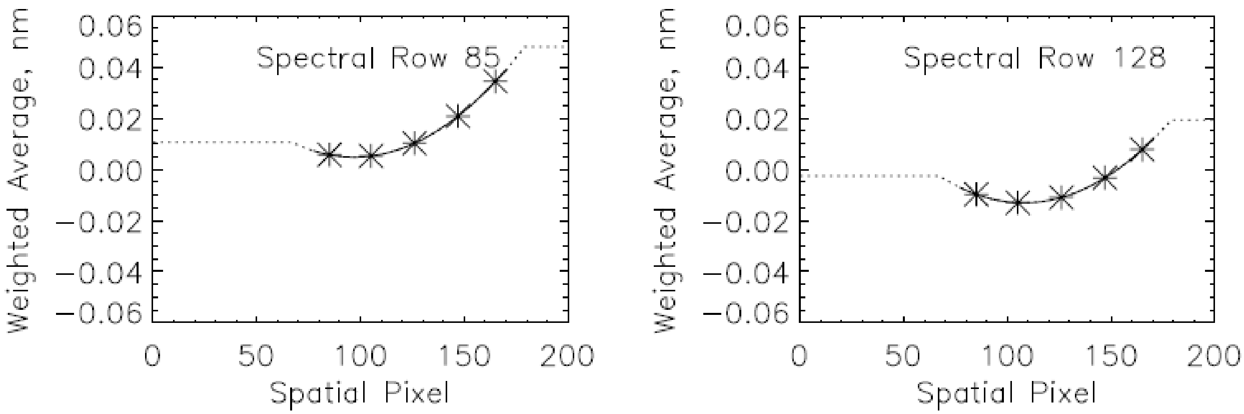
  $$sum\{BP_k*w_k\}/sum\{BP_k\}$$

  with w_k = (i-25)*0.1 and the sums taken over k=0 to 50, where BP is a set of 51 bandpass response values given every 0.1 nm centered at the pixel band centers from the earlier computations. Slices though the 2-D bandpass offset surface for NOAA-20 NP are displayed on the next two slides.
- The offsets for S-NPP are very small as evidenced by close agreement of the red and black dashed lines in Slide #3. That is the S-NPP bandpasses are centered in agreement with the wavelength scale.

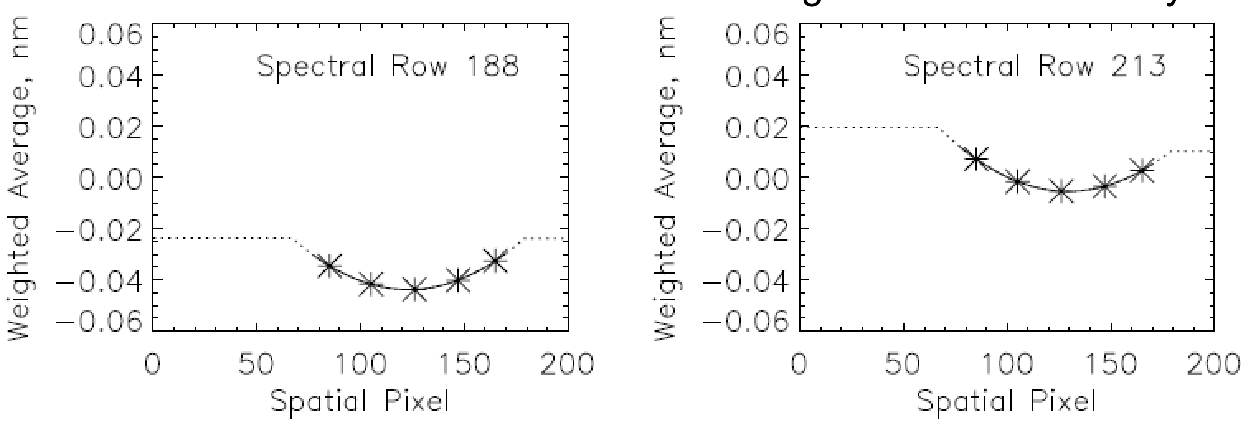
Weighted Average Bandpass Offsets for NOAA-20 Versus Wavelength Pixel



