**Beta Maturity Science Review
For V8TOz & V8TOS Total Column Ozone EDR**

*Presented by L. Flynn
Date: 3/30/2023*

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

2. Provisional
o 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.
o Product analyses are sufficient for qualitative, and limited quantitative, determination of product fitness-for-purpose.
o Documentation of product performance, testing involving product fixes, identified product performance anomalies, including recommended remediation strategies, exists.
o Product is recommended for potential operational use (user decision) and in scientific publications after consulting product status documents.

3. Validated
o Product performance has been demonstrated over a large and wide range of representative conditions (i.e., global, seasonal).
o 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.
o Product analyses are sufficient for full qualitative and quantitative determination of product fitness-for-purpose.
o Product is ready for operational use based on documented validation findings and user feedback.
o Product validation, quality assurance, and algorithm stewardship continue through the lifetime of the instrument.

- Product Requirements
- Pre-launch Performance Matrix/Waivers – None
- Beta Maturity Performance Validation
  - On-orbit instrument performance assessment
    - Identify all of the instrument and product characteristics you have verified/validated as individual bullets
    - Identify pre-launch concerns/waivers, mitigation and evaluation attempts with on-orbit data
- Users/Downstream-Products feedback
- Risks, Actions, Mitigations
  - Potential issues, concerns
- Path forward (to the next maturity stage)
- Summary

Maturity Review - Exit Criteria

- Beta Maturity Performance is well characterized and meets/exceeds the requirements:
  - On-orbit instrument performance assessment
    - Provide summary for each identified instrument and product characteristic you have validated/verified as part of the entry criteria
    - Provide summary of pre-launch concerns/waivers mitigations/evaluation and address whether any of them are still a concern that raises any risk.
- Updated Maturity Review Slide Package addressing review committee's comments for:
  - Cal/Val Plan and Schedules
  - Product Requirements
  - {Beta/Provisional/Validated} Maturity Performance
  - Risks, Actions, Mitigations
  - Path forward (to the next maturity stage)

BETA MATURITY REVIEW MATERIAL

- Algorithm Cal/Val Team Members
- Product Overview/Requirements
- Evaluation of algorithm performance to specification requirements
  – Algorithm version, processing environment
  – Evaluation of the effect of required algorithm inputs
  – Quality flag analysis/validation
  – Error Budget
- ~~User Feedback~~
- ~~Downstream Product Feedback~~
- Risks, Actions, and Mitigations
- Documentation (Science Maturity Check List)
- Conclusion
- Path Forward

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	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	Jeannette Wild	UMD	Applications, CDRs, validation
JAM	Starry Manoharan	JPSS/Aerospace	Coordination
Adjunct	Bigyani Das	STAR/ASSISTT	Deliveries to NDE / NCCF
PAL	Vaishali Kapoor	OSPO	Atmospheric Chemistry Product Area Lead

OMPS TC EDR Performance Characteristics

	Threshold	Objective
Ozone TC Applicable Conditions 1, 2.		
a. Horizontal Cell Size	50 x 50 km^2 @ nadir	10 x 10 km^2
b. Vertical Cell Size	0 - 60 km	0 - 60 km
c. Mapping Uncertainty, 1 Sigma	5 km at Nadir	5 km
d. Measurement Range	50 - 650 milli-atm-cm	50-650 milli-atm-cm
e. Measurement Precision	.	.
1. X < 0.25 atm-cm	6.0 milli-atm-cm	1.0 milli-atm-cm
2. 0.25 < X < 0.45 atm-cm	7.7 milli-atm-cm	1.0 milli-atm-cm
3. X > 0.45 atm-cm	2.8 milli-atm-cm + 1.1%	1.0 milli-atm-cm
f. Measurement Accuracy	.	.
1. X < 0.25 atm-cm	9.5 milli-atm-cm	5.0 milli-atm-cm
2. 0.25 < X < 0.45 atm-cm	13.0 milli-atm-cm	5.0 milli-atm-cm
3. X > 0.45 atm-cm	16.0 milli-atm-cm	5.0 milli-atm-cm
g. Latency	90 min.	15 min.
h. Refresh	At least 90% coverage of the globe Every 24 hours (monthly average)	24 hrs.
i. Long-term Stability	1% over 7 years	0.5 % over 7 years
1. Threshold requirements only apply under daytime conditions with Solar Zenith Angles (SZA) up to 80 degrees. 2. The EDR shall be delivered for all SZA. 3. SO2 exclusion removed.	1 milli-atm-cm = 1 DU	

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Product Overview/Requirements

- Product performance requirements from JPSS L1RD supplement (threshold) versus observed/validated/JERD Vol. II

Attribute	Threshold	Observed/Validated
Geographic coverage	90% Daily Global Earth	SZA < 80° (>90% coverage)
Vertical Coverage	0-60 km	0-60 km (RT tables, physics)
Vertical Cell Size	NA	NA
Horizontal Cell Size	50x50 km² at nadir	10x9 km² at nadir
Mapping Uncertainty	5 km at nadir	3 km at nadir (SDR Team)
Measurement Range	50 – 650 DU	90-700 DU (SDR range and past algorithm performance)
Measurement Accuracy		
X < 250 DU	9.5 DU	
250 DU < X < 450 DU	13.0 DU	
X > 450 DU	16.0 DU	
Measurement Precision	for 50x50 km² product	for 10x9 km² product
X < 250 DU	6.0 DU	
250 DU < X < 450 DU	7.7 DU	
X > 450 DU	2.8 DU + 1.1%	

Processing Environment and Algorithms

- Description of processing environment and algorithms used to achieve the maturity stage:

  – Algorithm version: NDE I&T V8TOz v4r2

                                                 STAR Offline V8TOz v4r2

  – Version of LUTs used: Pre-launch

                                                  Revised instrument radiative transfer table

  – Effective date: 3/24/2023

- Findings/Issues from {previous-maturity}/last Review
- Improvements since {previous-maturity}/last Review
  - Algorithm Improvements
  - LUT / PCT updates

- Algorithm performance evaluation
  - Validation data sets (type, periods, coverage)
  - Validation strategies / methods
  - Validation results
  - Long term monitoring readiness

- Inter-sensor comparison
  - Compare with S-NPP and NOAA-20
  - ~~Compare with other satellite product~~

Major changes since Launch

- Regular weekly dark table and biweekly Solar and wavelength table updates for both SDRs.
  - Solar and wavelength updates for ground-to-orbit wavelength shifts based on first solar measurements for both OMPS NM (-0.14nm) and NP SDRs (-0.09nm).
  - Solar and wavelength updates for three pixel offset error for OMPS NM SDR.
  - Minor solar and wavelength updates for nadir macro-pixels, expected 4/7/2023.
  - Minor sample table update for macro-pixel #177 is in Mx 8/9, expected 6/2023.
- OMPS NM SDR changes and performance are discussed in the OMPS NM SDR briefing.
- NOAA-21 OMPS NM & NP SDRs have all major updates as of 3/24/2023.
- No changes yet to the V8TOz or V8TOS EDR algorithm or tables.
  - Offline processing is using a corrected NOAA-21 Instrument Table.
  - This table will need to be implemented to achieve Provisional Maturity performance.

Comparison of Cross-track Retrieval Averages (STAR) NEW RT TABLE
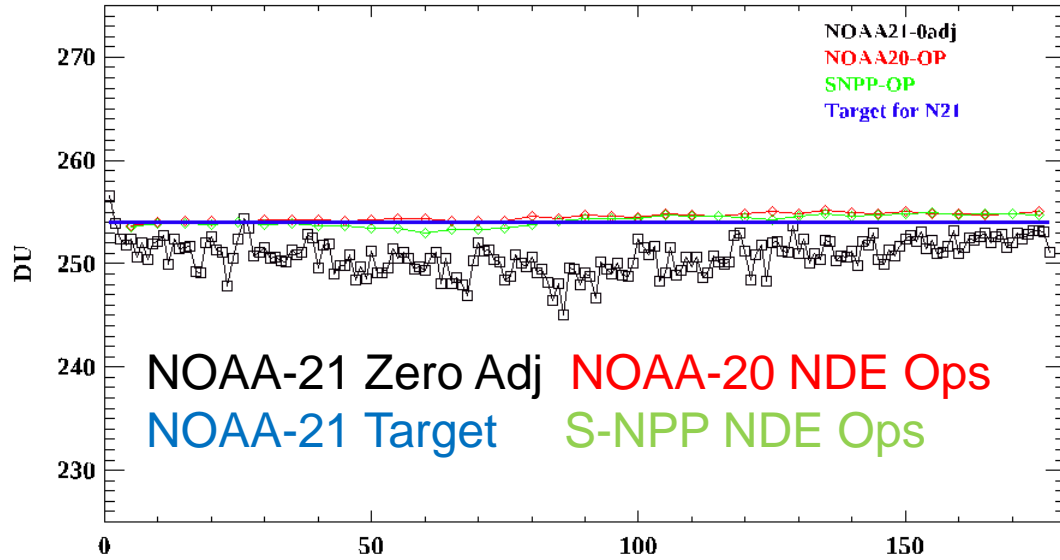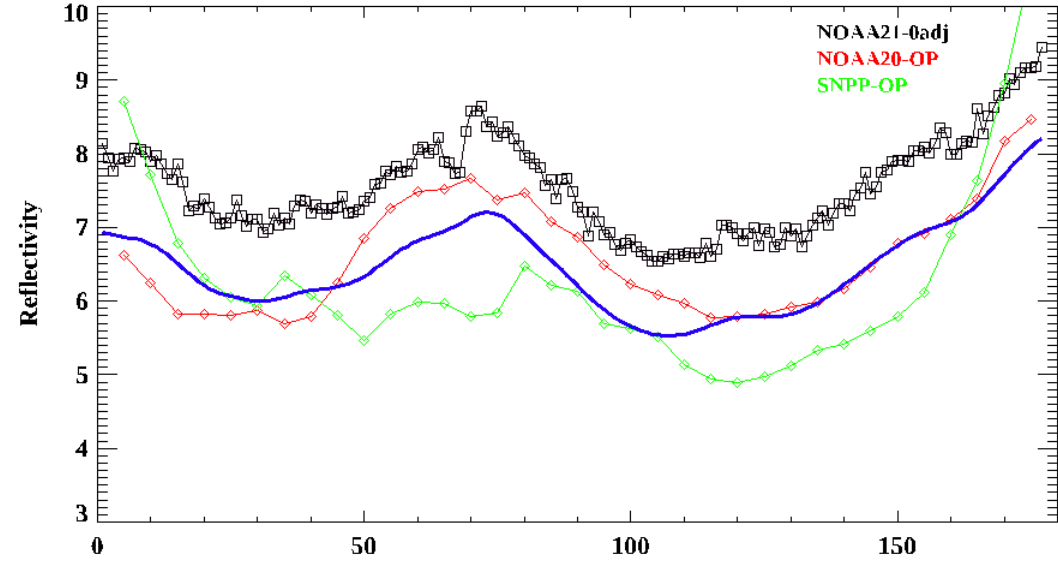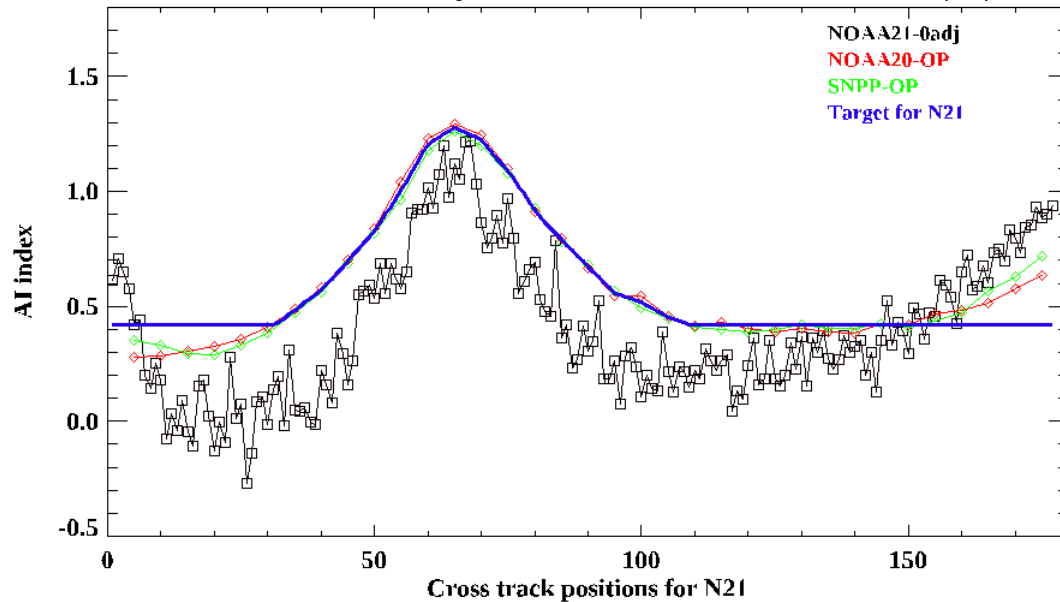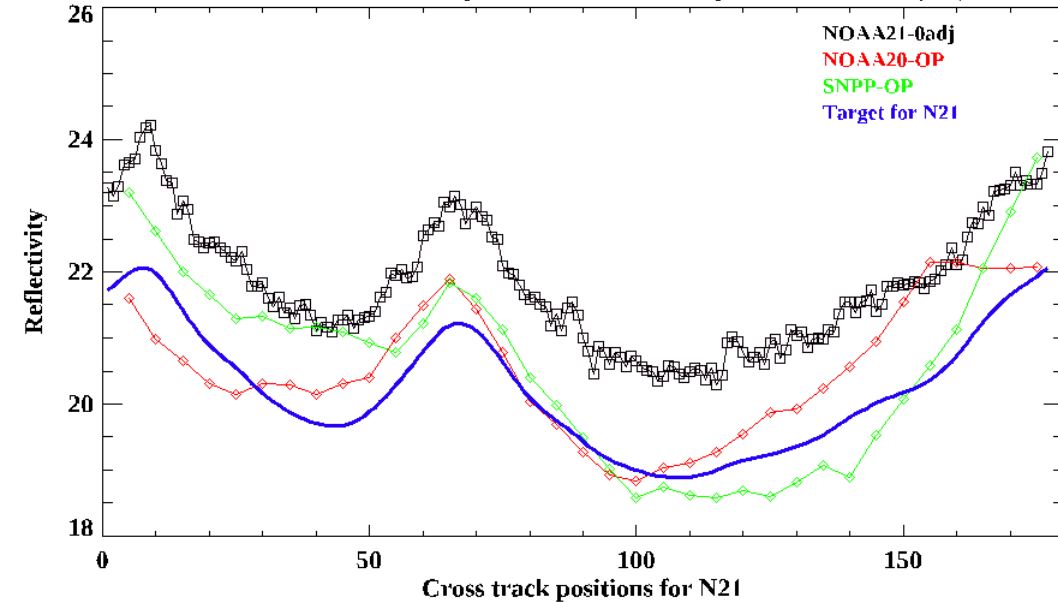
Current Bad RT Instrument Table

