Exploration of Retrieval Approaches For SLSTR

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20th ghrsst science team meeting

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European Union

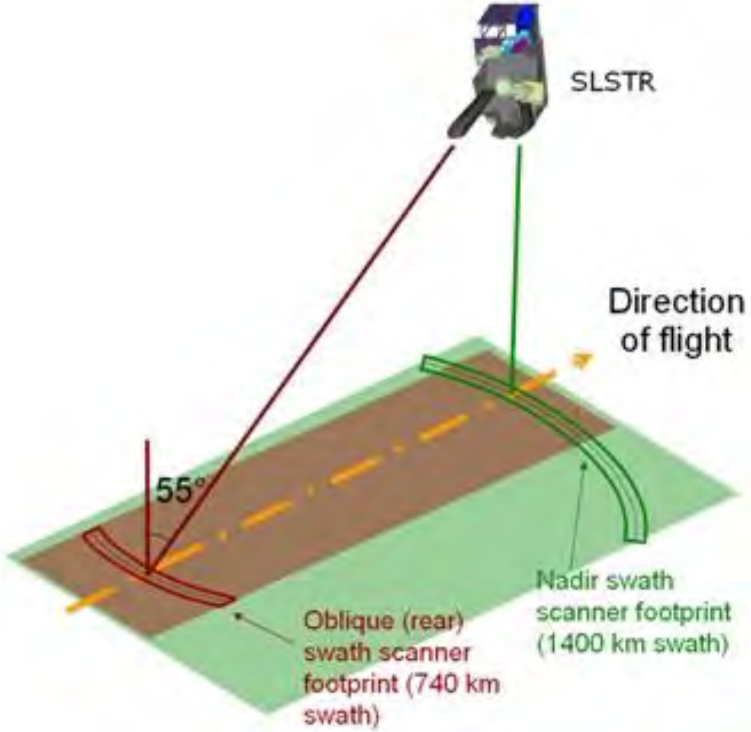
European Space Agency

Copernicus Europe's eyes on Earth

EUMETSAT

SLSTR: climate quality…

- SLSTR – continuation of (A)ATSR series
- (A)ATSR instruments
  - Dual-view to provide robust & accurate SST
  - Highly accurate thermal calibration (<0.03 K/decade)
  - Low thermal detector noise due to active cooling



SLSTR: climate quality…

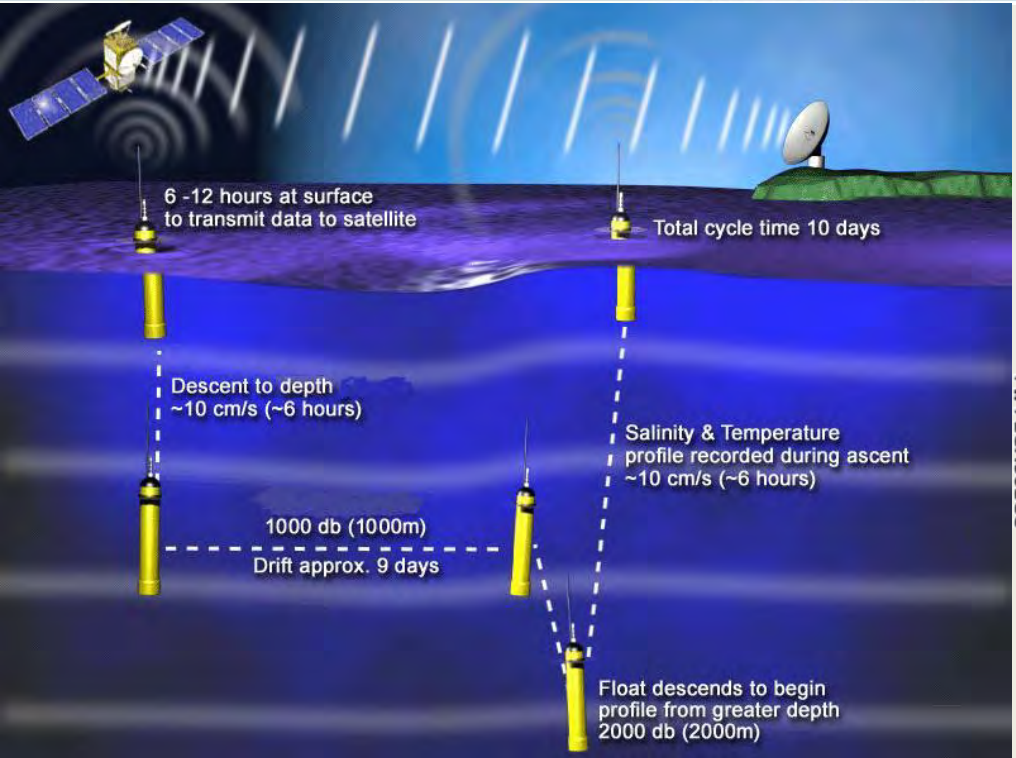
Climate accuracy requirements are very stringent

- Observing system stability <0.04 K/decade
    - Calibration drift
    - Retrieval (including cloud screening)
    - Requirements are no longer just global…
    - …Change, attribution, decadal forecasting…

How to validate product accuracy?

