Validated Maturity Science Review For NOAA-20 SST

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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 Criteria

- Product Requirements
- Pre-launch Performance Matrix/Waivers
- Validated 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/EDRs feedback
- Risks, Actions, Mitigations
  - Potential issues, concerns
- Path forward
- Summary

Validated Maturity Review - Exit Criteria

- Validated 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 Validated Maturity Slide Package addressing review committee's comments for:
  - Cal/Val Plan and Schedules
  - Product Requirements
  - Validated Maturity Performance
  - Risks, Actions, Mitigations
  - Path forward

VALIDATED MATURITY REVIEW MATERIAL

Outline

- 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

N20 SST Algorithm and Cal/Val Team

Name	Organization	Tasks
Ignatov, Sasha	STAR	JPSS Algorithm & Cal/Val Lead
DiGiacomo, Paul	STAR	JPSS Ocean Lead/CoastWatch
Lance, Veronica	STAR – GST	Coast Watch / JPSS Ocean Coordinator
Sapper, John	OSPO	NDE and OSPO Operations, Data distribution, Users, Archival
Kihai, Yury	STAR – GST	ACSPO SW/HW; Preprocessor; L2P Code; *In situ* match-ups; ARMS; R2O
Pennybacker, Matthew	STAR – GST	L3U/C/S Code/Algorithms; *i*Quam; SW/HW & SST cluster; AirFlow; Resampling/Pattern Recognition/Ocean Fronts Support
Jonasson, Olafur	STAR – GST	VIIRS SST Reanalysis (RAN); SST Quality Monitor (SQUAM)/Monitoring IR Clear-sky Radiances for SST (MICROS); In situ match-ups
Petrenko, Boris	STAR – GST	ACSPO Clear-Sky Mask; SST Algorithms; Error Characterization
Gladkova, Irina	STAR–CCNY CREST/GST	Data Fusion (L3C/S; C=Collated; S=Super-Collated); SST/Clear-Sky Mask and Resampling/Pattern Recognition/Ocean Fronts Algorithms

JPSS SST Requirements

EDR Attribute	Threshold	Objective
a. Horizontal Cell Size (Res)	1.6km[1]	0.25km
b. Mapping Uncertainty, 3σ	2km[1]	0.1km
c. Measurement Range	271 K to 313 K	271 K to 318 K
d. Measurement Accuracy[2]	0.2K	0.05K
e. Measurement Precision[2]	0.6K	0.2K (<55° VZA)
f. Refresh Rate	12 hrs	3 hrs
g. Latency	90 min	15 min
h. Geographic coverage	Global cloud and ice-free ocean; excluding lakes and rivers	Global cloud and ice-free ocean, plus large lakes and wide rivers

[1]Worst case scenario (corresponding to swath edge); both numbers are ~1km at nadir

[2]Represent global mean bias and standard deviation validation statistics against quality-controlled drifting buoys (for day and night, in full VIIRS swath, in full range of atmospheric conditions). Uncertainty is defined as square root of accuracy squared plus precision squared. Better performance is expected against ship radiometers.

ACSPO & VIIRS SST Bands

- VIIRS SST product is produced using the NOAA enterprise Advanced Clear-Sky Processor for Ocean (ACSPO) system
- ACSPO is also employed to process data of polar (AVHRR GAC/FRAC & MODIS) and geostationary (GOES-R ABI, Himawari-8/9 AHI) sensors

Sensor	SST Bands
Night: VIIRS & MODIS	**3.7 / 8.6 / 10.8 / 12 µm** **3.7 / 8.5 / 11.0 / 12 µm**
Day: VIIRS & MODIS	**8.6 / 10.8 / 12 µm** **8.5 / 11.0 / 12 µm**
ABI & AHI (Day & Night)	**8.5 / 10.3 / 11.2 / 12.3 µm**

- VIIRS/MODIS and ABI/AHI have new band(s) suitable for SST. In particular, M14 @8.6µm is now included in day and night retrievals (in addition to daytime split-window M15/16 centered at 11/12µm, and nighttime shortwave M12 @3.7µm)
- Two reflectance bands centered at 0.68/0.86 µm (VIIRS M5/7) are also employed in ACSPO for SST QC

VIIRS SST Algorithms

Night:

$$T_S = a_0 + a_1 T_{11} + a_2(T_{11}-T_{3.7}) + a_3(T_{11}-T_{8.6}) + a_4(T_{11}-T_{12}) + [a_5 + a_6 T_{11} + a_7(T_{11}-T_{3.7}) + a_8(T_{11}-T_{8.6}) + a_9(T_{11}-T_{12})]S_\theta + [a_{10}(T_{11}-T_{3.7}) + a_{11}(T_{11}-T_{8.6}) + a_{12}(T_{11}-T_{12})]T_S^0$$

Day:

$$T_S = a_0 + a_1 T_{11} + a_3(T_{11}-T_{8.6}) + a_4(T_{11}-T_{12}) + [a_5 + a_6 T_{11} + a_8(T_{11}-T_{8.6}) + a_9(T_{11}-T_{12})]S_\theta + [a_{11}(T_{11}-T_{8.6}) + a_{12}(T_{11}-T_{12})]T_S^0$$

$T_{3.7}$, $T_{8.6}$, T_{11}, T_{12}	BTs at 3.7, 8.6, 11 and 12 μm
$S_\theta = 1/\cos(\theta) - 1$	θ is VZA
T_S^0	L4 SST in °C (currently by Canadian Meteorological Center – CMC)
***a*'s**	regression coefficients, trained against drifters and mooring buoys

- Regressors are constructed from 3 (day) or 4 (night) radiometric bands, and VZA
- Potential instabilities of the regression coefficients are mitigated by taking special steps to keep only significant number of eigenvectors/values of the covariance matrix

Findings from Provisional Review (Apr 2018)

- **N20 SST reached provisional maturity. Performance comparable to NPP**
  - ✓ Product performance demonstrated through analysis of a large, but still seasonally limited number of independent global in situ matchups
  - ✓ Product analyses are sufficient for qualitative and limited quantitative, determination of product fitness-for-purpose
  - ✓ Necessary documentation exists
  - ✓ Product is recommended for potential operational use (user decision) and in scientific publications. Consulting with SST Team recommended
- **Path Forward**
  - 1) Complete ACSPO v2.60. 2) Deliver to NDE. 3) Reprocess available stable N20 time series. 4) Distribute via Coast Watch, PDA, EumetCast. 5) Work with PO.DAAC/NCEI to archive NDE & reprocessed N20 data.
  - Continue creating *in situ* matchups, perform product Val/Monitoring, NPP comparisons for representative seasonal domain. Tweak algorithms
- **Recommendation to the Program**
  - Minimize sensor instabilities to the extent possible. Ensure stable thermal regime of the N20 /NPP sensors (minimize/mitigate WUCDs etc.)