Total Colomn Ozone, NDE, N21-V8TOz, 2023/03/23

Dobson
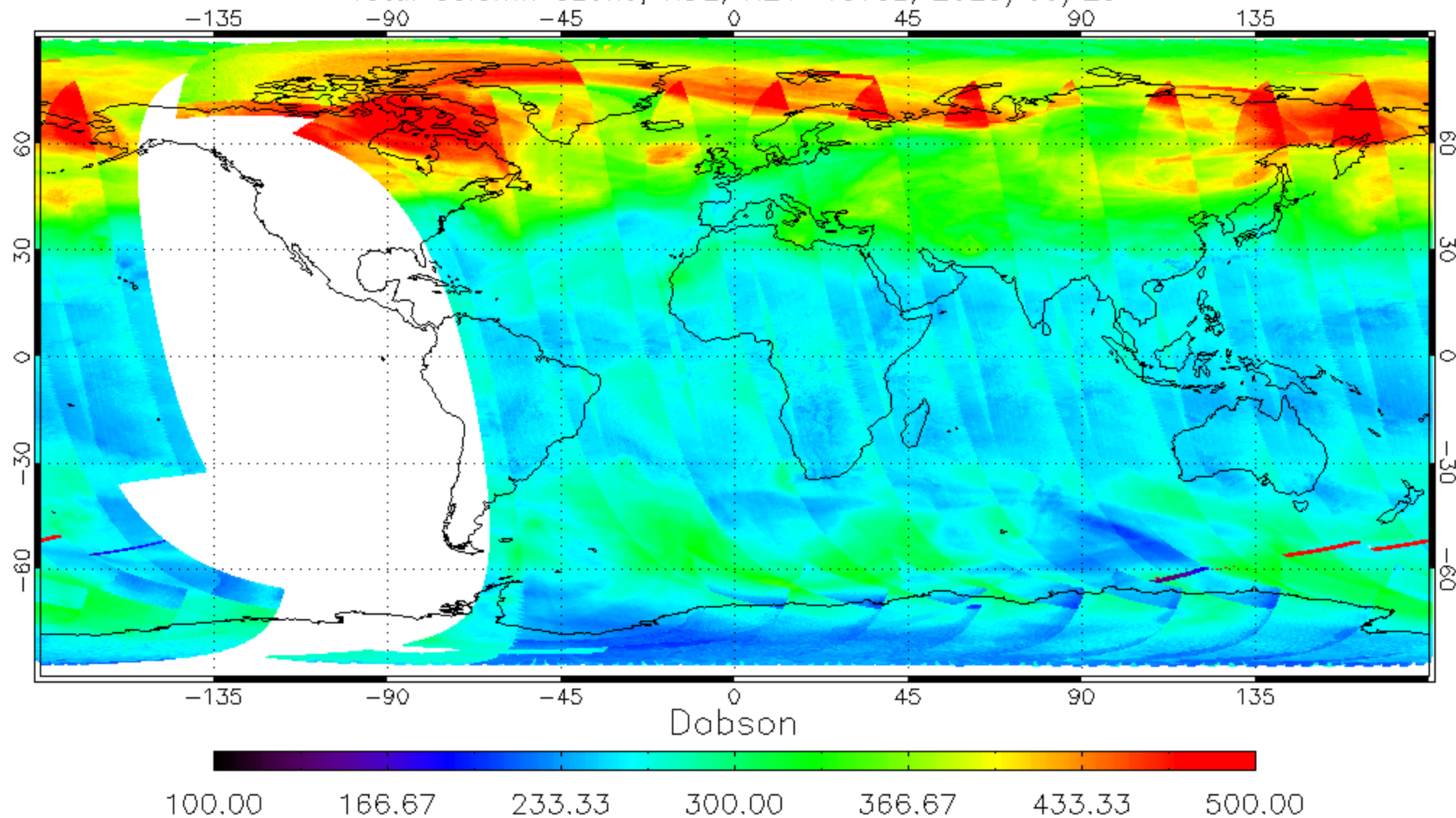
New Good N21 RT Instrument Table
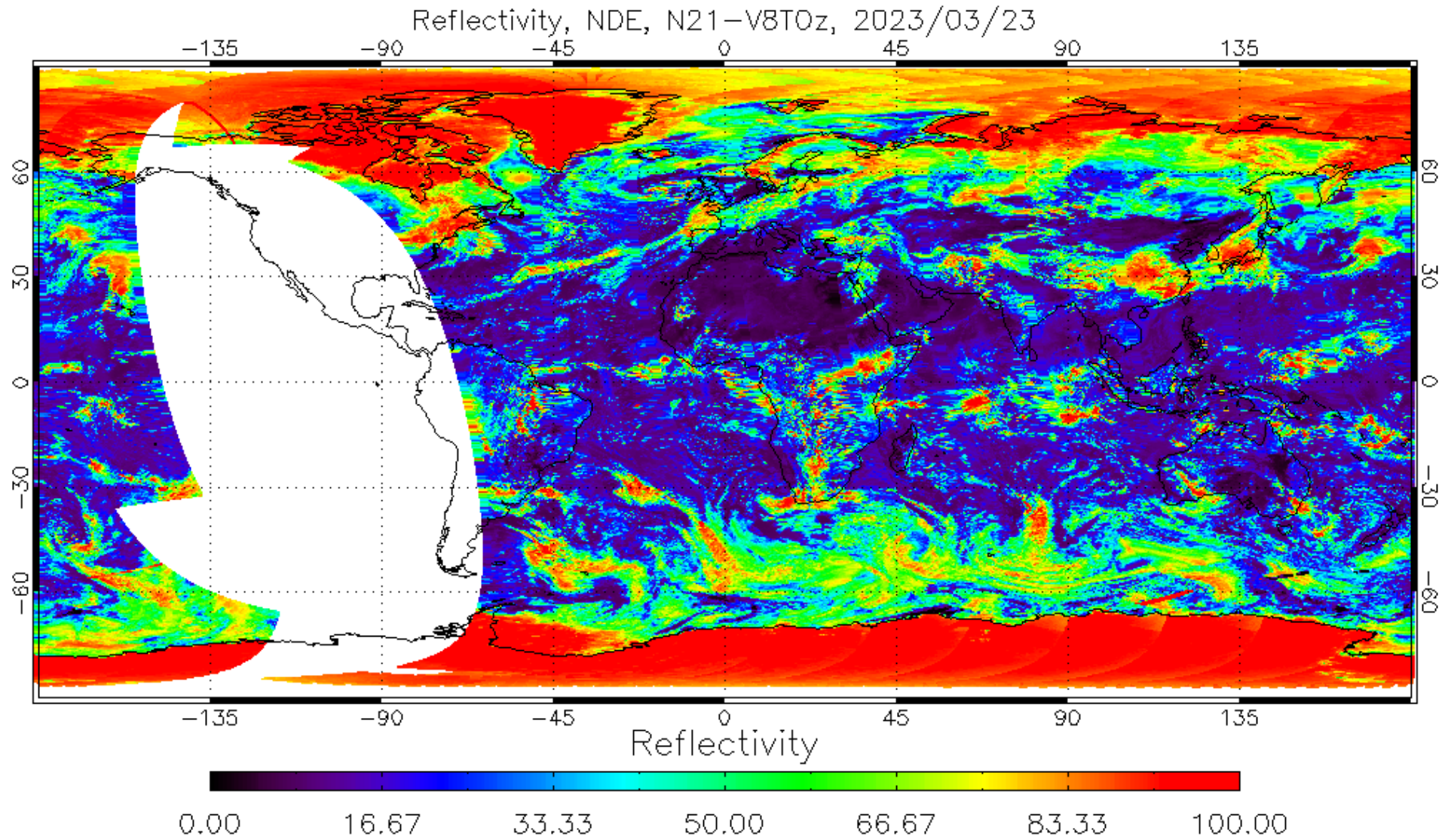