- Typical *in situ* accuracy ~0.2 K (drifting buoy)
    - Results tend to 0.2 K r.m.s. – hard to estimate below this
- Radiometers better (more accurate, closer to actual measurement)
    - Lack of coverage/matches
- ARGO array
    - Design accuracy <0.01 K

ARGO as a validation source



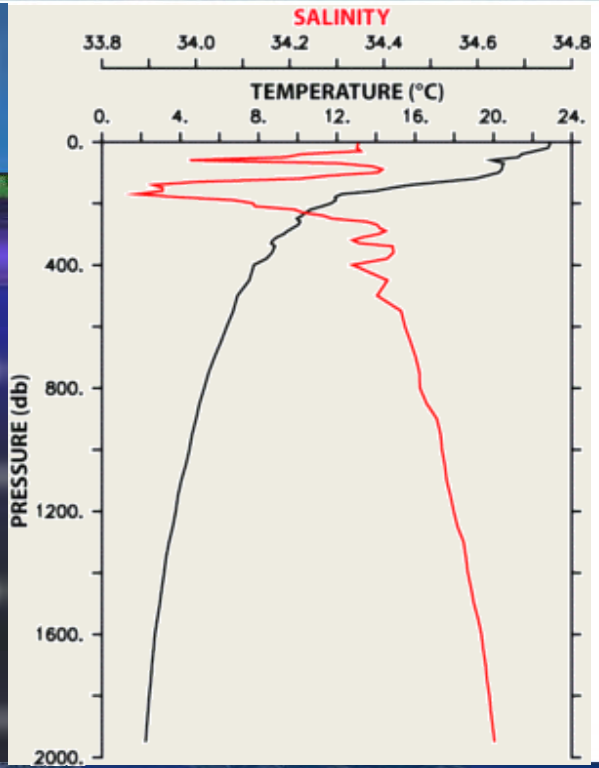
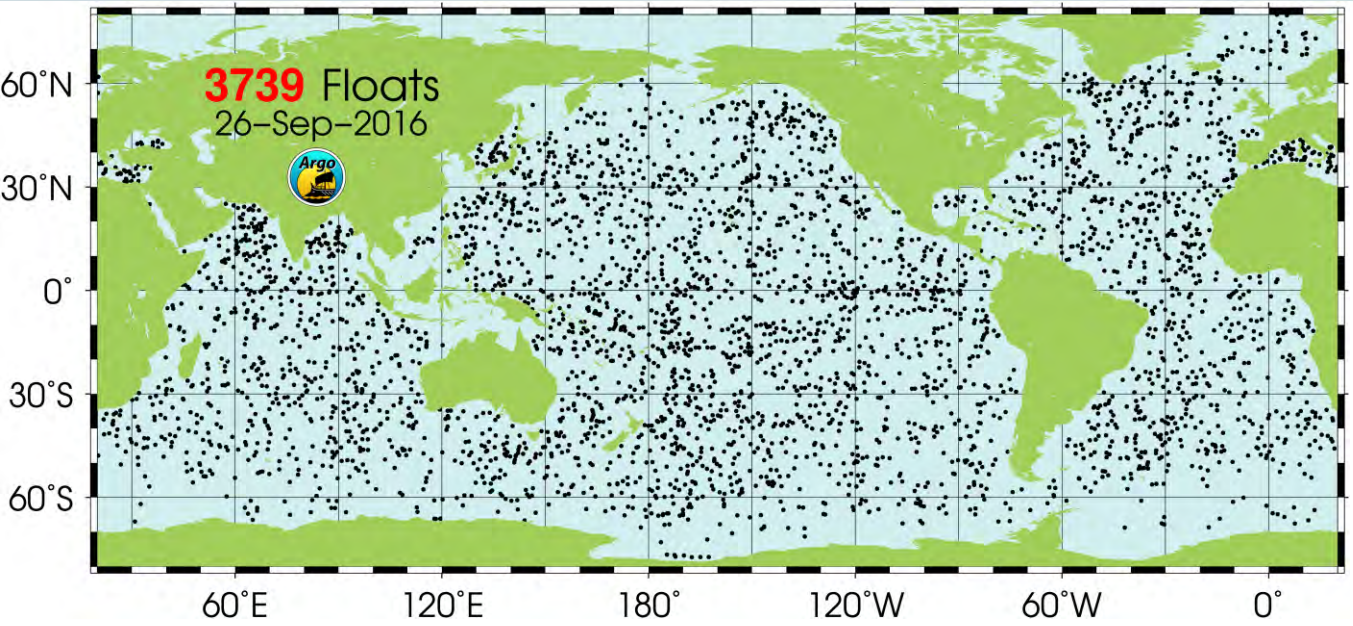