ACSPO Required Inputs

- **Required Algorithm Inputs**
  - No upstream algorithms (ACSPO is stand-alone)
  - Day: M14/15/16 (+ M5/7 for masking); Night: M12/14/15/16
  - SST LUT: 2 per platform/sensor (1 day, 1 night)
  - Ancillary Data: CMC L4 SST; GFS
- **Evaluation of the effect of required algorithm inputs**
  - Quality of BTs in SST bands is critical for SST
  - Sensitivity to N20 thermal IR anomaly and NPP/N20 WUCDs presented at the provisional review. They have been addressed by SDR Team and now quality of radiances is acceptable for SST
  - Effect of Missing/Delayed ancillary data is mitigated by using last available CMC/GFS file. There is no noticeable effect of this “graceful degradation” on the ACSPO SST – we do use prior SST/Atmosphere, but we do not force retrieved SST into it

Processing Environment, Data Products & Versions

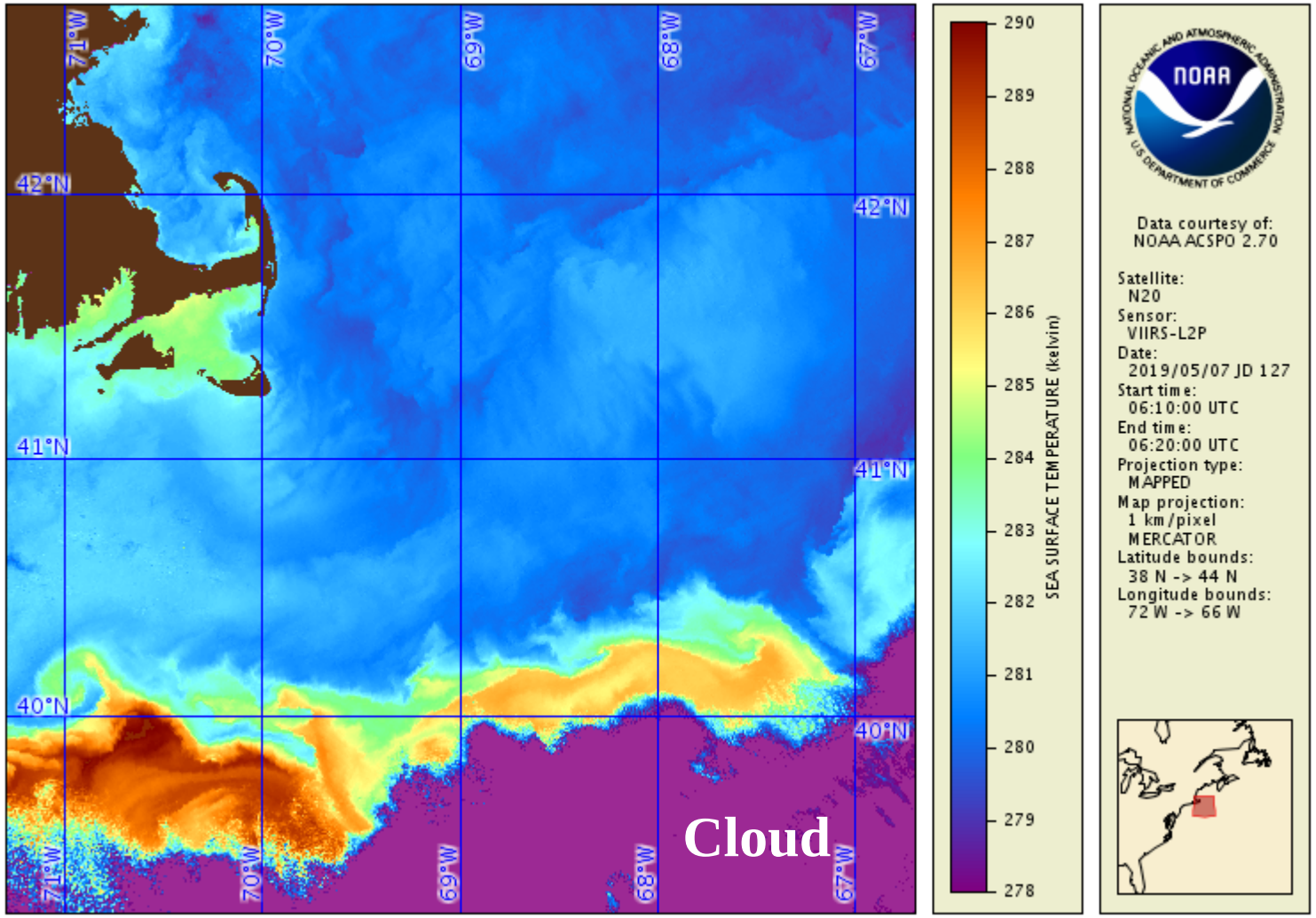
- **Today, both NPP and N20 are operational in NDE**
  - ACSPO v2.60 was used from 7 Nov 2018 – 23 Apr 2019
  - ACSPO v2.61 implemented on 23 Apr 2019 and used to-date. It corrected high-latitude bias. The 2.61 code is identical to 2.60 but uses an updated version of SST LUTs, to minimize the hi-lat bias
  - Both v2.60 and 2.61 are distributed via CW & PDA (not sure if on EumetCast yet) and archived in PO.DAAC & NCEI. RAN2 with 2.61 back-fills to the beginning of both NPP and N20 missions
- **Two products from both NPP & N20 (10min granules; 144/day)**
  - L2P (original swath projection; 26GB/day); and
  - Equal-grid 0.02° L3U (U=uncollated; 0.45GB/day)
- **Majority of VIIRS SST users prefer L3U (EumetCast, NOS, BoM, JMA, Met Office, Coast Watch)**
  - There is only one L2P user: STAR geo-polar blended group. Work is underway to convince GPB to switch over to L3U, to facilitate reprocessing, and data assimilation from multiple sensors/platforms

Evaluation of SST performance to specs

- **Improvements since Provisional**
  - ACSPO was updated from v2.41 to 2.60 (Operational: 7 Nov 2018).
  - 2.60: Resamples BT imagery, corrects bow-tie deletions & distortions: Ready for pattern recognition & front detection. Clear-sky mask tweaked. New N20 LUTs have been added
  - 2:61: LUTs updated to minimize hi-lat biases (Oper: 23 Apr 2019).