Total Colomn Ozone, NewLUT, N21-V8TOz, 2023/03/23

Dobson
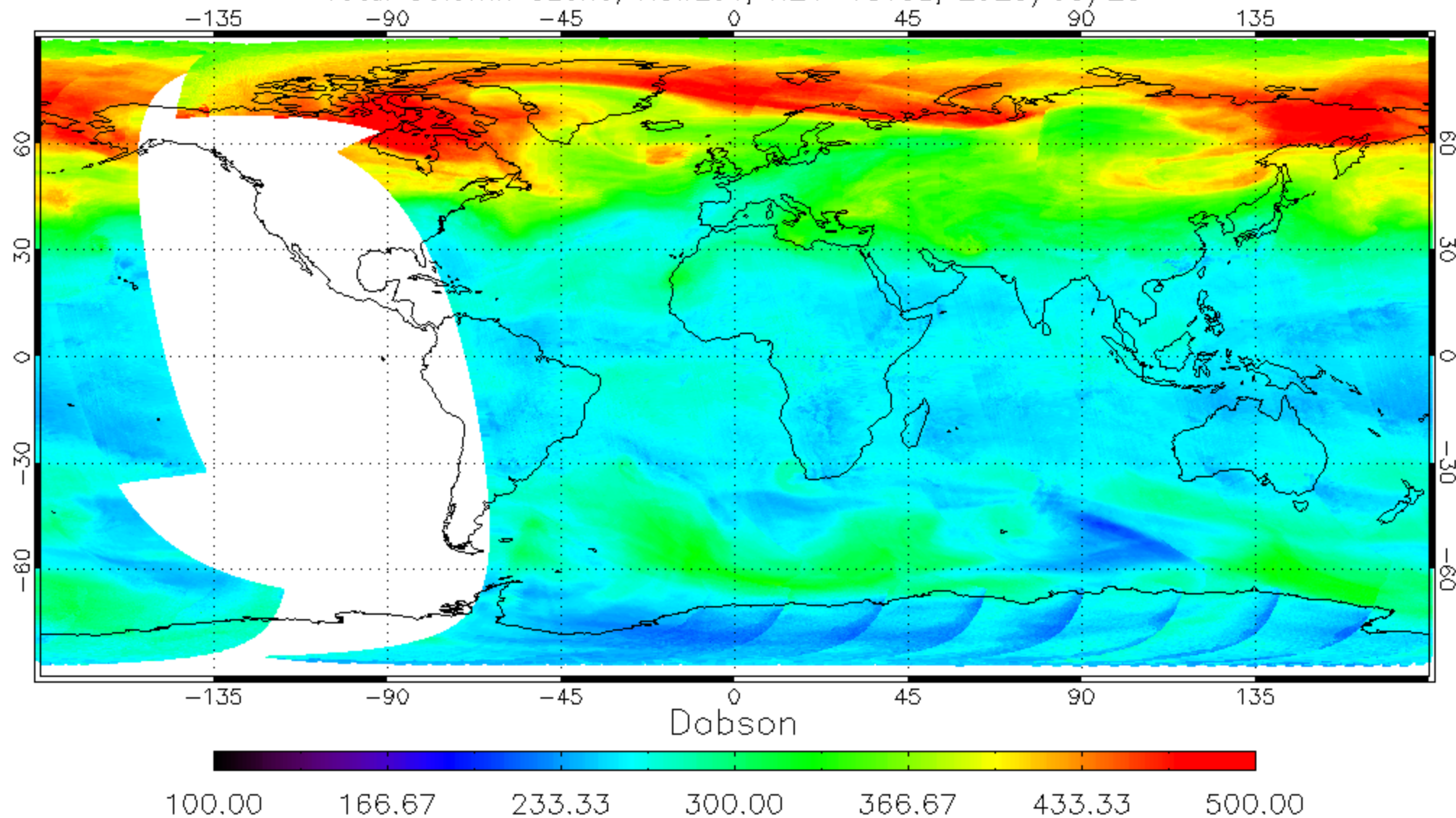
NOAA-20 RESULTS
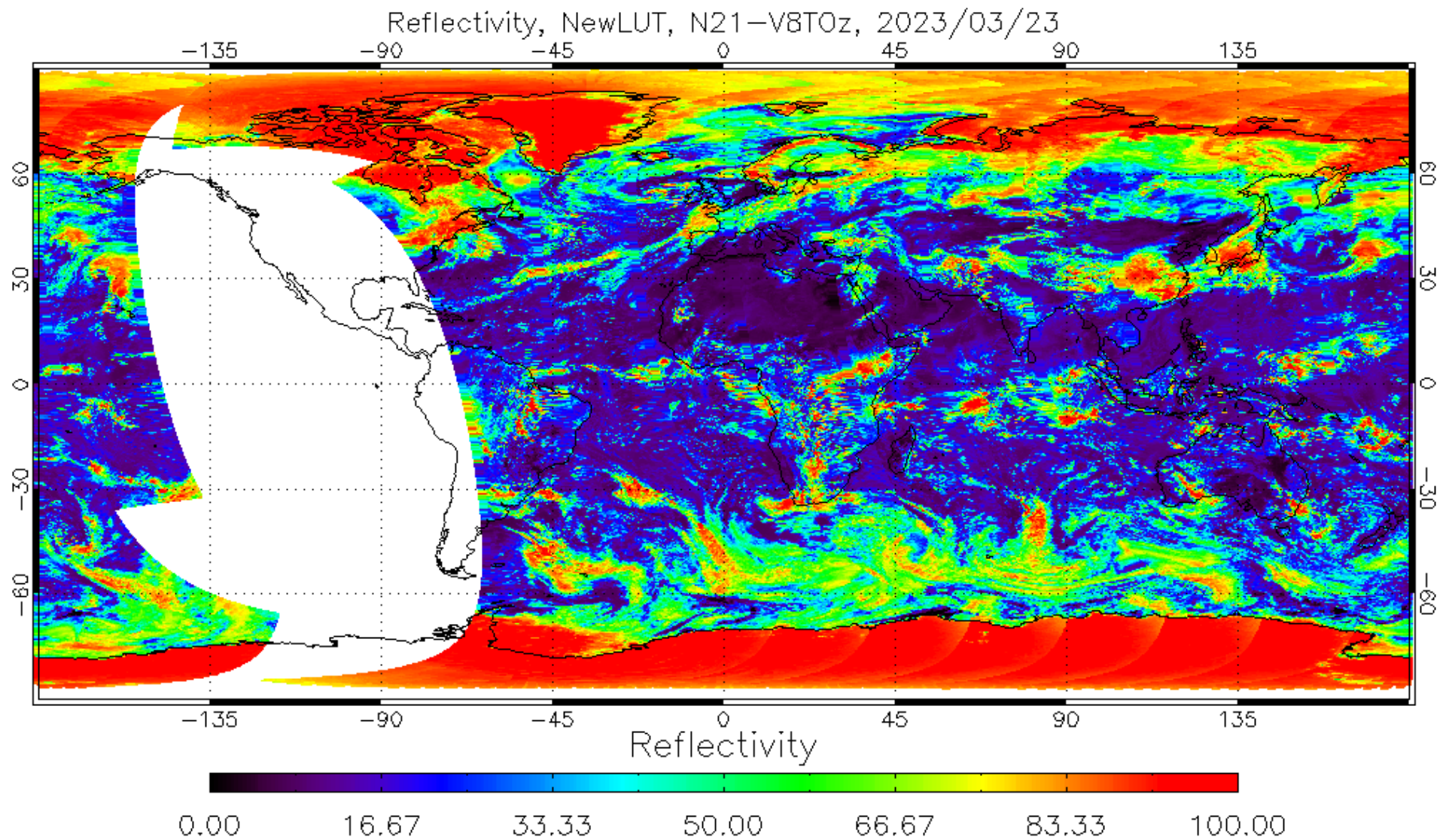

Total Colomn Ozone, NDE, N20-V8TOz, 2023/03/23
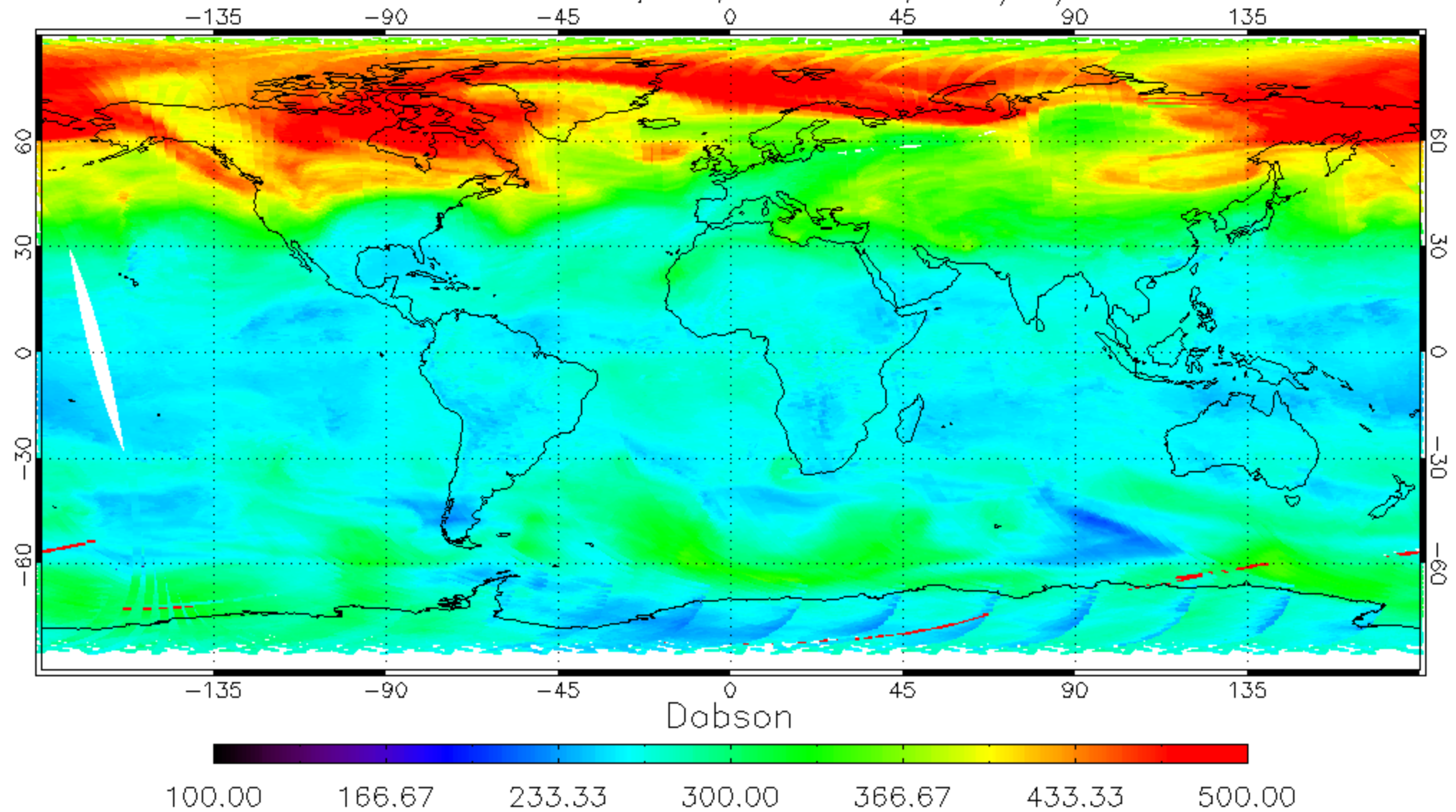
Dobson