Image credit
argo.ucsd.edu

SLSTR: climate quality…



~400 near-surface measurements per day

Usually, pump is shut off ~few metres from **surface…**

- 'High-resolution' floats sample <1 m

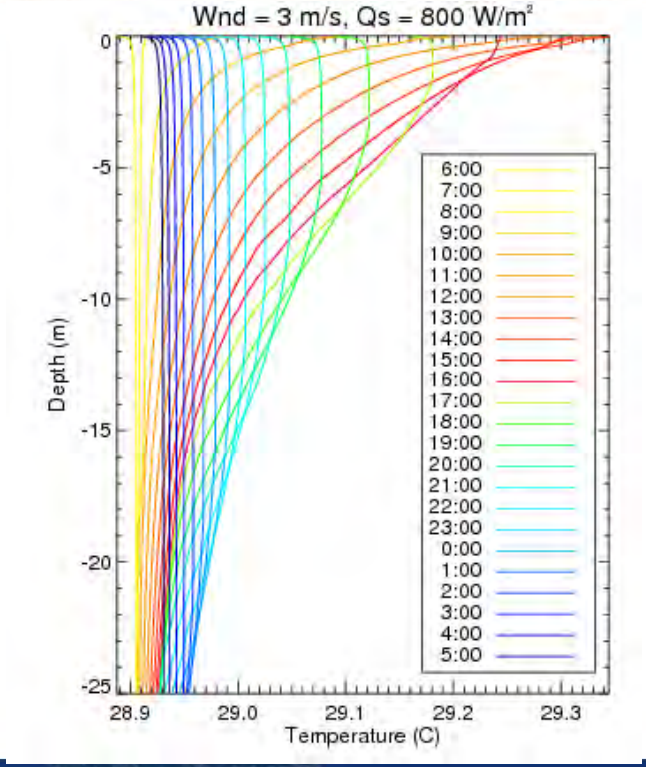
Must account for surface effects <u>down to ARGO depth</u>

Diurnal Warming Correction – Sample Model Profile of Warming with Depth

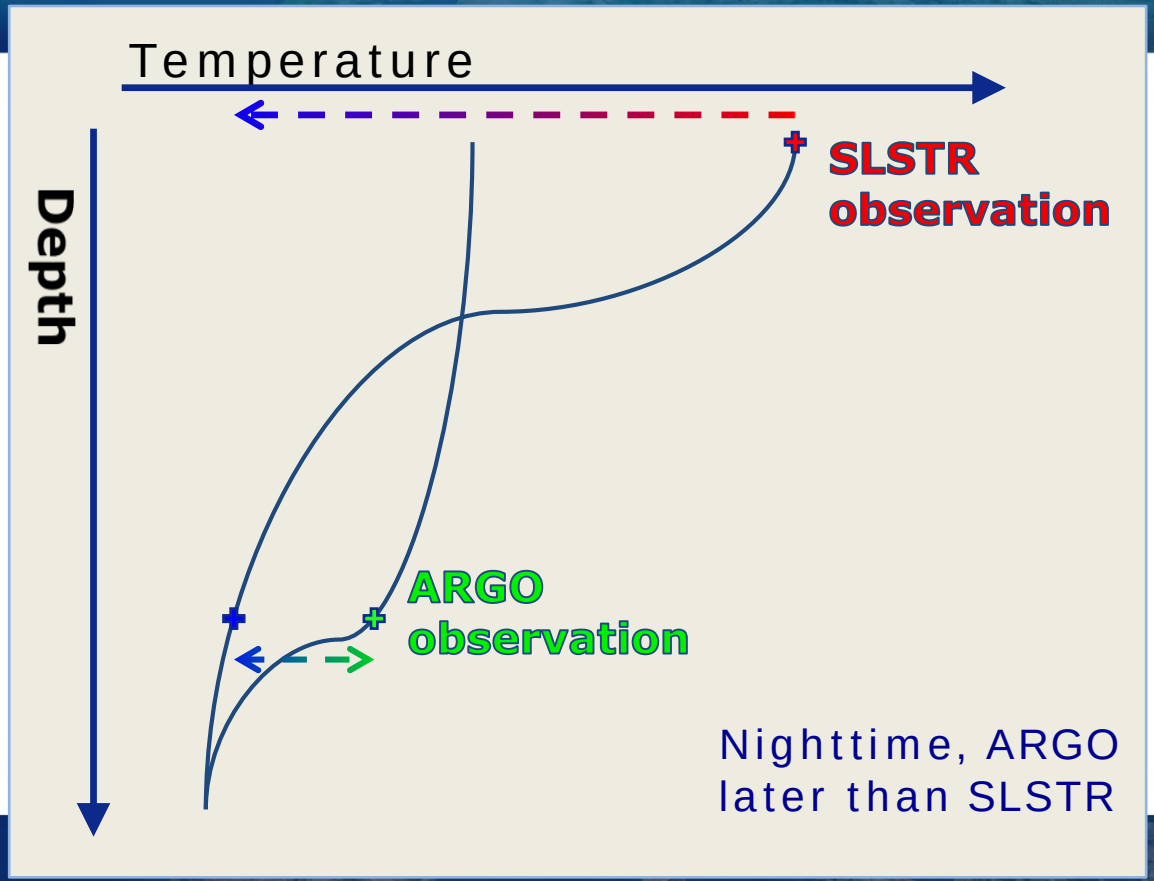
Model simulates full vertical profile of warming

- Enables estimation of warming at arbitrary depth
- Model presently run to a depth of 50 m