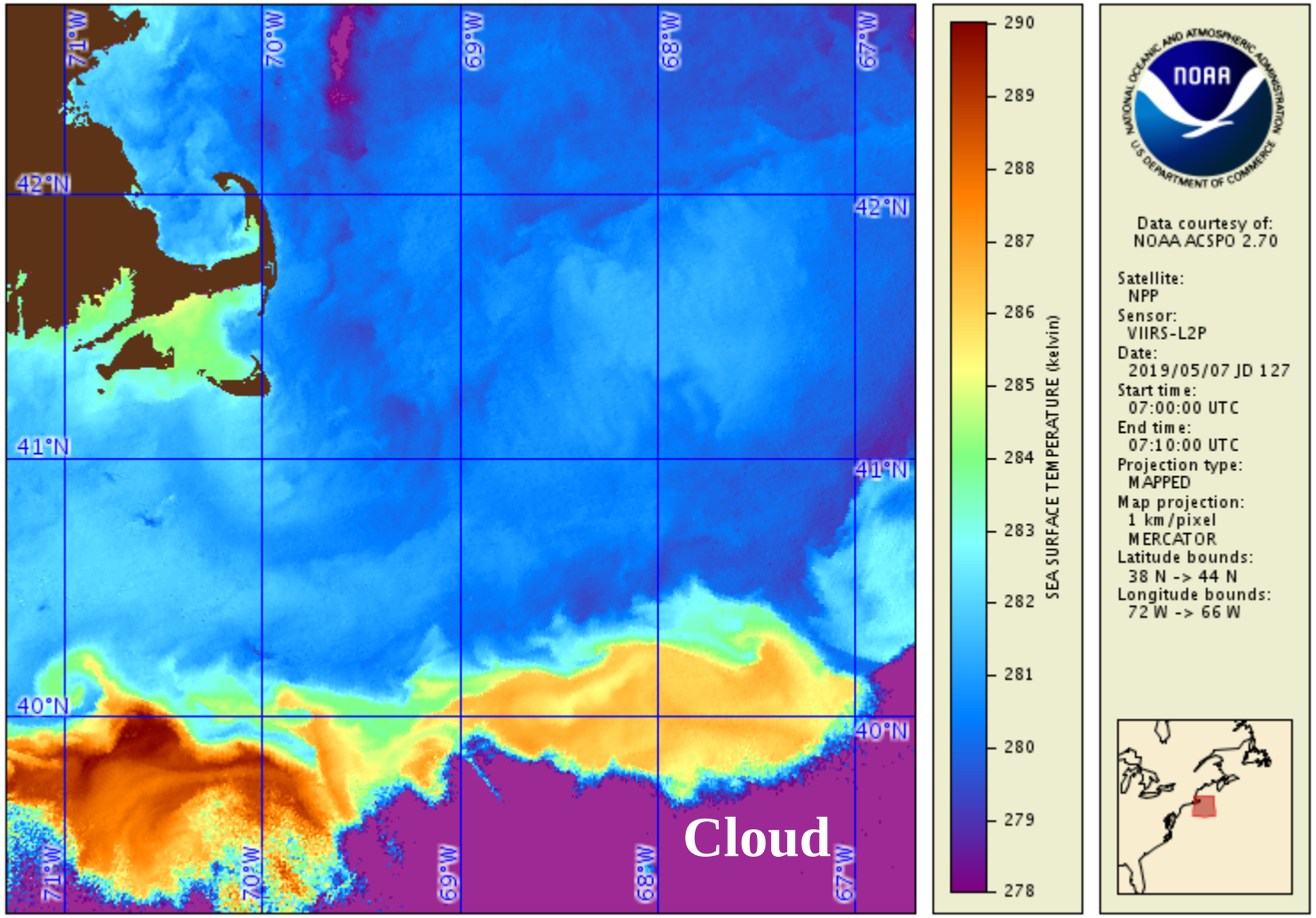
- **Product performance evaluation**
  - Global and Regional, for a complete N20 period from Jan 2018 (since opening cryoradiator doors of N20 VIIRS) – present
  - Validation strategies:
    1. Global comparisons with several high-quality L4 SST analyses;
    2. Validation vs. global QC'ed drifters & tropical moorings, and ARGO Floats from the NOAA *in situ* Quality Monitor (*i*Quam; www.star.nesdis.noaa.gov/sod/sst/iquam/);
    3. Comparisons w/NPP, Aqua/Terra MODIS, Metop-A/B/C AVHRR FRAC.
  - Long term monitoring:
    1. SST Quality Monitor (SQUAM; www.star.nesdis.noaa.gov/sod/sst/squam/);
    2. ACSPO Regional Monitor SST (ARMS; www.star.nesdis.noaa.gov/sod/sst/arms/)

NPP/N20 SST Imagery: Consistency/Complementarity



- Georges Bank/Nantucket Shoals 7 May 2019: N20 @6:10UTC
- VIIRS provides very high resolution & quality SST imagery

NPP/N20 SST Imagery: Consistency/Complementarity



- Georges Bank/Nantucket Shoals 7 May 2019: NPP @7:00UTC
- Cloud & SST patterns move. Fusion requires normalizing overpass time

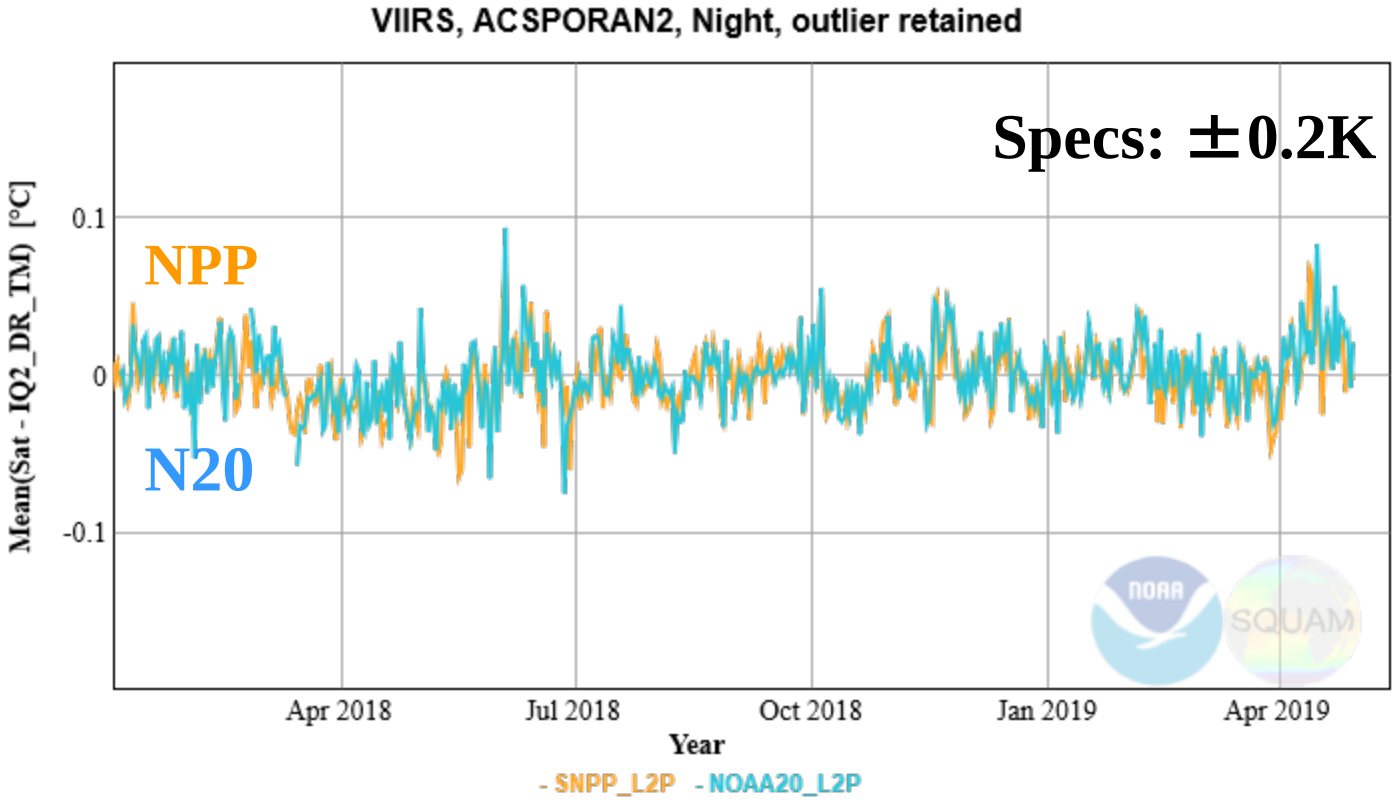
Quality Control Analysis/Validation

- **Defined Quality Flags**
  - ACSPO has quality levels (QLs). QL=5: Recommended to users; QL=0: Missing data; QL=1: Non-SST (cloudy, probably cloudy, land, etc.); QL=2,3,4 – not used
- **ACSPO Follows GHRSST Data Specifications and provides error characterization of SST in each pixel**
  - SST uncertainty in each QL=5 pixel is defined by the two extra layers in data files: Singe Scanner Error Statistics (SSES) Bias and SSES Standard Deviation (SD)
  - So far, users use SSES Bias and it is mostly validated
  - The SSES SD is also reported. However, it has not been independently evaluated by users yet