Current Bad RT Instrument Table

Reflectivity, NDE, N21-V8TOz, 2023/03/23

Reflectivity

New Good N21 RT Instrument Table

Reflectivity, NewLUT, N21-V8TOz, 2023/03/23

Reflectivity

0.00 16.67 33.33 50.00 66.67 83.33 100.00

Reflectivity, NDE, N20−V8TOz, 2023/03/23

Reflectivity

Current Bad RT Instrument Table

Aerosol Index, NDE, N21-V8TOz, 2023/03/23

New Good N21 RT Instrument Table

Aerosol Index, NewLUT, N21-V8TOz, 2023/03/23

Aerosol Index

Aerosol Index, NDE, N20–V8TOz, 2023/03/23
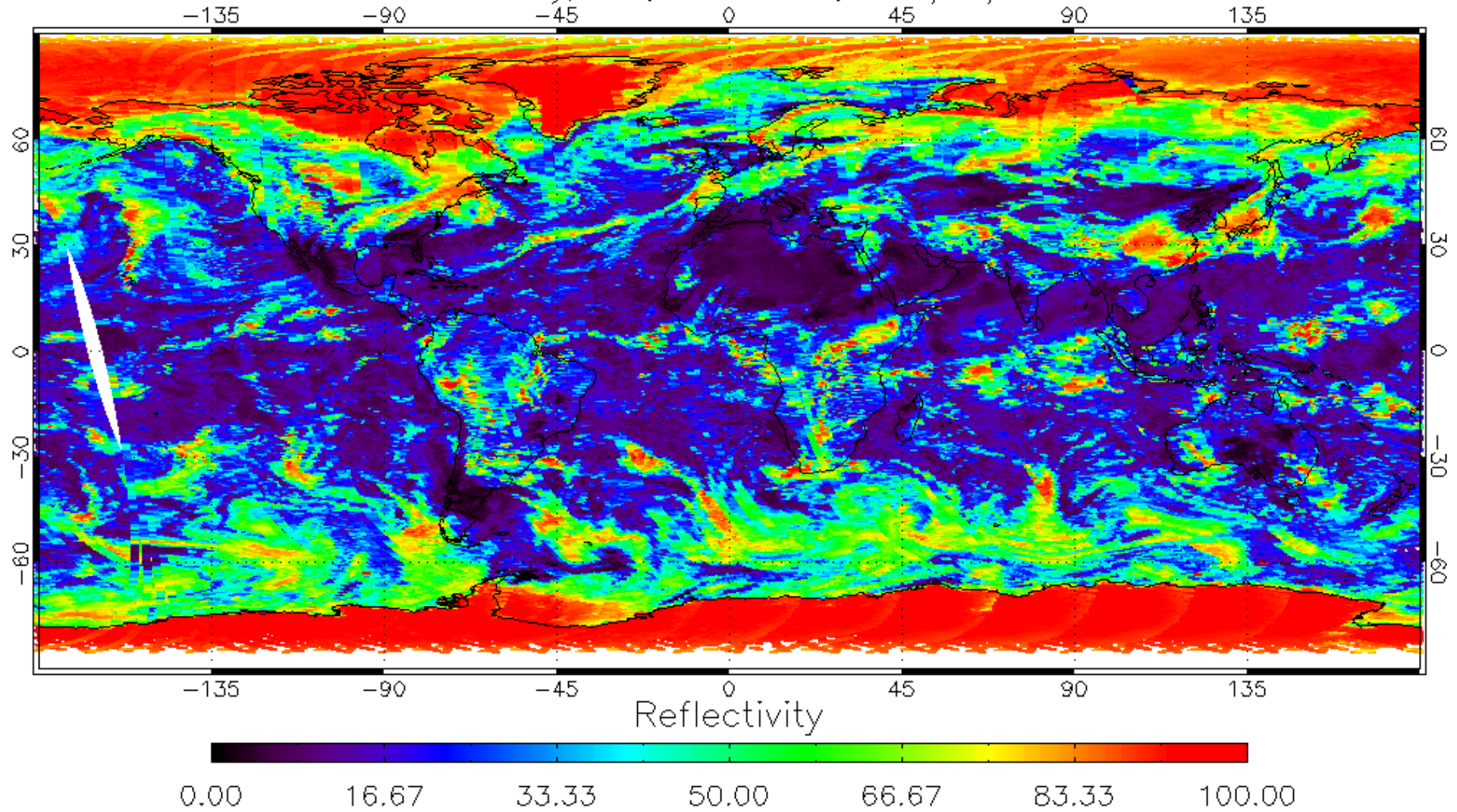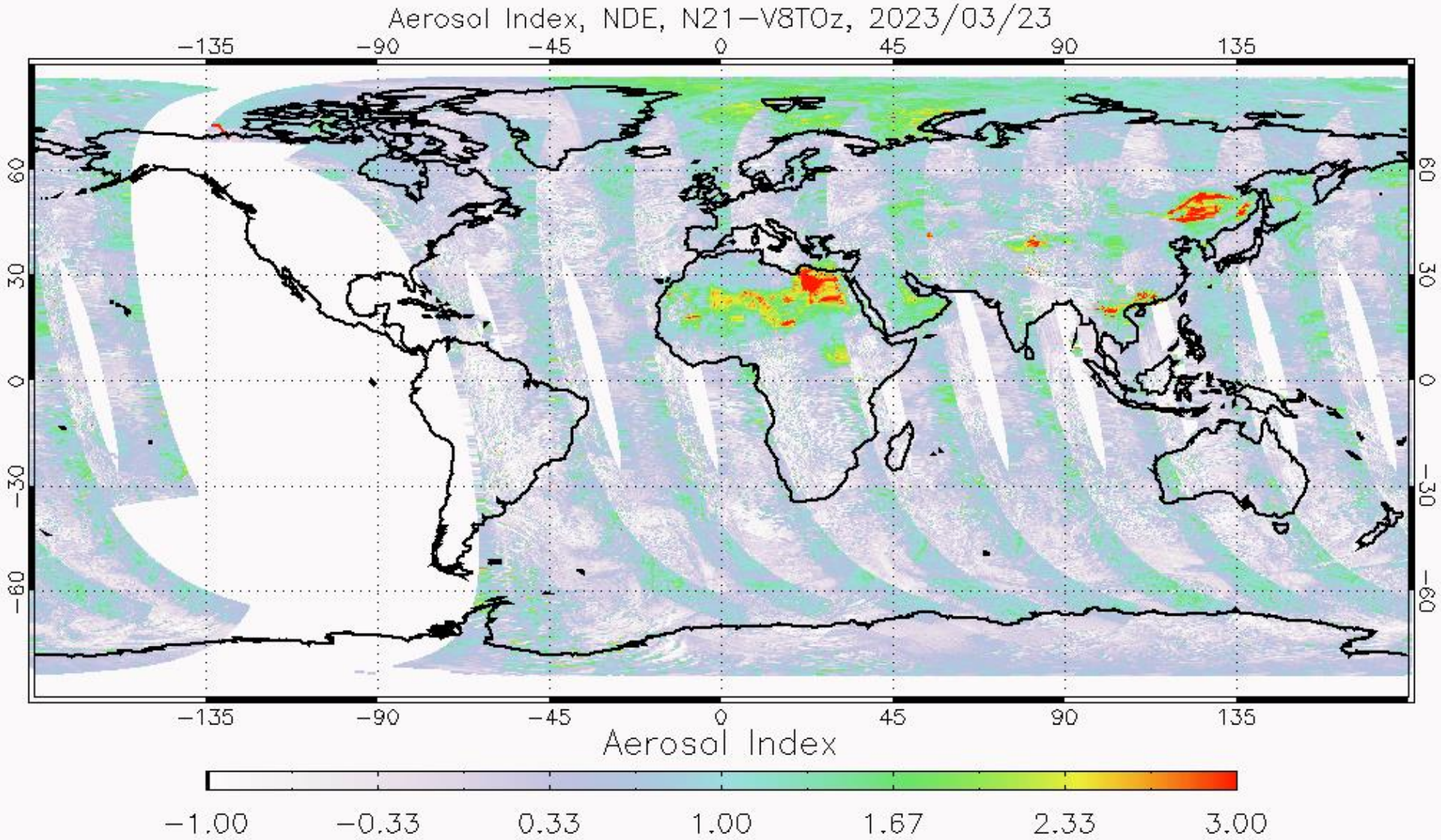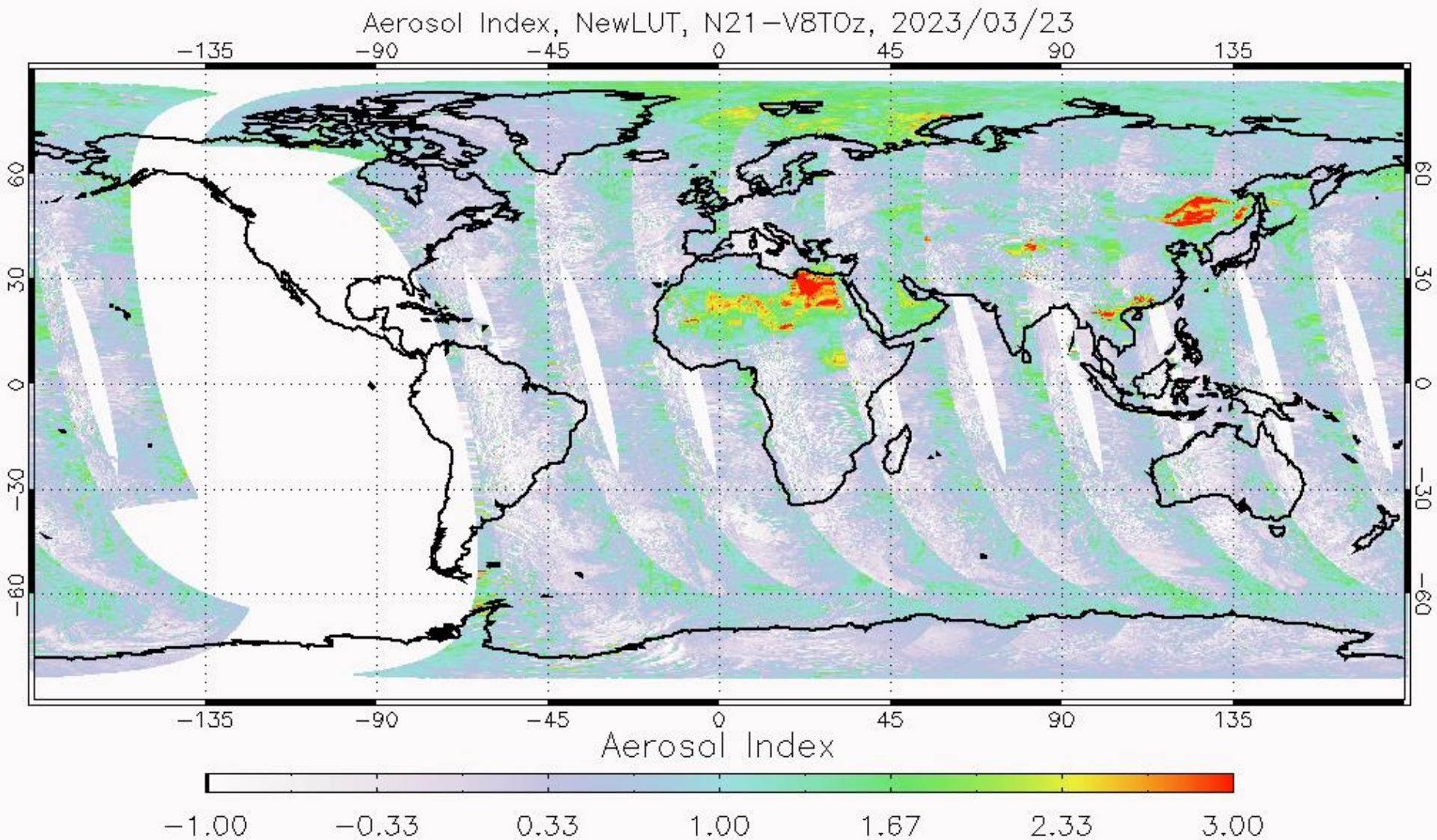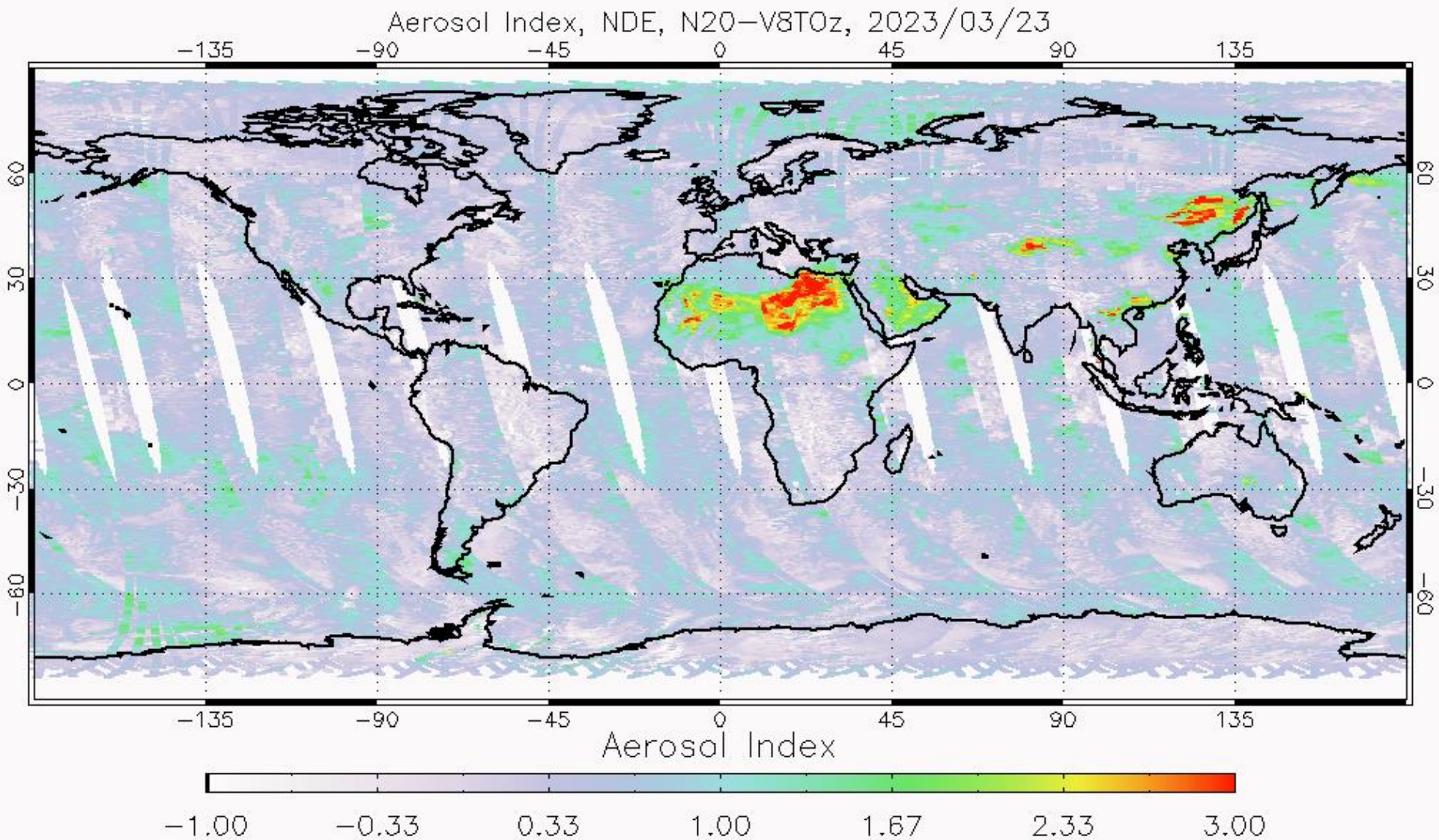
- Defined Quality Flags
  - Variable
  - Description
  - Value