Weighted-Average Bandpass Offsets for NOAA-20 Versus Cross-track Spatial Pixel

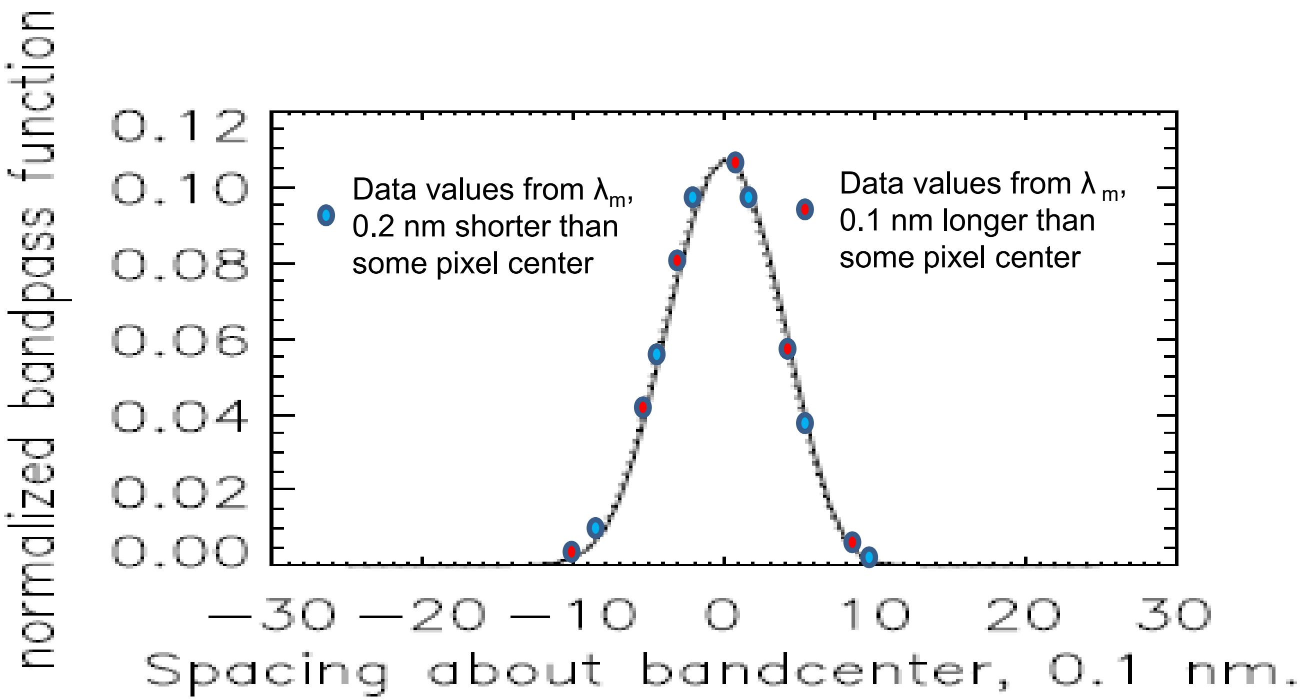


Solid lines denote the active region of the CCD array.



Bandpass Estimation (1)

- The same data used to get the wavelength scales can be used to get the non-wavelength-throughput-dependent bandpasses. One takes the measurements for a given laser wavelength input and again normalizes the total counts over some localized spectral and spatial region. The result is used to provide data points by using the laser input wavelength relative to the pixel centers computed earlier.



Bandpass Estimation (2)