The following 8 charts show the time series of the two major metrics (global mean bias and SD), stratified by day and night, without and with SSES bias correction

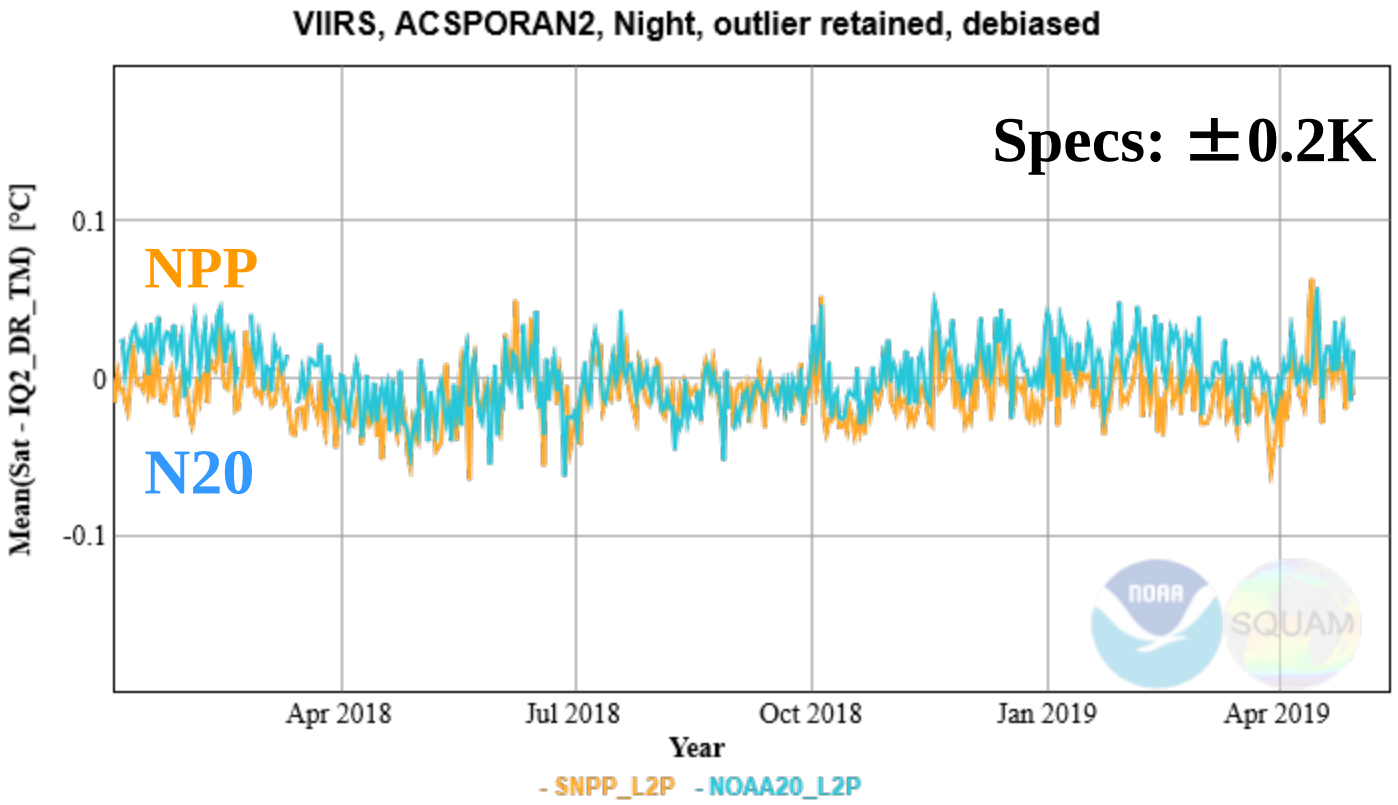
Global SST Bias wrt. *i*Quam *in situ*: NIGHT
No SSES Bias Correction

Each Data point: Global 24hr statistic supported by ~150K match-ups



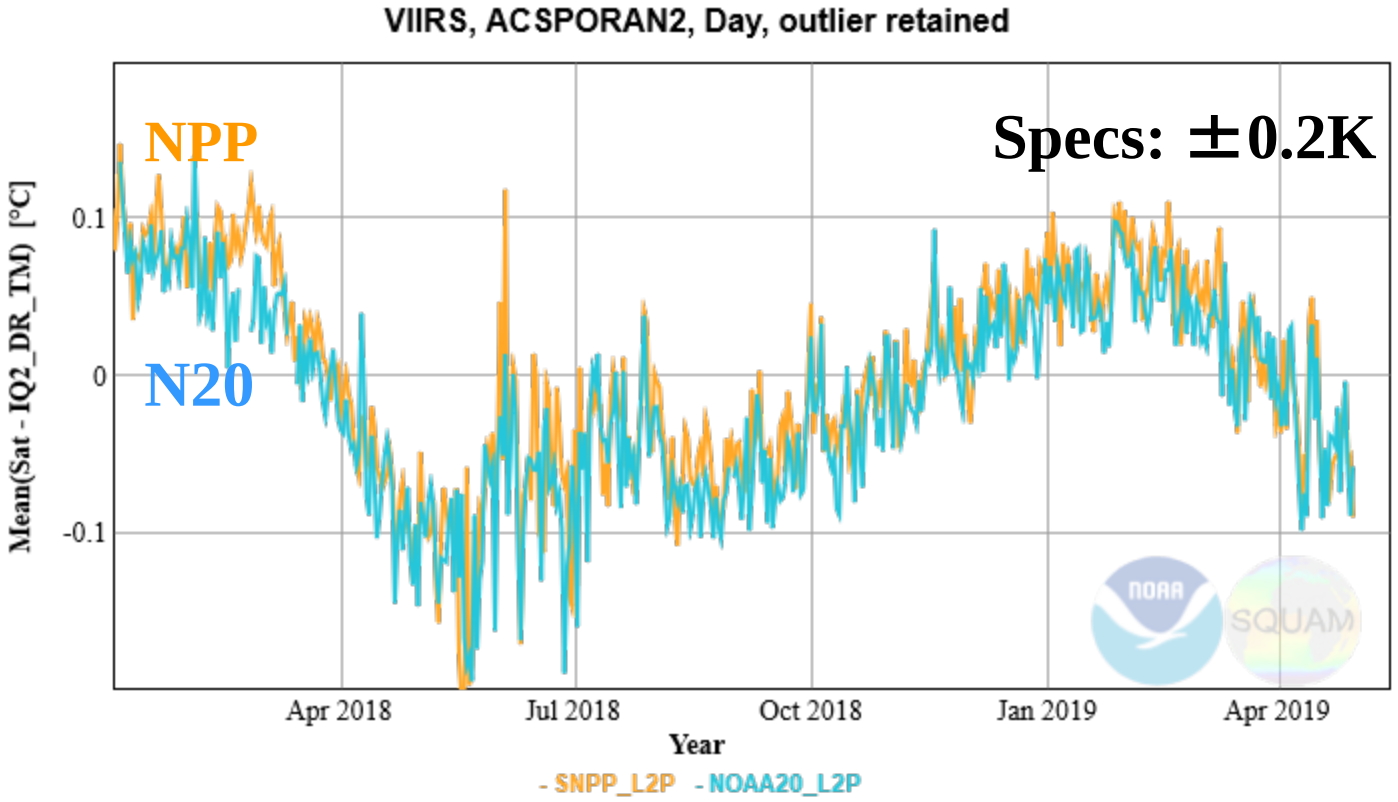
- Nighttime biases are centered at ~0, typically within ±0.05K
- NPP and N20 statistics are very consistent