- Quality flag analysis/validation
  - Test / example / ground truth data sets
 - Analysis / validation results
  - Analysis / validation plan

Quality Flags V8TOz Error Codes

| Output	Type	Description	
ErrorFlag		Good – 0	Good retrieval SZA <= 84°
		Sun Glint Geometry – 1	Good retrieval, open water with sun glint geometry present
		High SZA – 2	Good retrieval SZA > 84°
		Large Aerosol Index – 3	360 nm residual > threshold
		Profile Shape Error – 4	Residual at unused ozone wavelength > 4 σ
		High SO$_2$ – 5	SO$_2$ Index > 4 σ
		Non-Convergence – 6	Algorithm does not converge
		Large Residual – 7	Absolute residual > 32
		Bad Radiances – 8	Negative or missing radiances (Partial Granule Fix)
EclipseFlag*		0 – Good, 1 – Eclipse	Solar Eclipse Condition

Current Bad RT Instrument Table

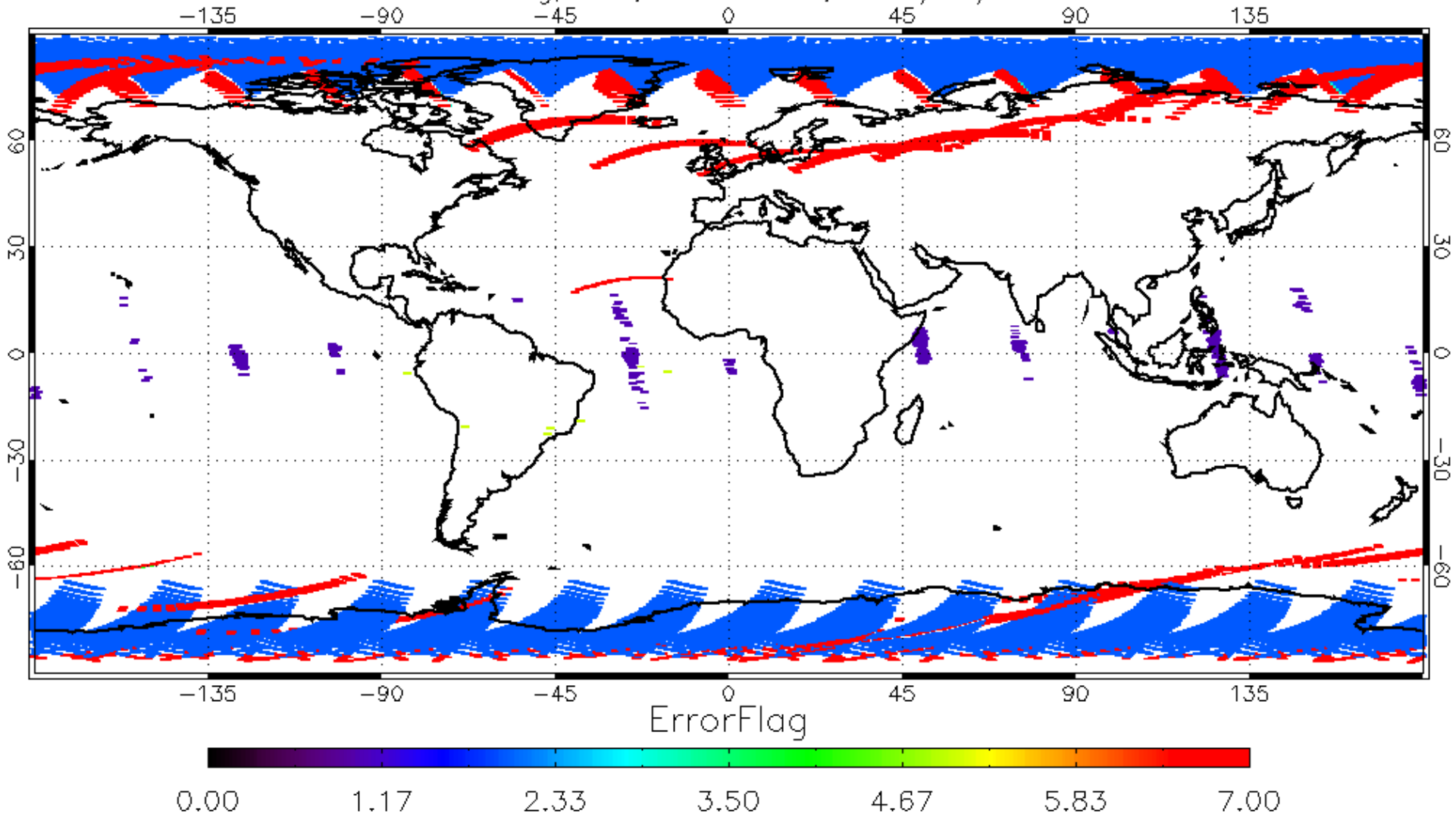ErrorFlag, NDE, N21–V8TOz, 2023/03/23
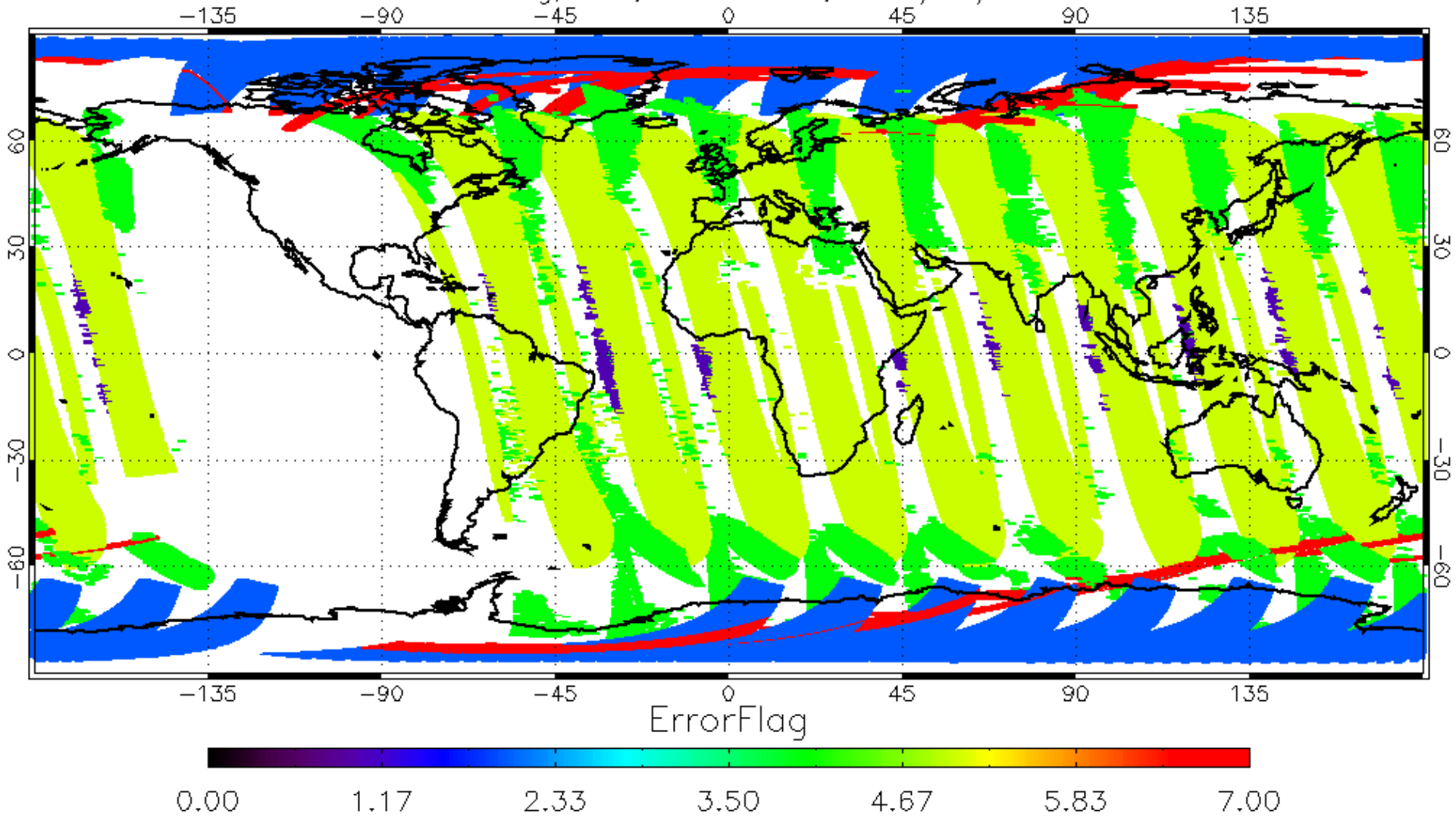
ErrorFlag