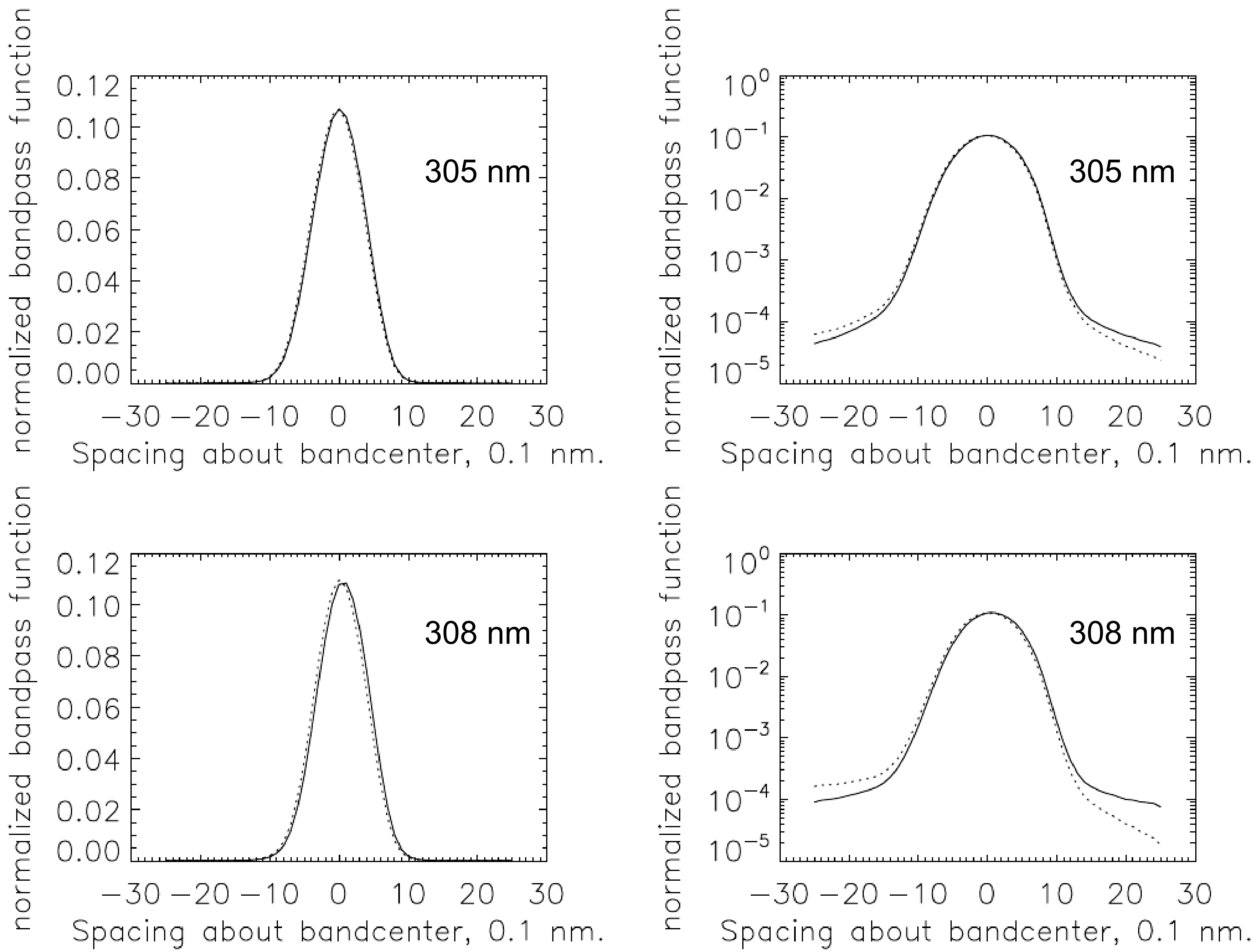
- There are two implicit key assumptions in this approach:

1. That the bandpasses change slowly in both spectral and spatial dimension so one can work with measurements over 12 spectral pixels and 8 spatial pixels.
2. That the normalization of a bandpass as sampled every 0.42 nm provides comparable values as the sampling is shifted relative to the center. (For the JPSS bandpasses, I have checked this by comparing the sums of every fourth bandpass value and it holds at the 0.2% level.)

- There is the further assumption that the corrected count responses for different pixels are consistent for a given specific photon energy / wavelength over the local analysis region.