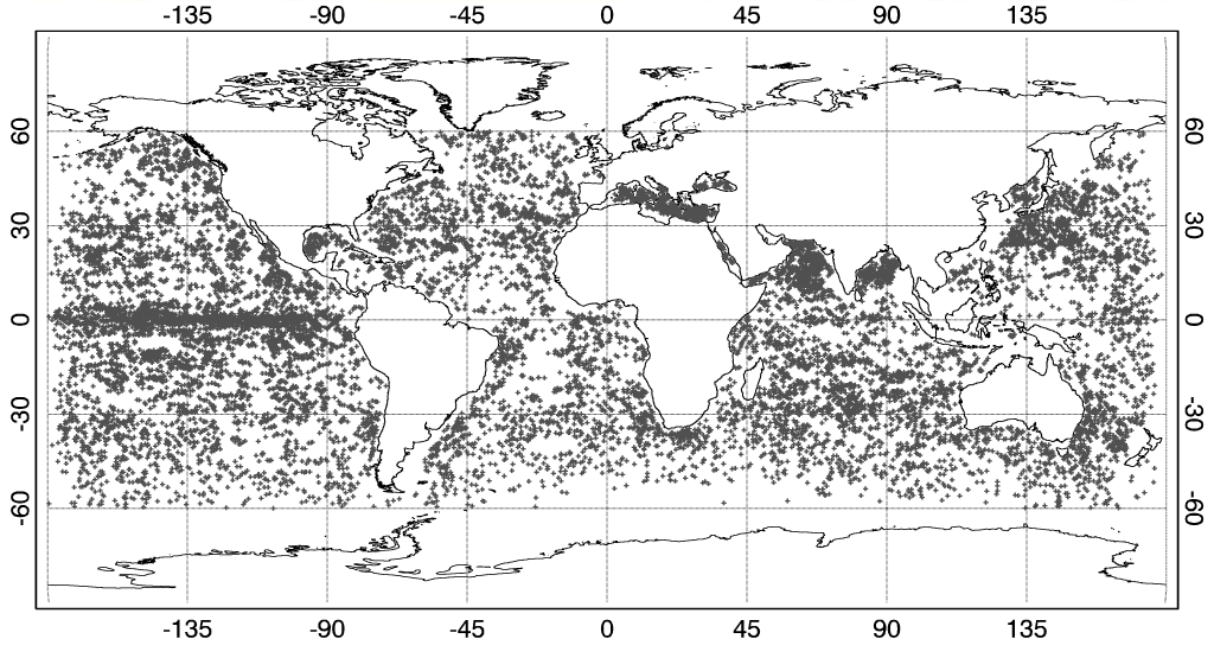
Time evolution of vertical temperature profile shown here for idealized forcing with a constant wind speed of 3 m/s and a peak insolation of 800 W/m2



Revised depth adjustment



Matchup distribution

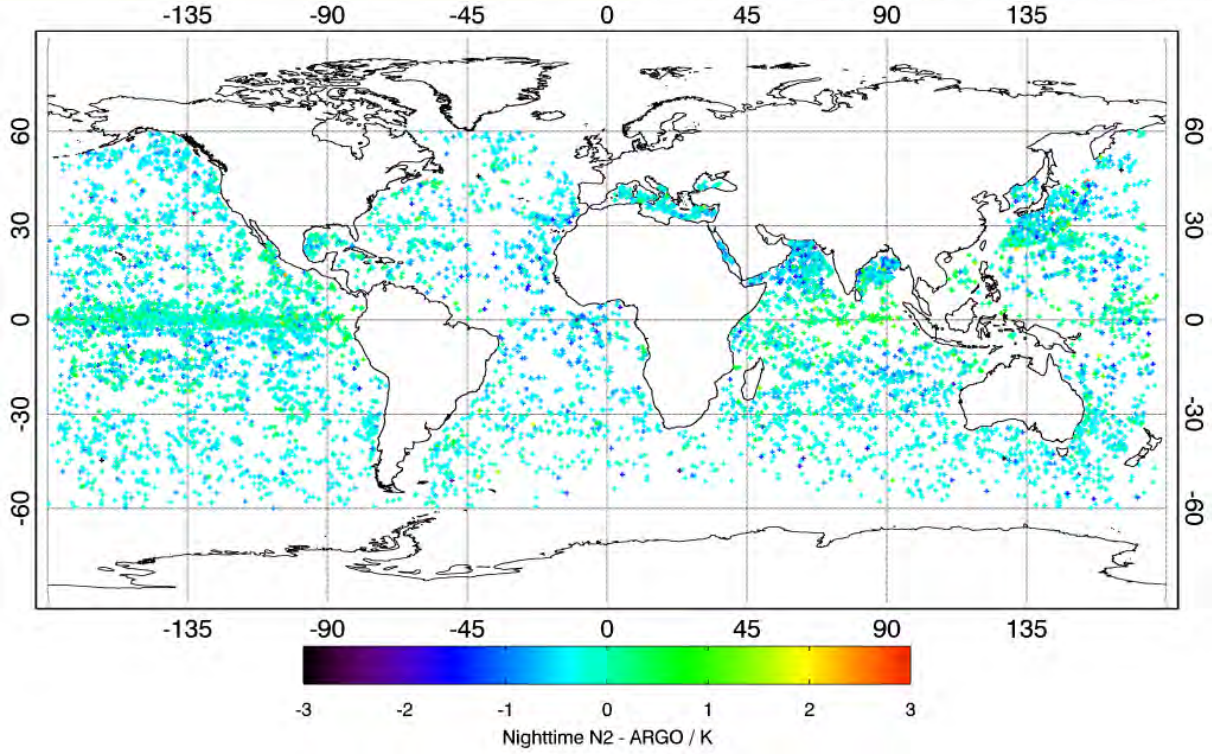


SLSTR - ARGO match locations

Reprocessed S3A data, Aug 2016 – Apr 2018 (~177,000 matches)