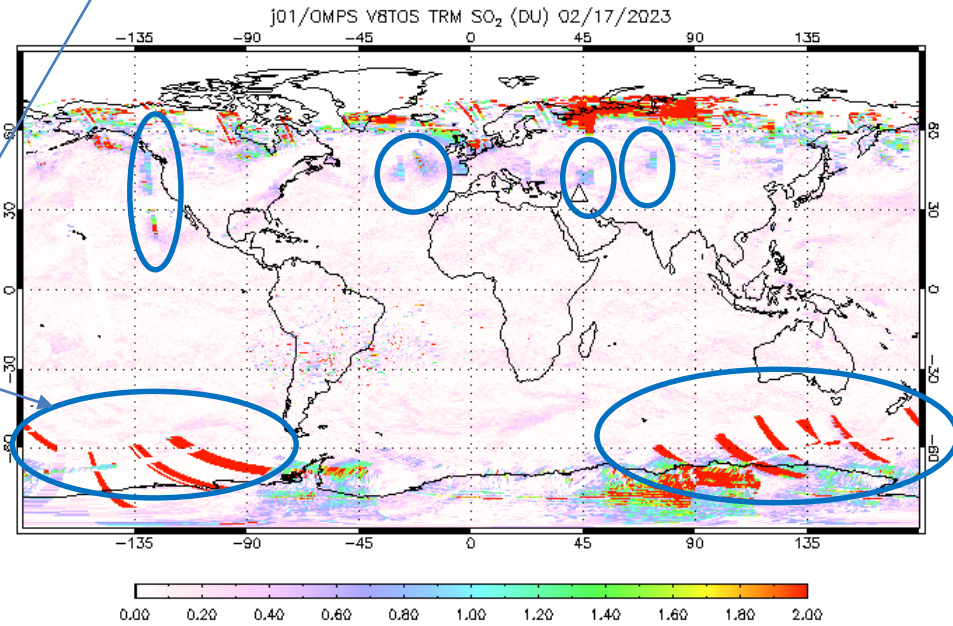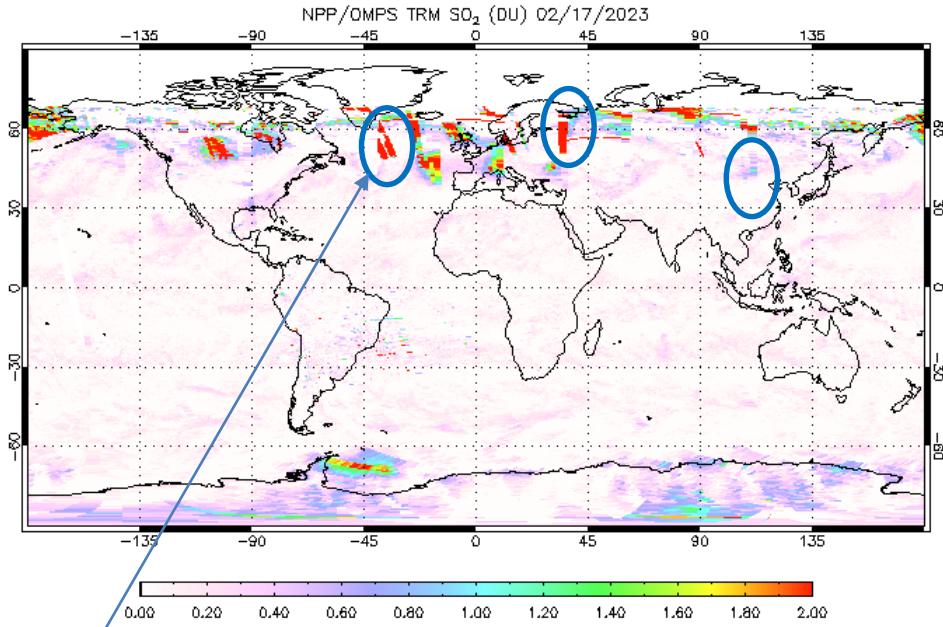# New Good N21 RT Instrument Table
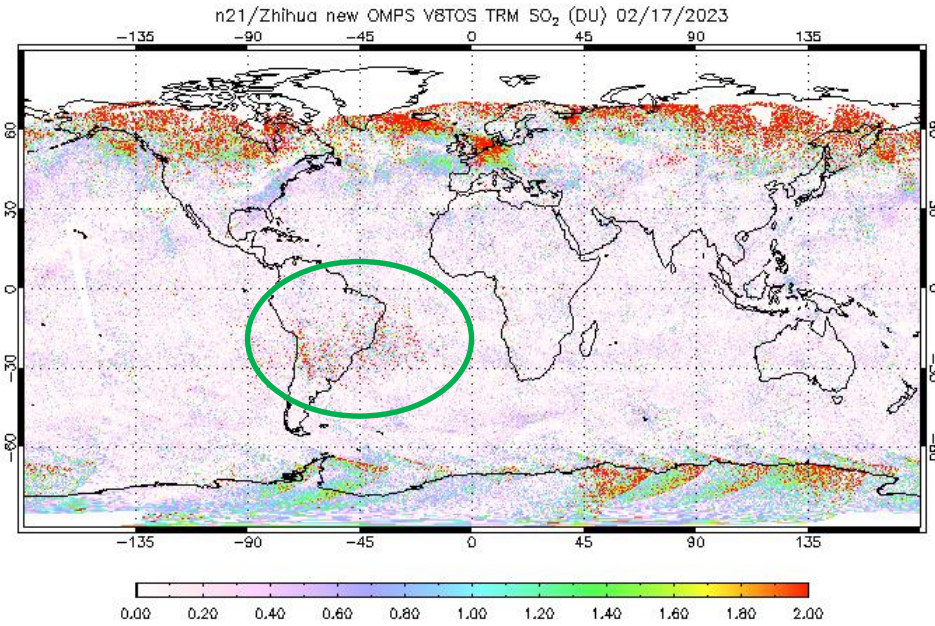

ErrorFlag, NewLUT, N21-V8TOz, 2023/03/23
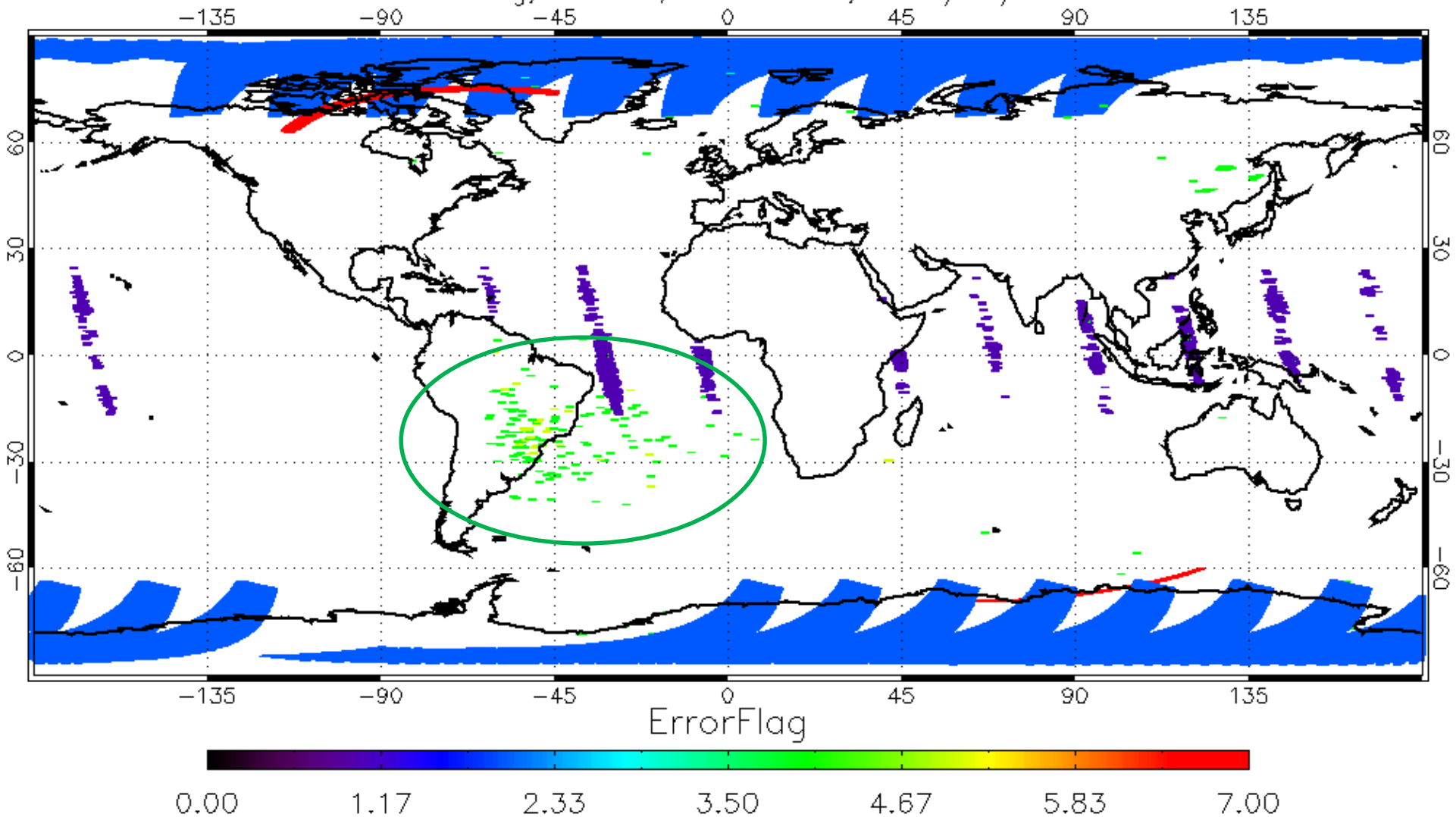
ErrorFlag

Smaller FOVs show increased flagging in the SAA

ErrorFlag, NDE, N20-V8TOz, 2023/03/23
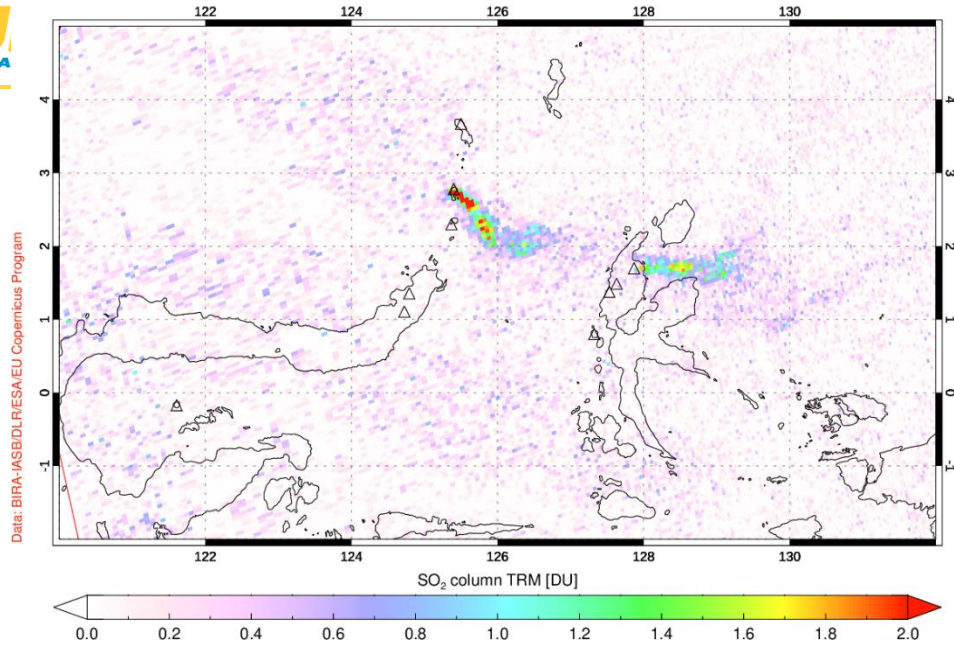
SO2 Results for STAR processing
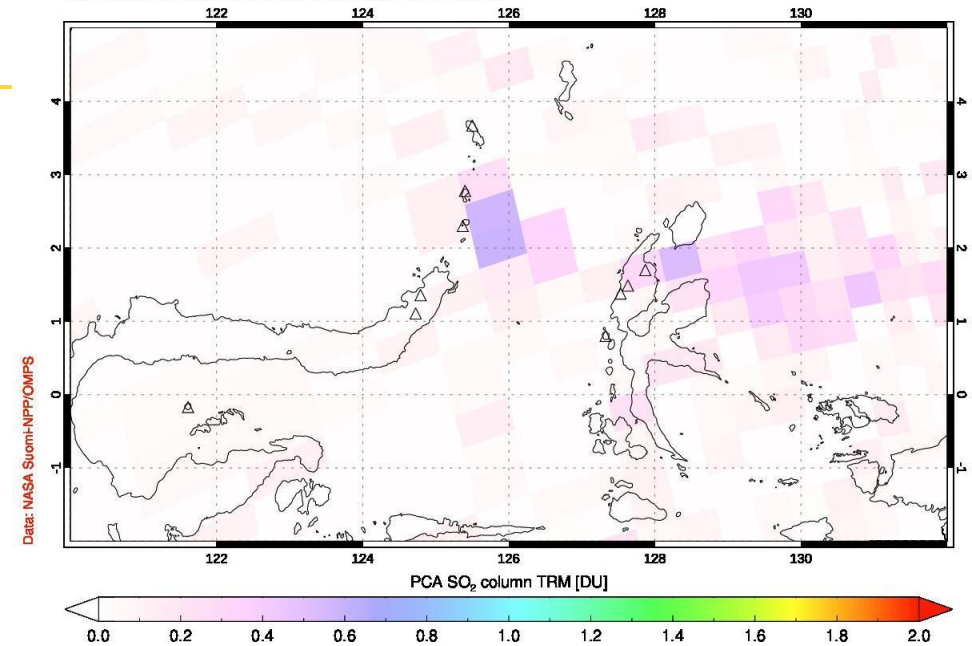NOAA-21 top left
S-NPP top right
NOAA-20 bottom right

Smaller FOVs show increased noise in the SAA

Artificial patterns

Sentinel-5P/TROPOMI - 02/17/2023 04:42-04:45 UT

SO2 mass: 0.2495 kt; SO2 max: 4.03 DU at lon: 125.43 lat: 2.75 ; 04:44UTC

SO2 column TRM [DU]