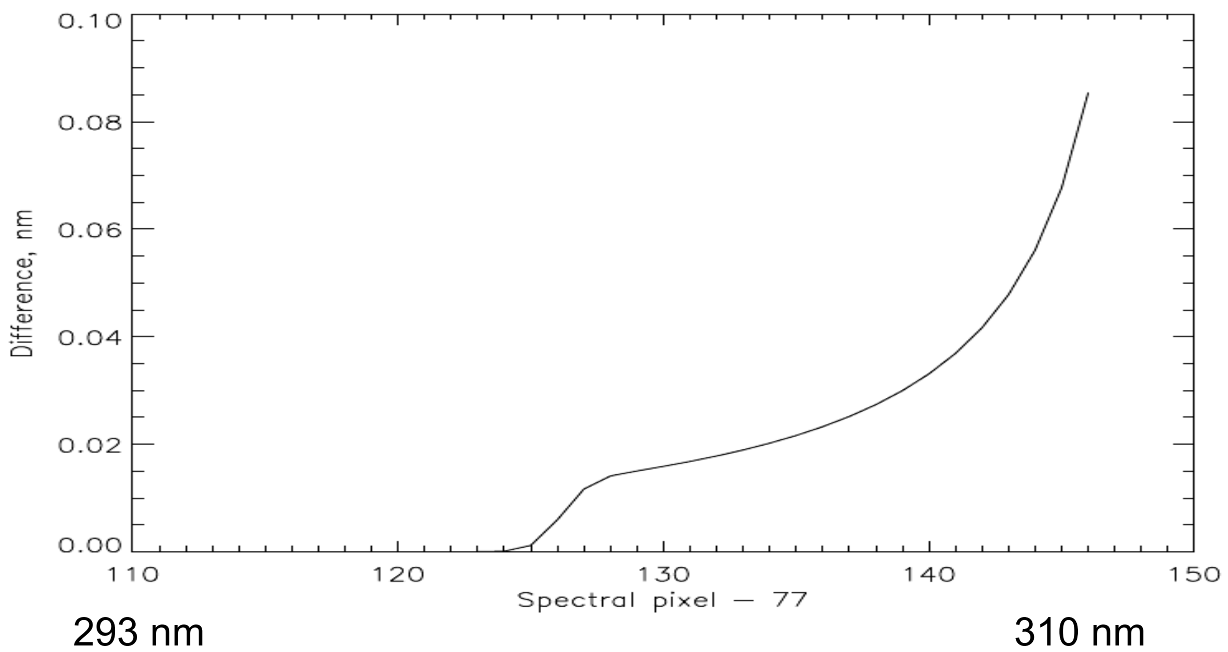
Bandpass Estimation (3)

- Again, these bandpasses will be the idealized instrument response functions without taking into account the wavelength-dependent throughput. One can adjust the bandpasses by using the relative wavelength dependent throughput to create the expected instruments bandpasses but this requires some assumptions about how the pixel count to radiance data are constructed from measurements.
- The pixel-dependent calibration constants were used as a proxy for wavelength-dependent throughput variations to see how much the real bandpasses would be changed. The pixel level constants were used by assigning the conversion value to the central wavelength. These were linearly interpolated to create a set of values with 0.1-nm spacing about the central wavelength of a pixel. The full set of values are convolved with the current bandpass data for that pixel and central wavelength to produce throughput-weighted bandpass values.
- The figures on the next page compare unadjusted (Solid) and adjusted (Dotted) bandpasses with linear (Left) and log (Right) scales for 305 nm (Top) and 308 nm (Bottom) for S-NPP OMPS NP.


305 nm
305 nm
308 nm
308 nm
normalized bandpass function
Spacing about bandcenter, 0.1 nm.
0.12
0.10
0.08
0.06
0.04
0.02
0.00
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
−30 −20 −10 0 10 20 30