Global SST Bias wrt. *i*Quam *in situ*: NIGHT
With SSES Bias Correction



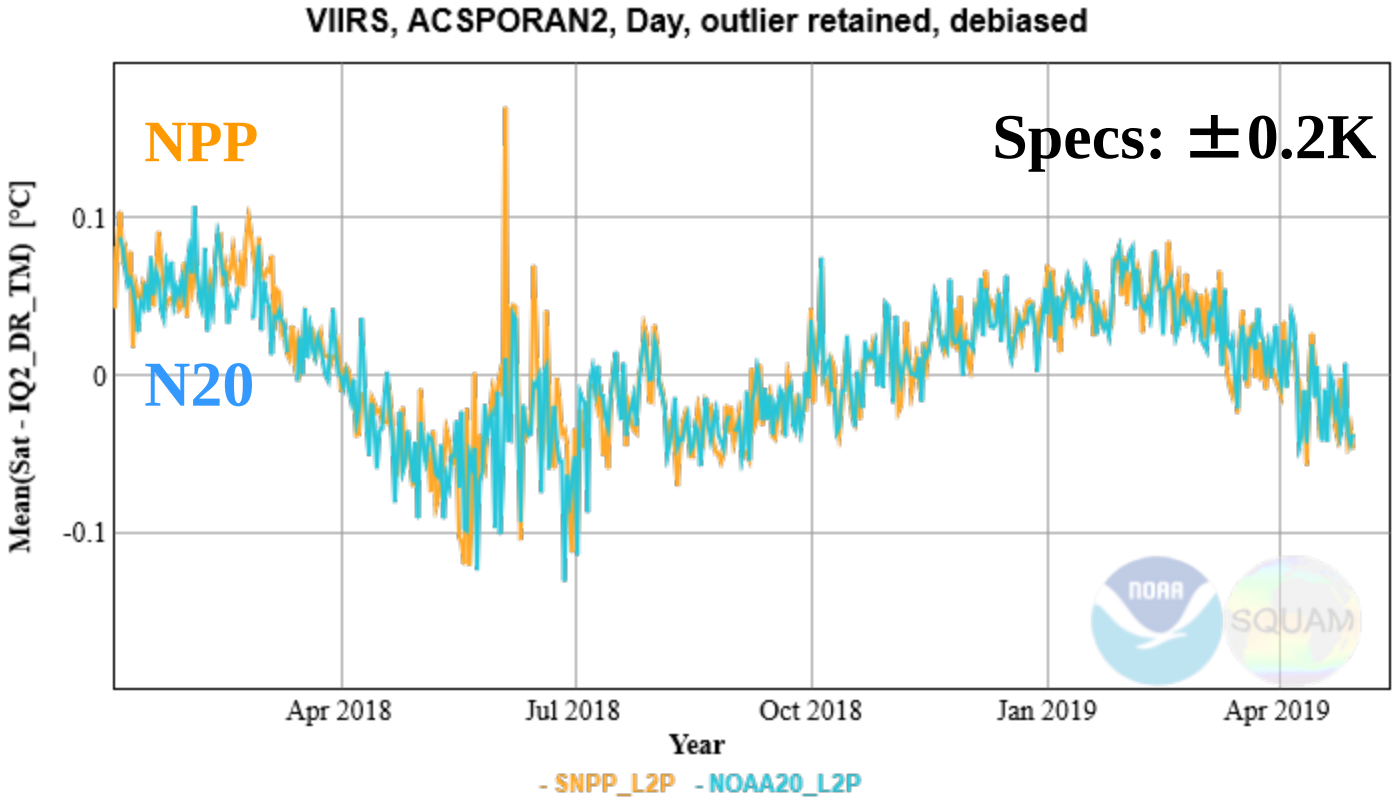
- SSES Bias correction at night results in comparable biases
- NPP and N20 remain consistent