Suomi NPP/OMPS - 02/17/2023 04:38-04:41 UT

SO2 mass: 0.036 kt; SO2 max: 0.59 DU at lon: 125.89 lat: 2.05 ; 04:39UTC

PCA SO2 column TRM [DU]

n21/Zhihua new OMPS V8TOS TRM SO2 (DU) 02/17/2023

The increased noise in the NOAA-21 SO2 estimates is expected. We are investigating methods to use local fits (wavelength channel intervals) of radiance / irradiance rations to identify outliers and filter the measurements to reduce the noise.
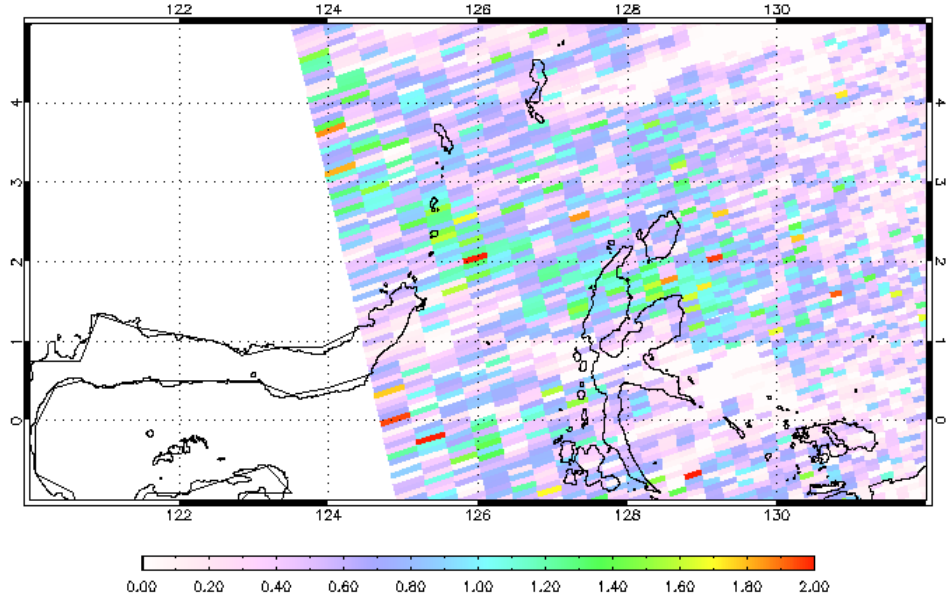
Comparisons of UV Absorbing Aerosol Index estimates from NOAA-20 OMPS (left) and NOAA-21 OMPS (right) for one day showing Saharan Dust (upper feature) and biomass burning (lower).


Aerosol Index, OMPS N20, 2023/02/18 over lat(−10,30) lon(−20,20)

Aerosol Index, OMPS N21, 2023/02/18 over lat(−10,30) lon(−20,20)

Aerosol Index

−2.00   −0.92   0.17   1.25   2.33   3.42   4.50
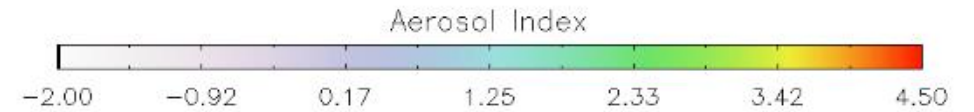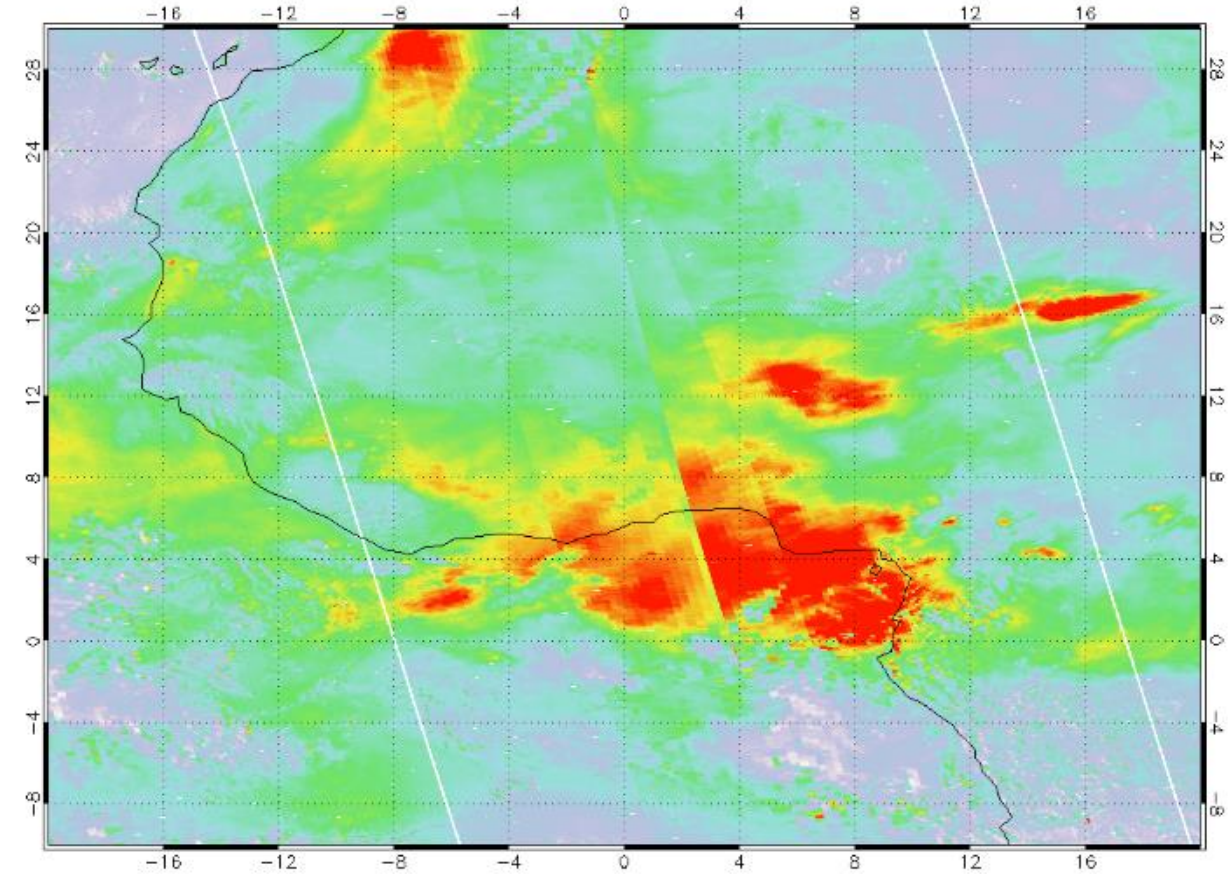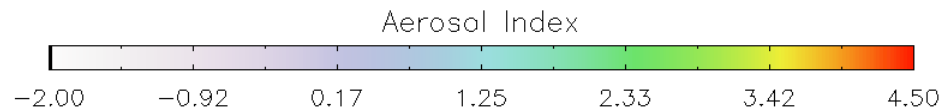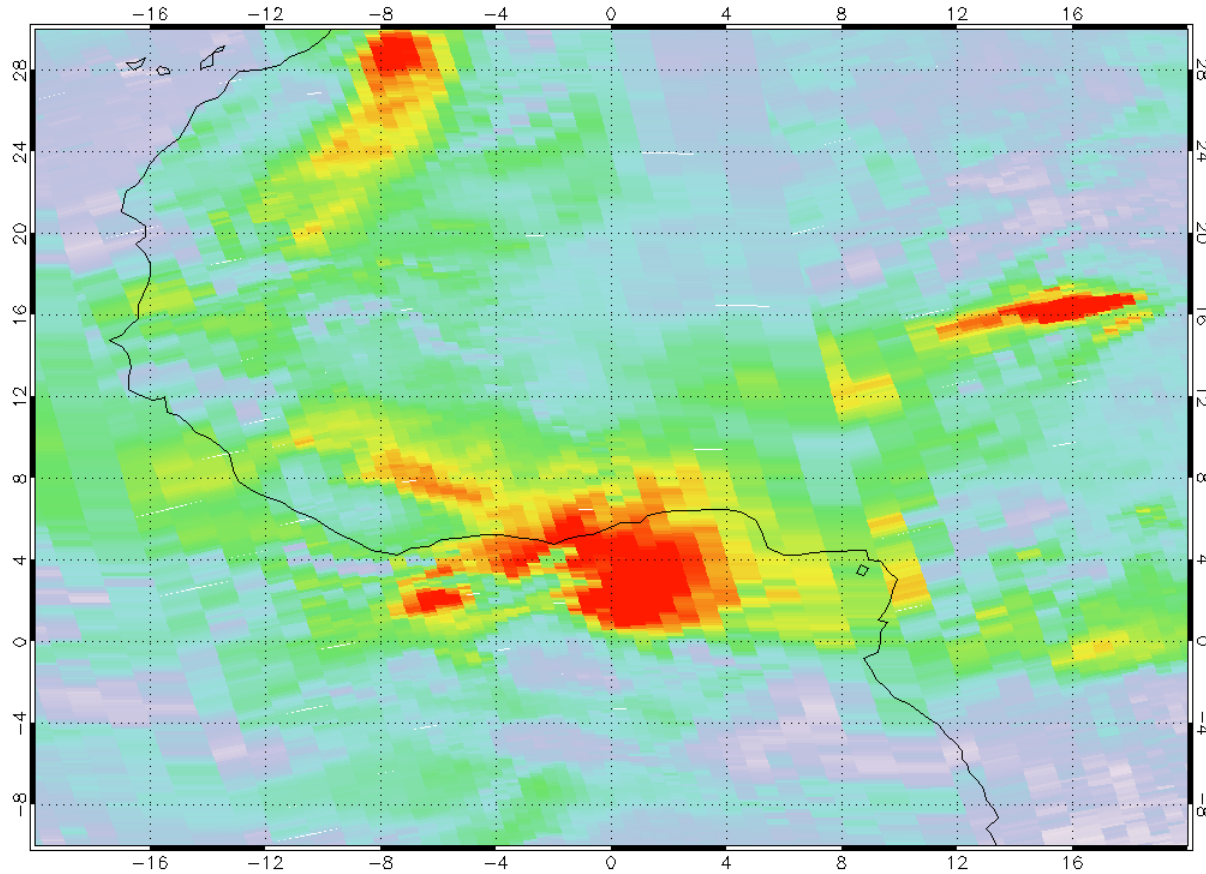
While the NOAA-21 product shows cross-track calibration biases in the initial calibration, the much improved spatial resolution with the small Fields-of-View is obvious.

- Required Algorithm Inputs
  - OMPS Nadir Mapper SDR and GEO
  - Instrument Radiative Transfer Tables
  - Soft Calibration Adjustment Tables

- Evaluation of the effect of required algorithm inputs
  - Study / test cases
  - Results