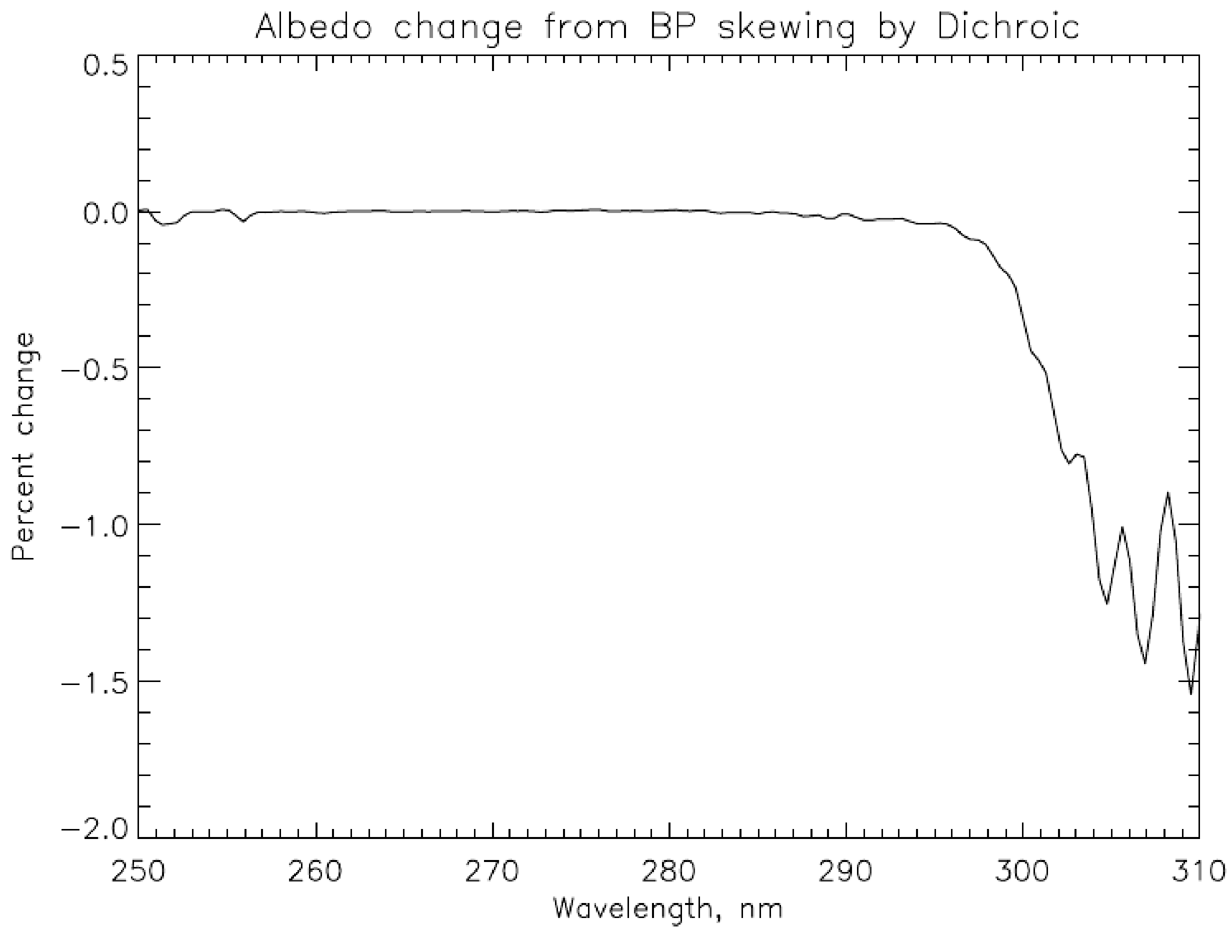
Bandpass Offsets from the Dichroic

- The throughput adjustments creates bandpasses with different centering – different weighted-average bandpass wavelength offsets. The figure below shows the differences in the weighted-average bandpass centers, old – new,



Applying the new Bandpasses

- Since the albedo is rapidly changing over the 300 nm to 310 nm interval, changing the bandpasses will affect the Solar and Earth View data differently leading to changes in the expected albedo. That is, there will be significant differences in an RT instrument table created by the two sets of bandpasses.
- The figure on the next slides uses a single set of measured NP radiance and irradiance spectra interpolated to higher density and convolved with the old and new bandpasses to estimate the albedo changes.
- The sign of these changes will switch from the NP to the NM over the 300 nm to 310 nm interval, as the throughput gradients from the dichroic are in the opposite directions.