Global SST Bias wrt. *i*Quam *in situ*: DAY
No SSES Bias Correction



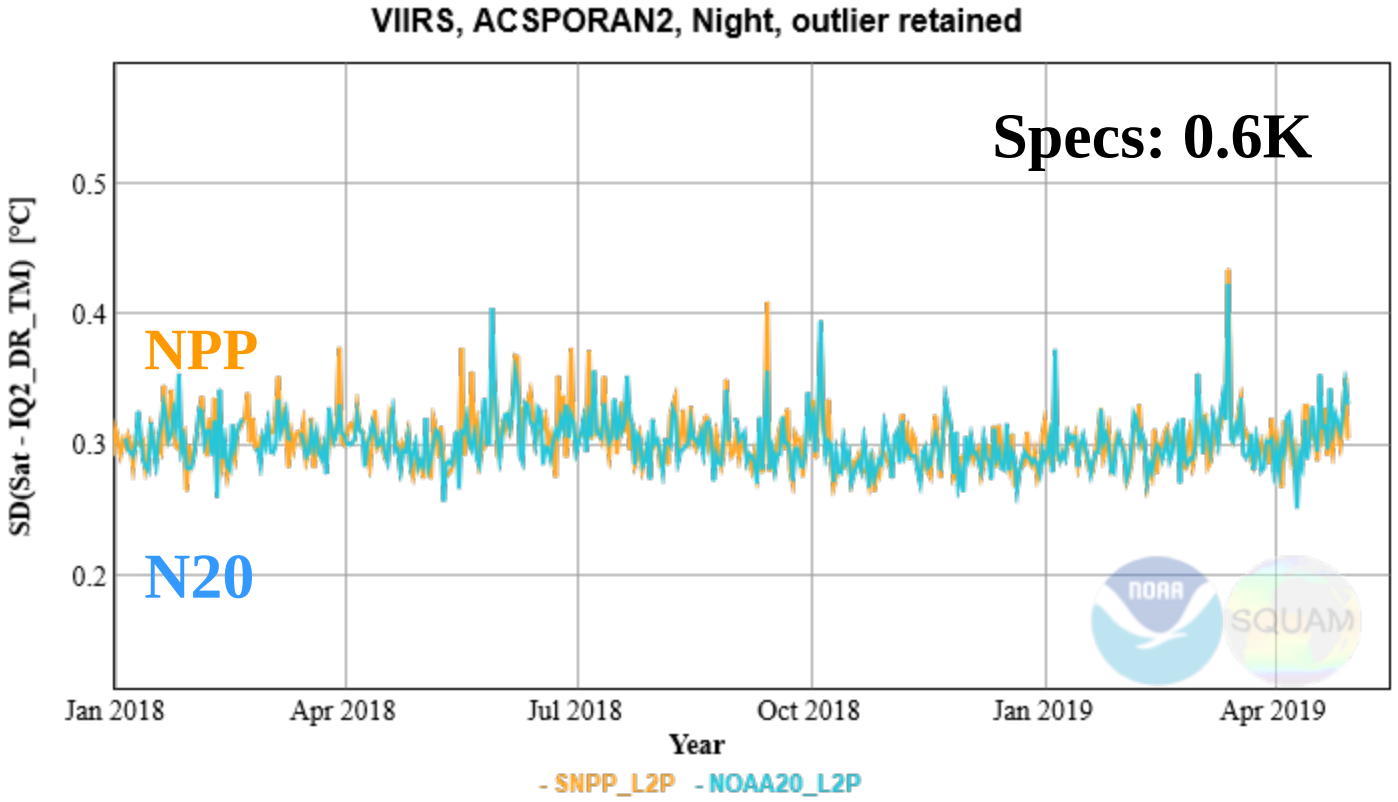
- Daytime biases are centered at ~0 and typically within ±0.1K
- Seasonal cycle (likely due to skin-bulk SST difference)
- Periodic disturbance in Val statistics consistent in NPP/N20 likely due to *in situ*
- NPP and N20 statistics are very consistent

Global SST Bias wrt. *i*Quam *in situ*: DAY With SSES Bias Correction



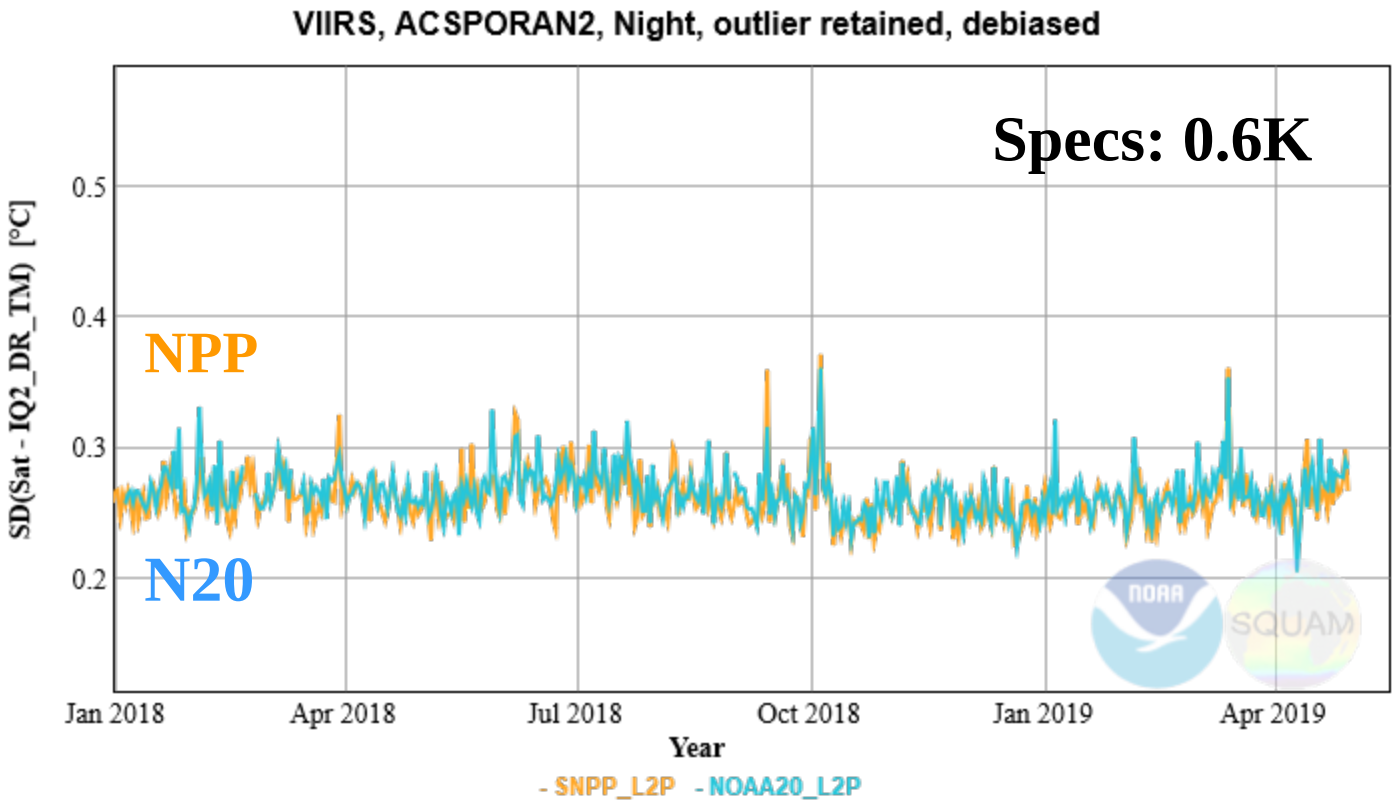
- Daytime SSES Bias correction reduces biases to ±0.07K
- Seasonal cycle is reduced (because SSES is trained against *in situ* data)
- Biases remain very consistent across NPP and N20