Nvalue LUT lgi0 for 318nm channel
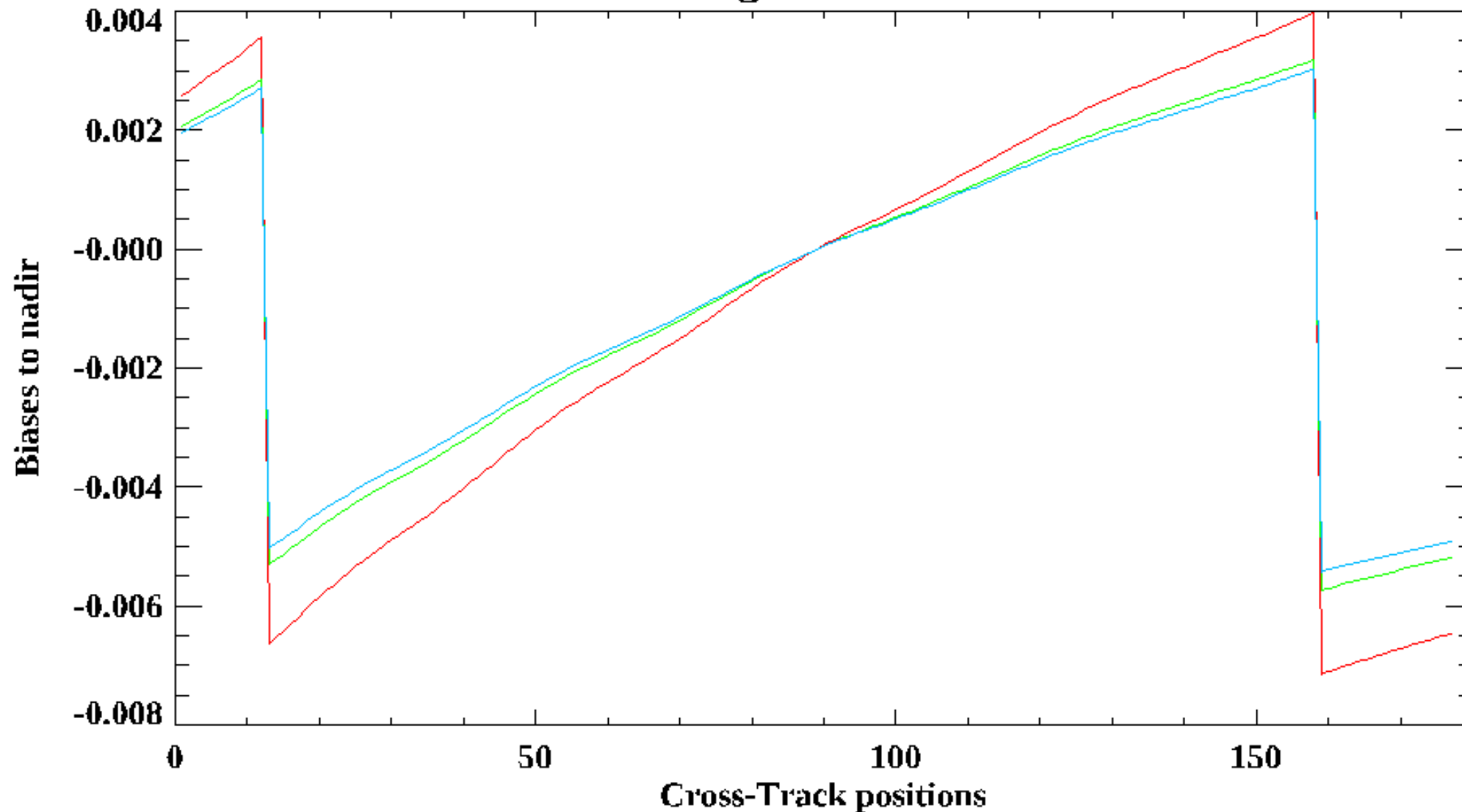
NOAA-21 OMPS NM has a smaller intra-orbital wavelength scale variation than NOAA-20 OMPS NM. Both are well-characterized by the granule-level adjustments in the SDR processing, the adjustments are good.
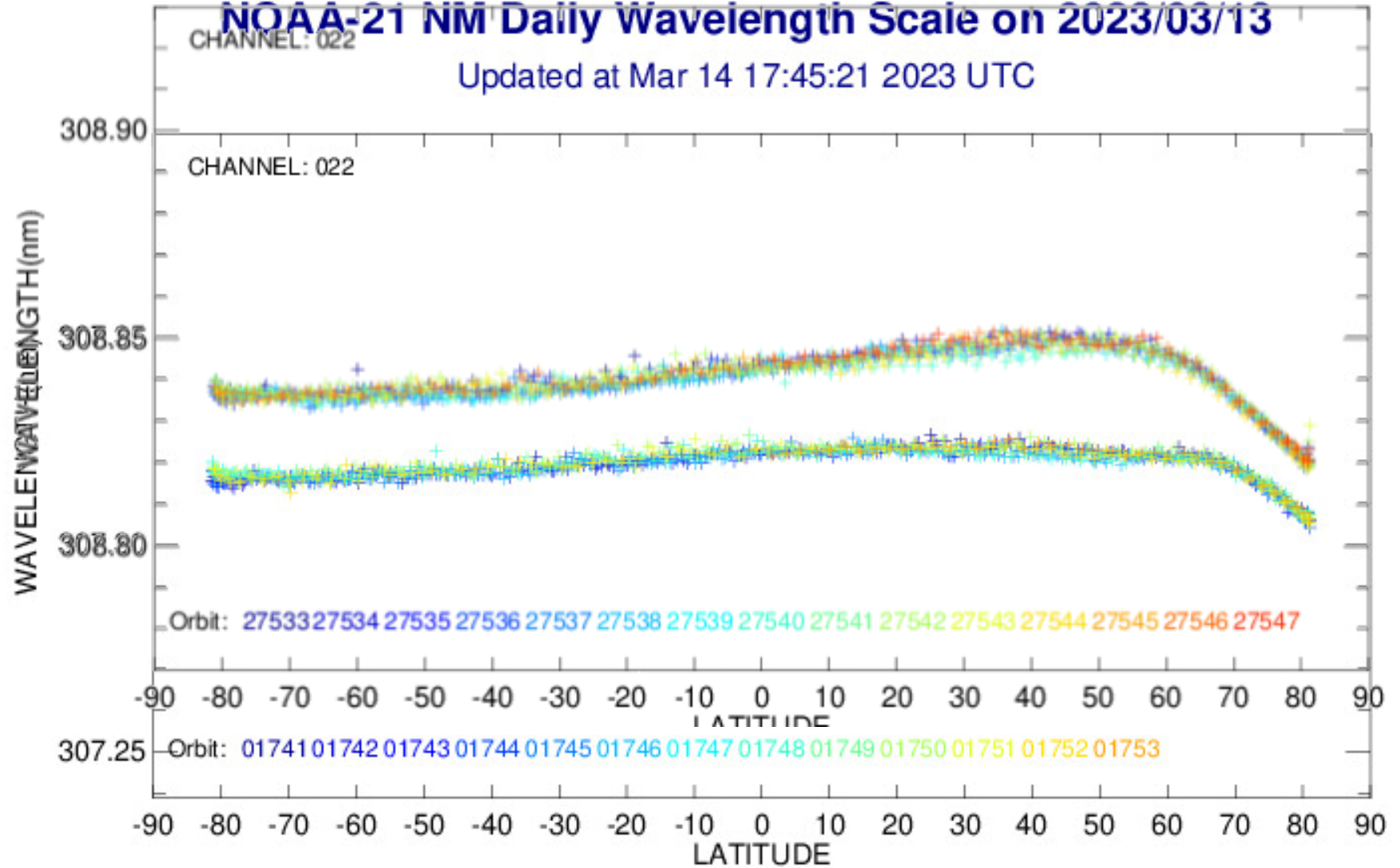
Smaller FOV have noisier measurements as expected

Noise estimates from triple centered differences.

—— Solid NOAA-21

······ Dot S-NPP

- - - Dash NOAA-20

SO$_2$ Channels
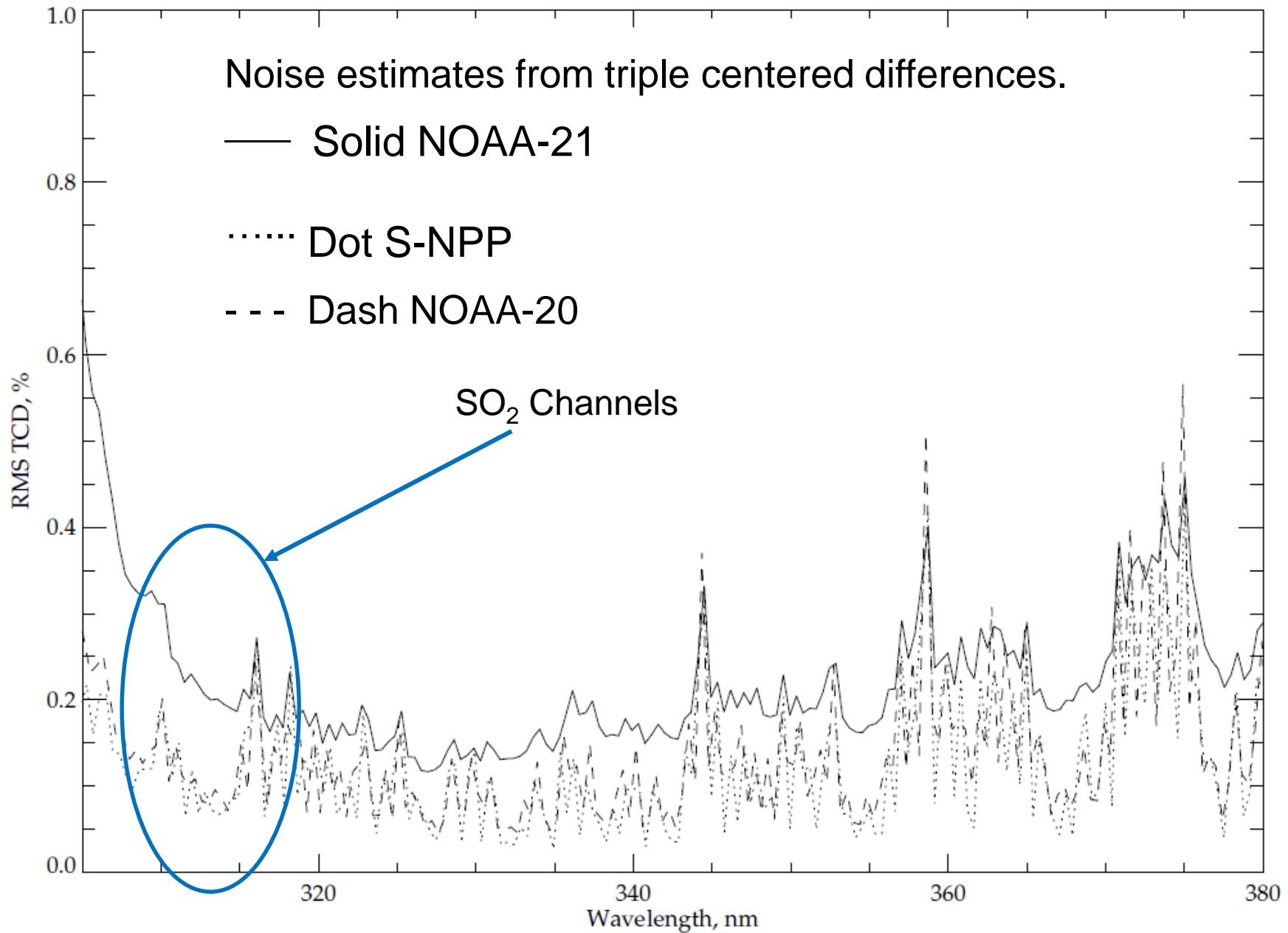
Risks, Actions, and Mitigations

- Provide updates for the status of the risks/actions identified during the previous maturity review(s); add new ones as needed

Identified Risk	Description	Impact	Action/Mitigation and Schedule

Documentations (Check List, 1 slide)

Science Maturity Check List	Yes ?
ReadMe for Data Product Users	Yes (after approval)
Algorithm Theoretical Basis Document (ATBD)	Yes
Algorithm Calibration/Validation Plan	Yes
(External/Internal) Users Manual	Yes
System Maintenance Manual (for ESPC products)	Yes
Peer Reviewed Publications (Demonstrates algorithm is independently reviewed)	Yes
Regular Validation Reports (at least annually) (Demonstrates long-term performance of the algorithm)	

Beta Maturity End State	Assessment
Product is minimally validated, and may still contain significant identified and unidentified errors	NDE I&T product has significant errors from an error in creating the prelaunch Instrument Radiance Table.
Information/data from validation efforts can only be used to make initial qualitative or very limited quantitative assessments regarding product fitness-for-purpose	Ozone values should only be used for qualitative assessment due to instrument table error.
Documentation of product performance and identified product performance anomalies, including recommended remediation strategies, exists	New RT Instrument and Soft Calibration Adjustment Tables will be delivered to advance to Provisional Maturity.

Conclusion & Caveats

- The NOAA-21 OMPS NM SDRs have good performance.
  - The OMPS NM SDRs have a small error in the wavelength / solar table for three near-nadir FOVs. This will be fixed with the fast-track table updates on 4/7/2023.
  - The OMPS NM SDRs will have a sample table update for macro-pixel #177 in Mx 8/9, expected 6/2023.
- We recommend that the NOAA-21 V8OTz v4r2 EDRs from NDE I&T be reported at Beta Maturity as of 3/24/2023. The instruments are still making extensive calibration and diagnostic measurements, so the Earth Science coverage is less than for regular operations. Regular operations will begin next month.
- While the NDE I&T NOAA-21 V8TOz v4r2 EDRs are reasonable
  - The ozone values have large cross-track errors from a mistake in the wavelength centers used in the creation of the Instrument Table. A new table has been tested and will be implemented to achieve Provisional Maturity.
  - Error codes checking residuals are set for most retrievals due to poor calibration of the shorter wavelength channels. Soft calibration adjustments to force agreement with S-NPP and NOAA-20 V8Pro EDRs are under development. This has to be done in concert with possible SDR changes to the calibration coefficients and stray light corrections as they progress from provisional to fully validated.
  - The smaller FOV measurements show increased noise especially in the SAA and for SO2 retrievals. We are developing outlier detection and local fitting processes to increase the SNRs of the values used in the retrieval algorithm. We will also be checking whether aggregation / averaging of the smaller FOVs recovers the performance obtained for NOAA-20.