After QC checks (7×7 pixel box: Pclr>0.9, QL=5, ±4h) ~15,300 matches

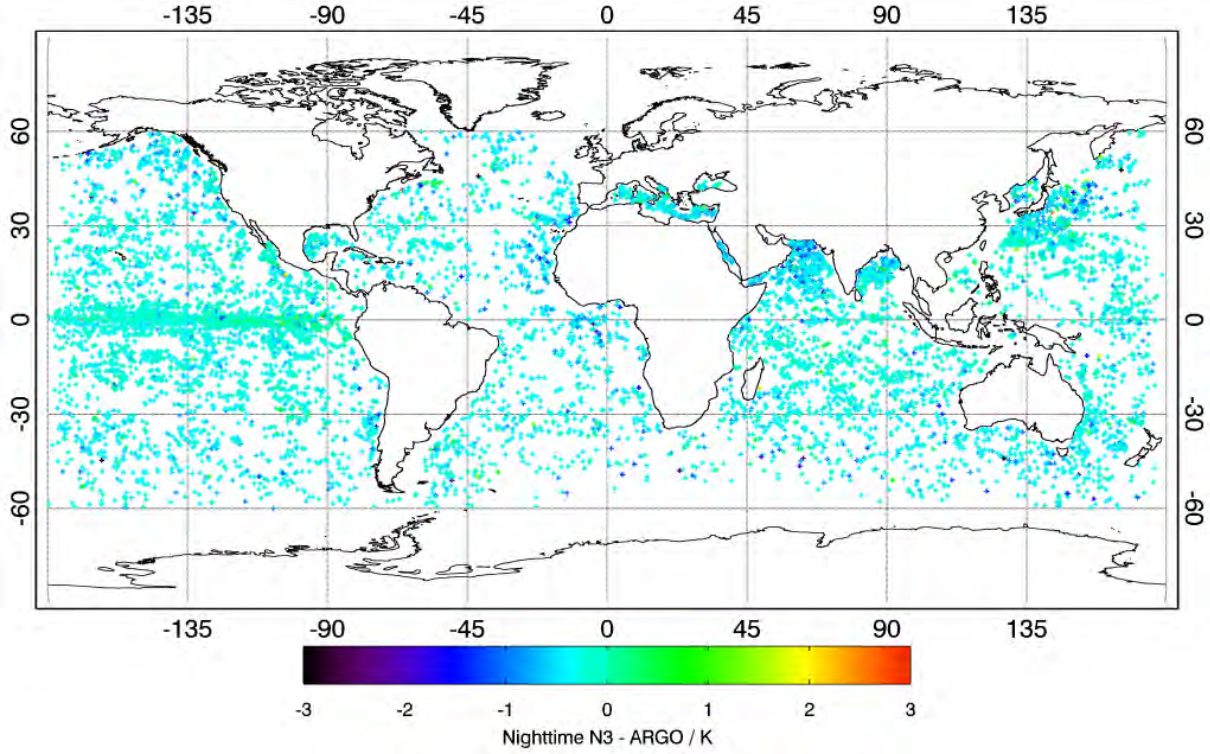
Nighttime N2



Warm bias in tropics

Cool aerosol bias evident