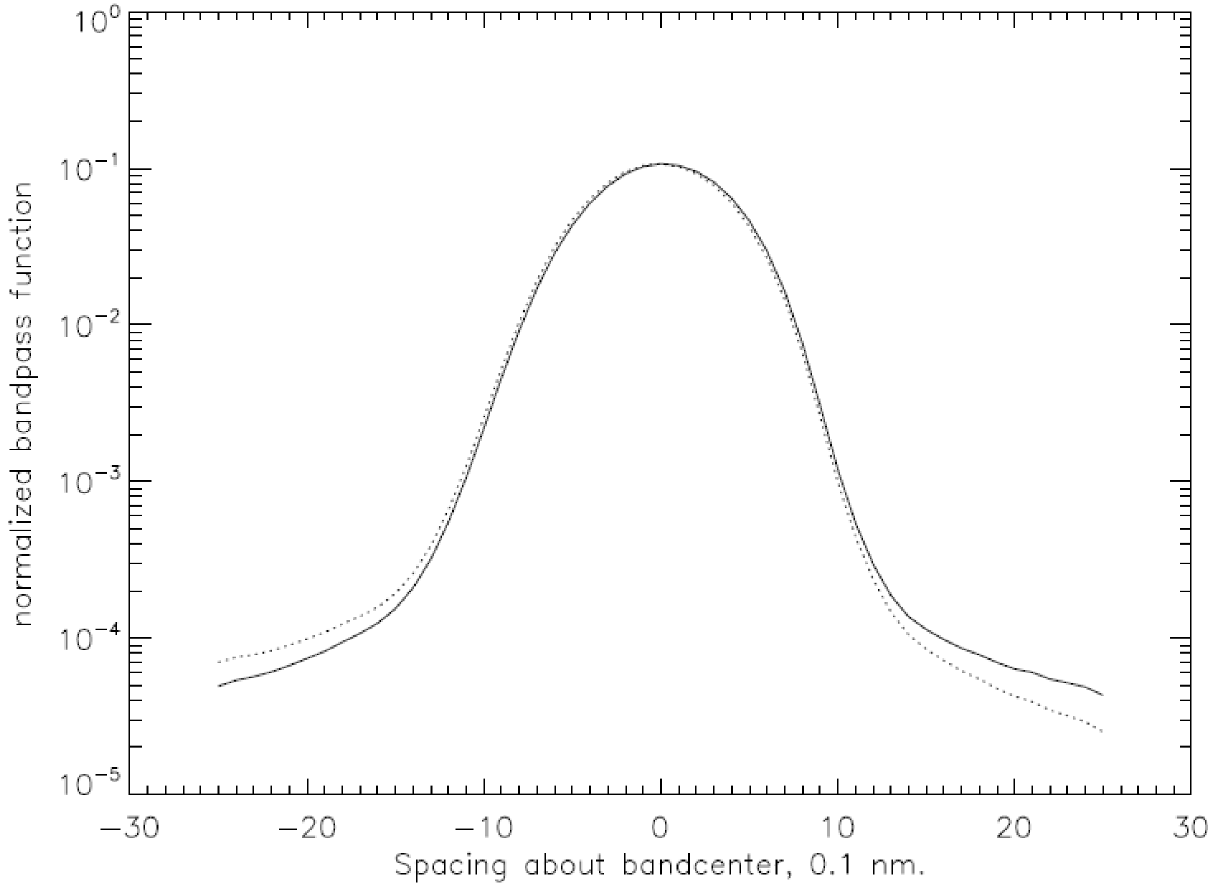

Albedo change from BP skewing by Dichroic
Percent change
Wavelength, nm
0.5
0.0
−0.5
−1.0
−1.5
−2.0
250
260
270
280
290
300
310

Open Questions

- Why does the S-NPP data show a good fit by a quadratic in wavelength and the bandpasses have small offsets*? Or, Why do the NOAA-20 data need a quartic to get a good fit and the bandpasses have large offsets^?
- Why don't the provided bandpasses show the dichroic skewing? Will the throughput adjustments by using skewed bandpasses improve the RT forward model albedo comparisons and OMPS NM/NP agreement in the overlap region for S-NPP?
- How accurately can we estimate the wavelength scales in-orbit?

* I still need to check the S-NPP data to see how well the observed values are fit by the provided characterizations.

^ I expect/assume that the bandpasses should be consistent with the bandcenters from the analysis of the same set of laser measurements.



normalized bandpass function
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
−30
−20
−10
0
10
20
30
Spacing about bandcenter, 0.1 nm.