Global SST SD wrt. *i*Quam *in situ*: NIGHT
No SSES Bias Correction



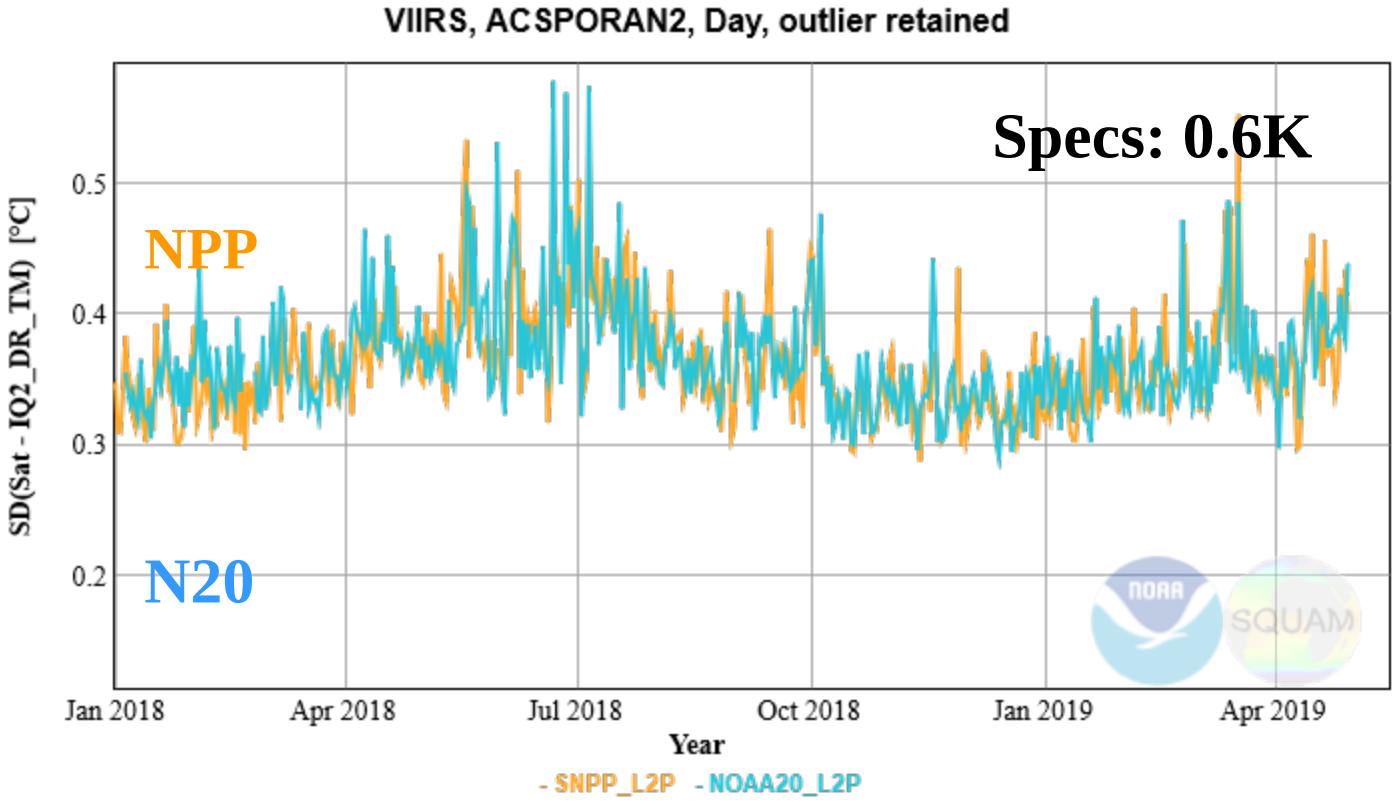
- Nighttime SDs are ~0.3K
- Seasonal cycle is minimal (at night, skin SST is close to bulk SST)
- NPP and N20 statistics are very consistent

Global SST SD wrt. *i*Quam *in situ*: NIGHT With SSES Bias Correction



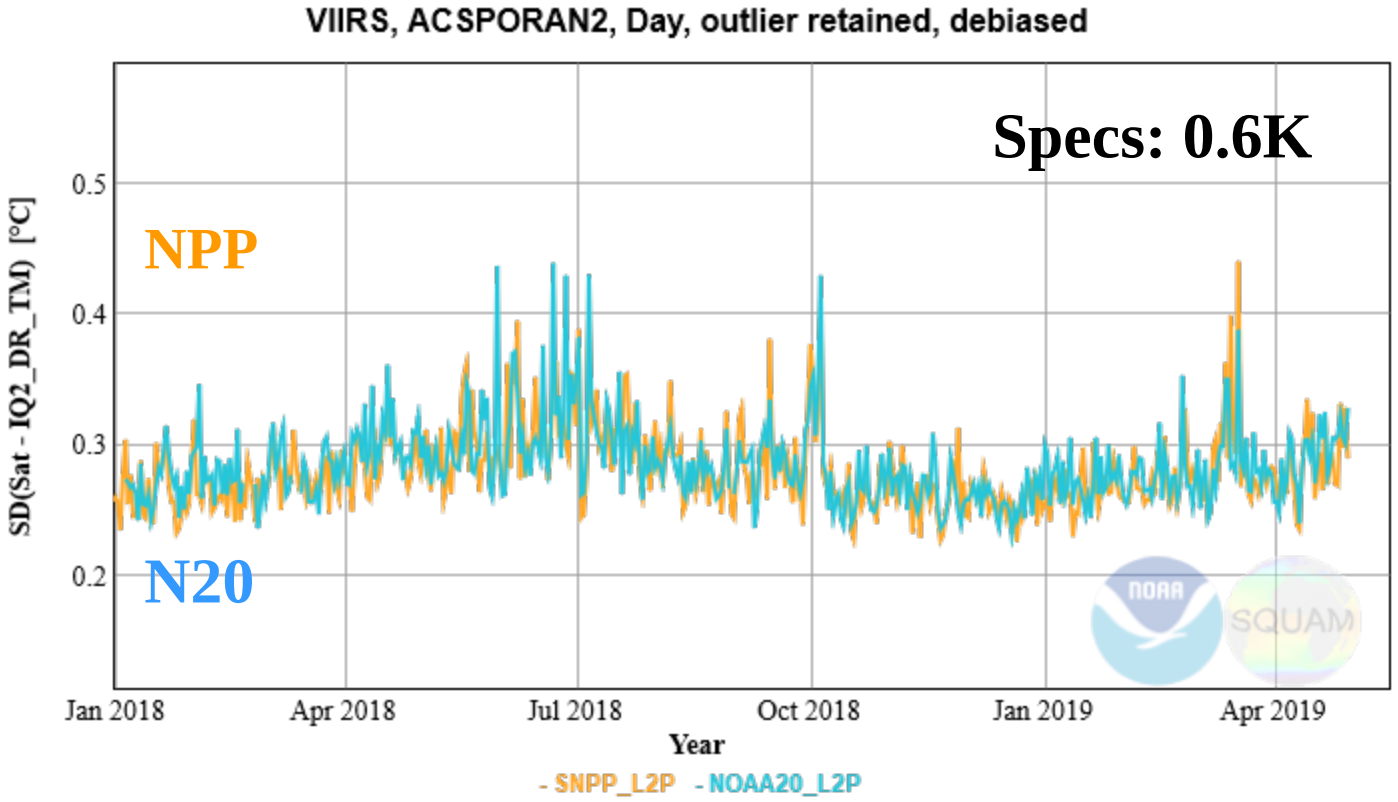
- Nighttime SSES Bias correction reduces SDs to ±0.26K
- Seasonal cycle is minimal (if present at all; skin close to bulk at night)
- SDs remain very consistent across NPP and N20

Global SST SD wrt. *i*Quam *in situ*: DAY
No SSES Bias Correction



- Daytime SDs have seasonal cycle and typically are bracketed by 0.33-0.45K
- Seasonal cycle is likely due to skin-bulk SST difference
- NPP and N20 statistics are consistent
- Disturbance in Val statistics consistent across NPP/N20 are likely due to in situ

Global SST SD wrt. *i*Quam *in situ*: DAY
With SSES Bias Correction



- Daytime SSES Bias correction reduces SDs to ±0.35K
- Seasonal cycle is reduced, because SSES is trained against *in situ* data
- SDs remain very consistent across NPP and N20