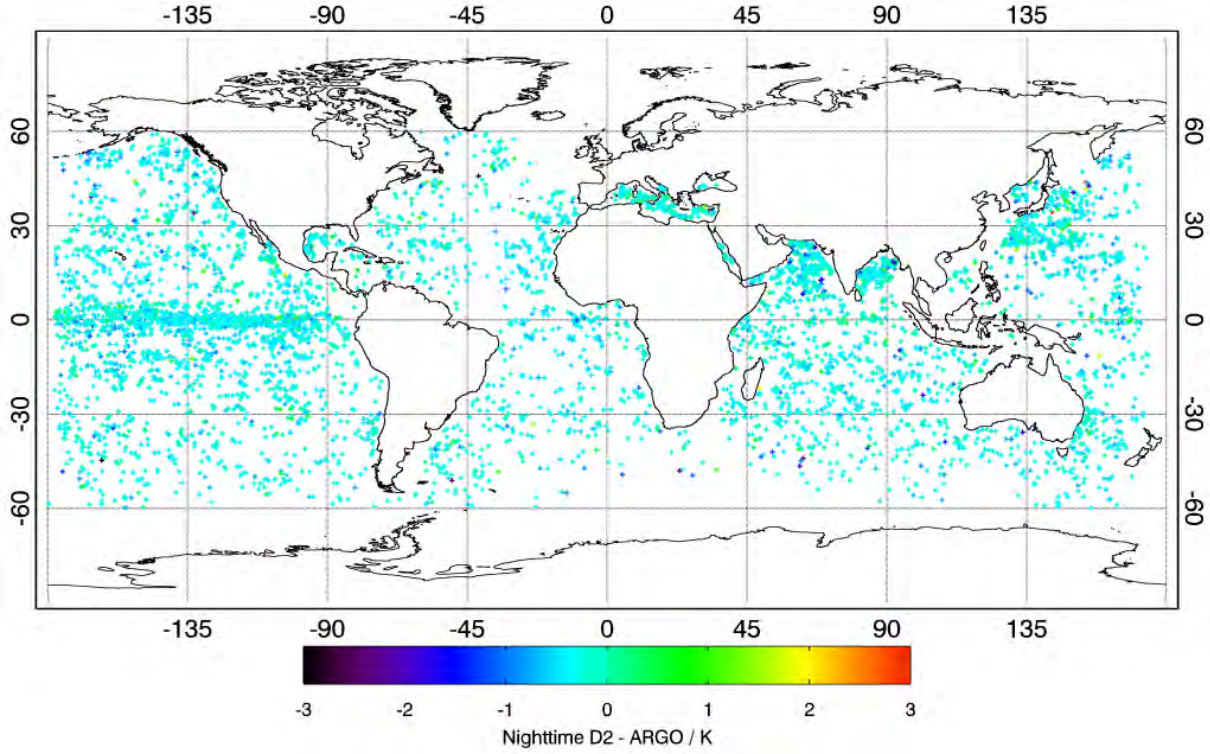
Nighttime N3



Reduced regional differences

Some aerosol-related bias still evident

Nighttime D2

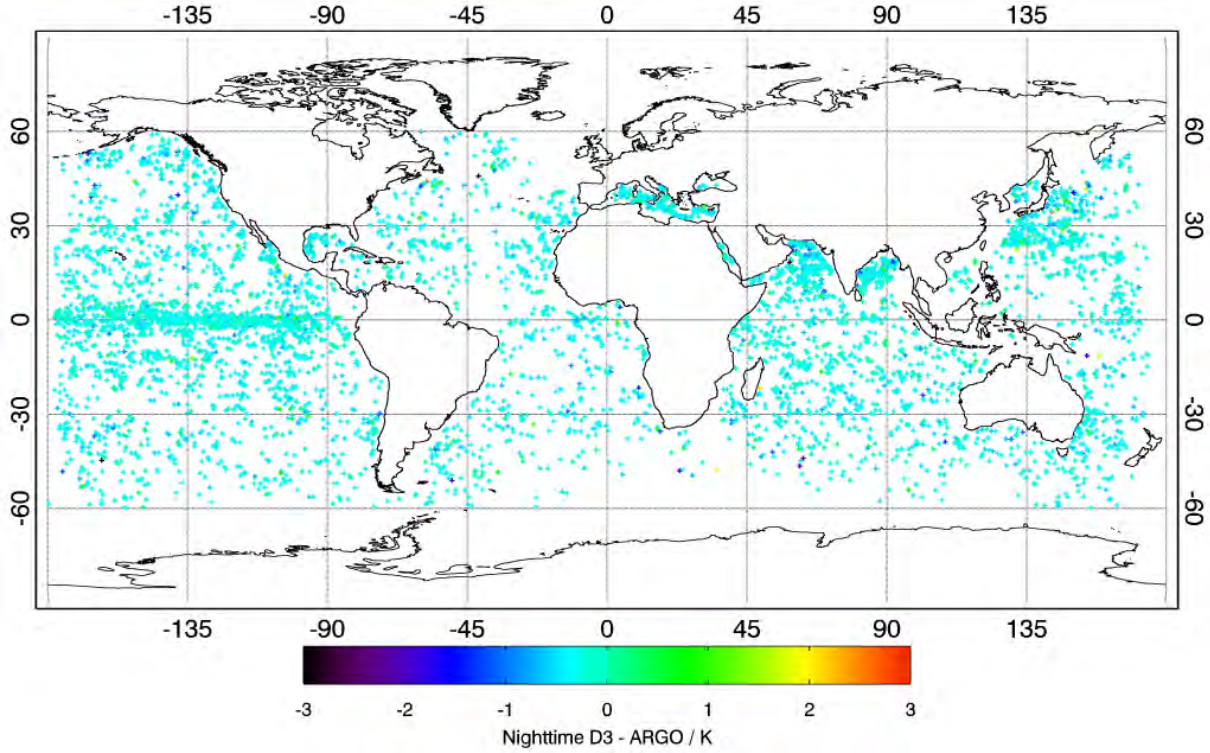


Fewer matches (narrower swath)

Greatly reduced aerosol-related bias

Still some regional biases

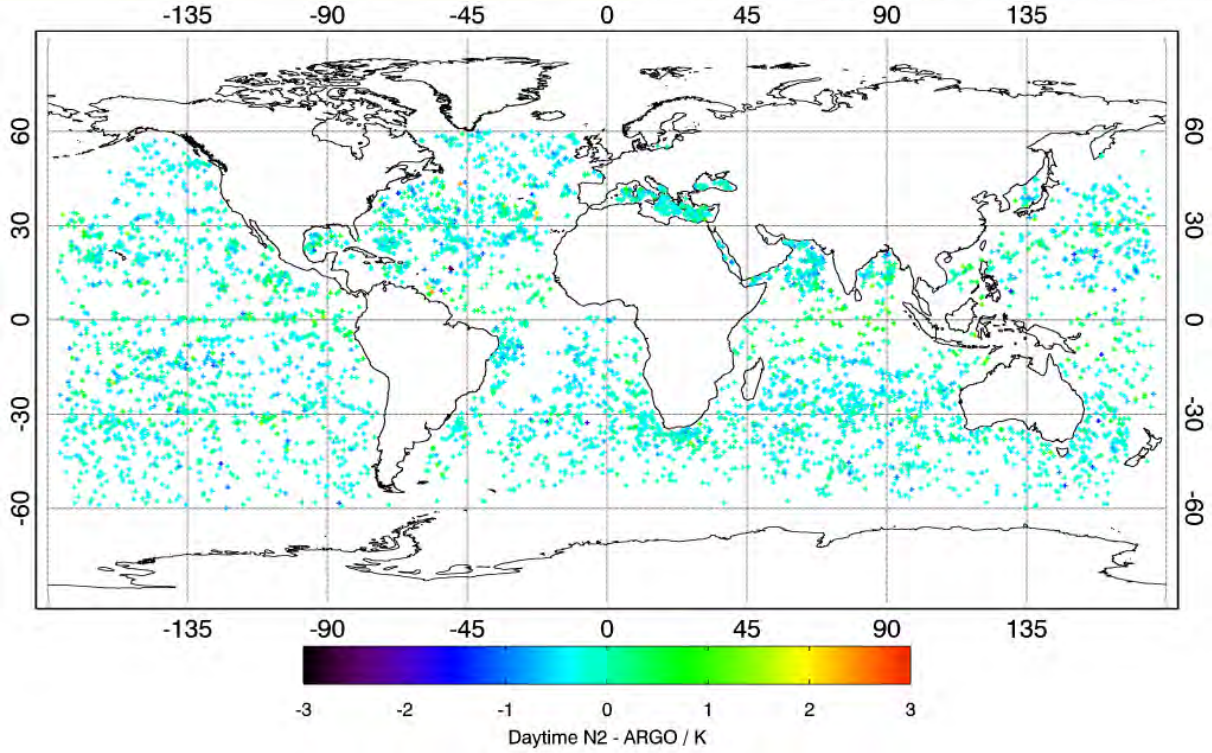
Nighttime D3



Issues largely resolved

Low noise

Daytime N2

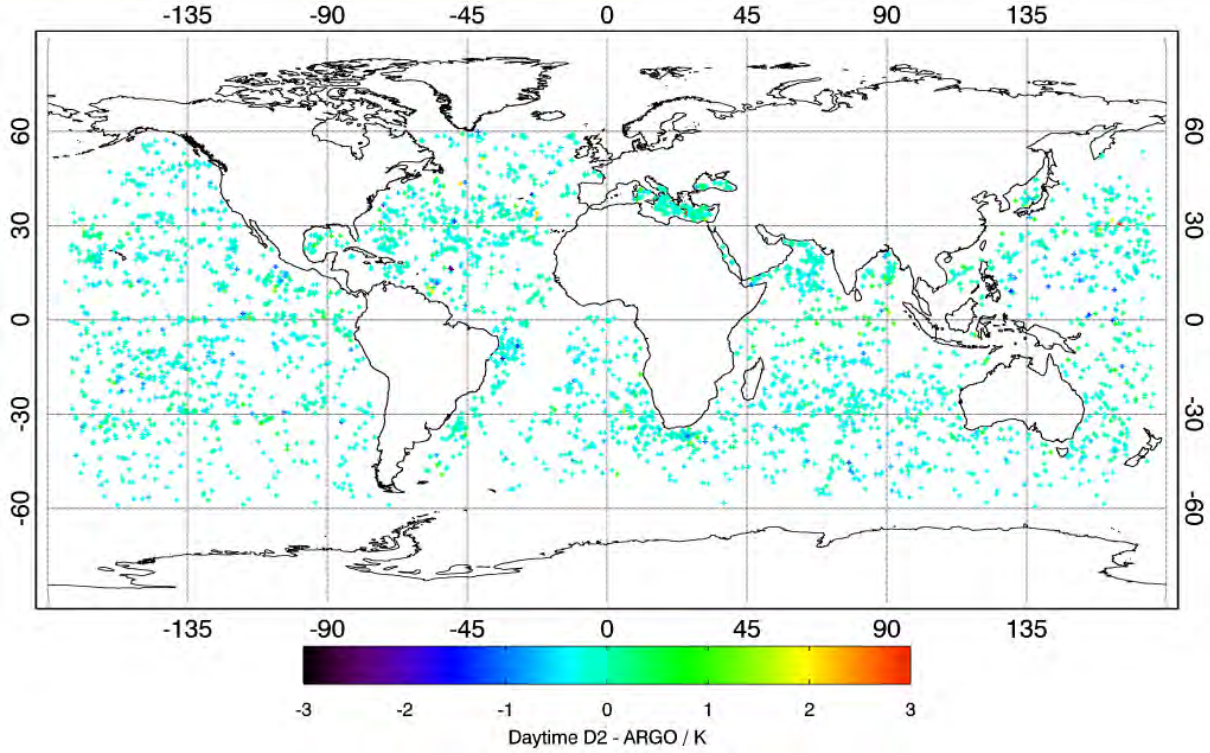


Warm bias in tropics still evident

Less prominent aerosol-related bias

- Cloud screening?