SST Error Budget

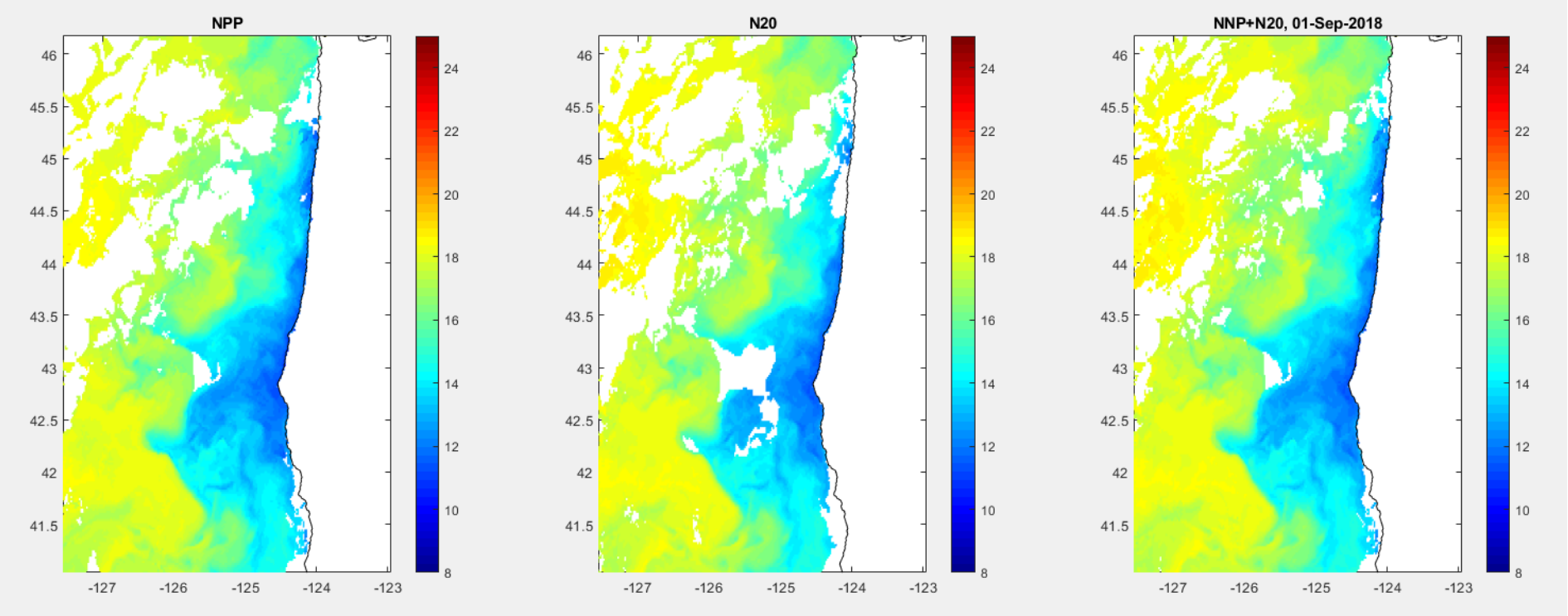
Attribute Analyzed	L1RD Threshold	Pre-Launch Performance	On-orbit Performance	Meet Requirement?	Additional Comments
Bias (no SSES Bias Correction)	±0.2 K	N/A	±0.05 K ±0.10 K	Yes	Meets/Exceeds User's Expectations
Bias (with SSES Bias Correction)	±0.2 K	N/A	±0.05 K ±0.07 K	Yes	Meets/Exceeds User's Expectations
SD (no SSES Bias Correction)	0.6 K	N/A	0.30 K 0.37 K	Yes	Meets/Exceeds User's Expectations
SD (with SSES Bias Correction)	0.6 K	N/A	0.26 K 0.28 K	Yes	Meets/Exceeds User's Expectations

User Feedback

Name	Organization	Application	User Feedback - User readiness dates for ingest of data and bringing data to operations
Paul DiGiacomo/ Veronica Lance	NOAA STAR	Coast Watch	Data distributed via CW to users
Alexander Kurapov	NOS	WCOFS	N20 data not included in the data assimilation process yet, but scripts to acquire the data created and preliminary assessments done
Eileen Maturi/ Andy Harris	STAR	Geo-Polar Blended Analysis	N20 already assimilated. Moderate-to-positive impact on analysis.
Simon Good	Met Office	OSTIA Analysis	Pending adding N20 SST on EumetCast
Helen Beggs	Australian Bureau of Met	RAMSSA, GAMSSA, L3S	Working with PO.DAAC to pull the data
Dorina Surcel-Colan	Canadian Met Centre	CMC Analysis	Working with PO.DAAC to pull the data

Example Feedback from NOS WCOFS

Improved coverage of the Oregon Coast (part of the West Coast Ocean Forecast System domain) by two VIIRSs from NPP and N20 (daily mosaic) (1-Sep-2018)



- Scripts to pull N20 data off CW THREDDS written
- Consistency/Complementarity of NPP/N20 SSTs preliminarily assessed
- Work is underway to include in data assimilation

Downstream Product Feedback

Algorit	duct	Downstream Product Feedback - Reports from downstream product teams on the dependencies and impacts

No Downstream Products Use SST

Risks, Actions, Mitigations

Identified Risk	Description	Impact	Action/Mitigation and Schedule
1	N20 VIIRS Thermal IR anomalies	High	SDR team mitigated
2	Frequent WUCDs (NPP & N20)	High	SDR team mitigated
3	Operational correction of WUCDs	High	SDR Team Mitigated

Documentations

Science Maturity Check List	Yes ?
ReadMe for Data Product Users	Yes
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)	Yes

Check List - Validated Maturity

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

Cal/Val Summary & Conclusion

- SST Team recommends algorithm validated maturity
- Both N20 & NPP Products are highly consistent, and meet/exceed JPSS specs & users expectations
- Both are distributed to users via PDA and CW, and archived at PO.DAAC/NCEI. No negative feedback received from users
- All sensors performance issues have been properly addressed by the SDR team, including
  - Resolved initial thermal IR anomaly;
  - Reduced frequency of WUCDs from quarterly to annual;
  - Delivered to ops the WUCD mitigation algorithm, so that the effect of future (reduced frequency) annual WUCDs on BT is significantly minimized
- No N20-specific caveats or reservations have been observed.
- Users are encouraged to use the N20 product the same way they use NPP

Path Forward

- **Lessons learned from N20 and NPP Cal Val**
  - Taken in isolation, both NPP and N20 SST products fully meet and exceed NOAA requirements and users expectations. Both NPP & N20 products are accurate and consistent
  - Moving forward with new tasks (pattern recognition, frontal detection, data fusion), requires minimization of residual cloud leakages and mitigating SST biases (cross-platform, angular, regional), in each individual sensor product
- **Planned improvements**
  - Minimize residual cloud leakages in each individual product. Potentially, revisit clear-sky mask, add new tests
  - Minimize cross-platform, angular, regional SST biases. Potentially, revisit the current MC/NLSST algorithms
- **Future Cal/Val activities / milestones**
  - Preliminarily minimize cloud leakages. Implement pattern recognition. Derive new thermal fronts product (FY20)
  - Work towards data fusion. Revisit SST algorithms/clear mask. Generate collated and super-collated ACSPO products (FY21+)