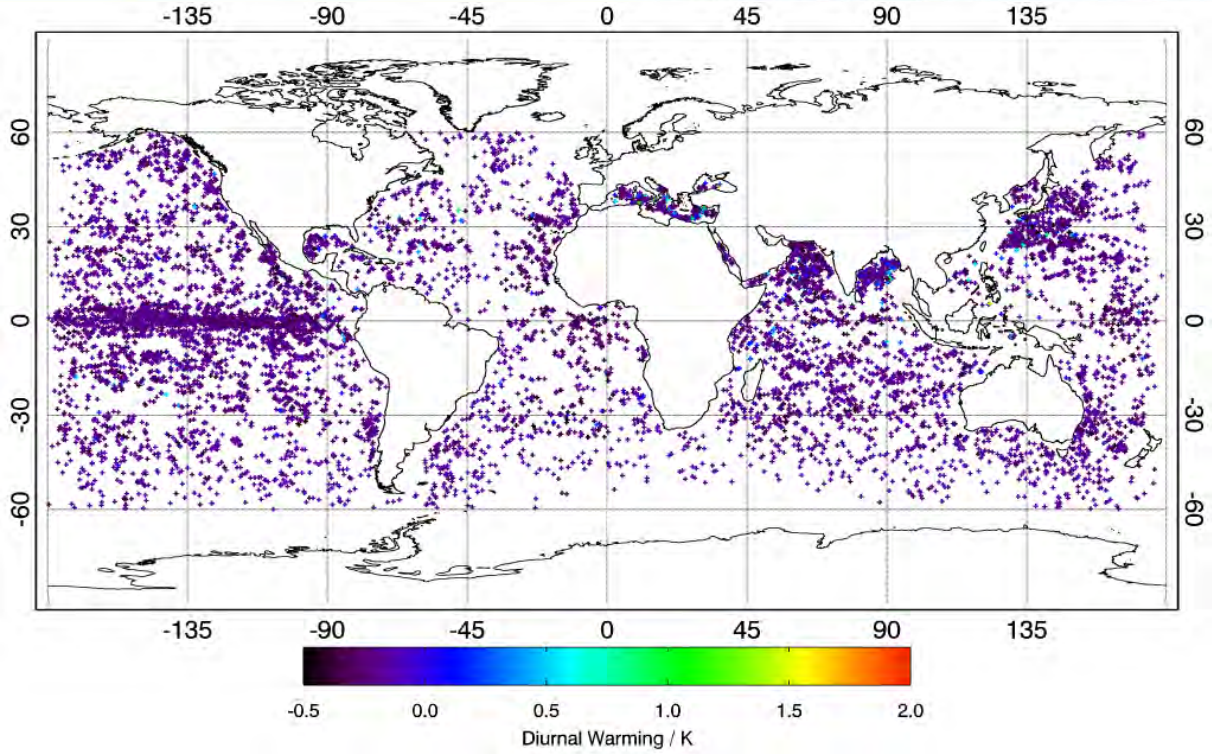
Daytime D2



Subtle regional biases still evident

Aerosol issue largely managed

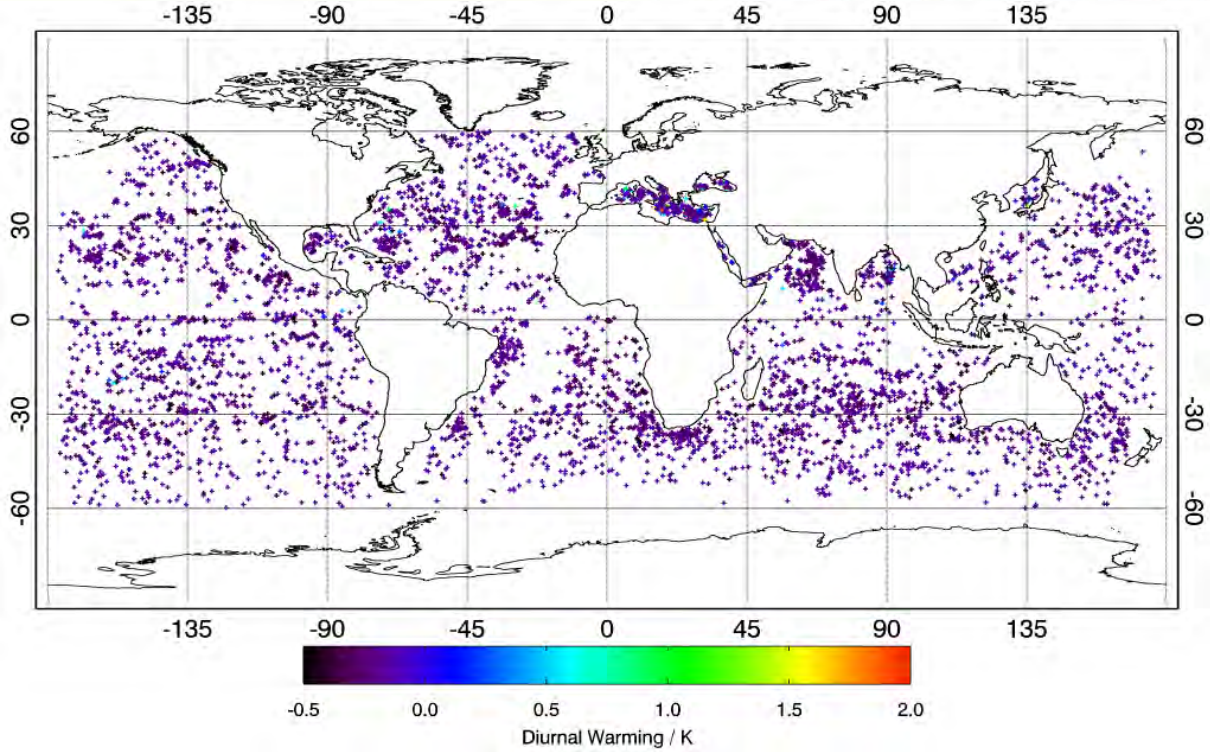
Nighttime depth adjustment



Mostly negative (skin effect)

Some residual warming

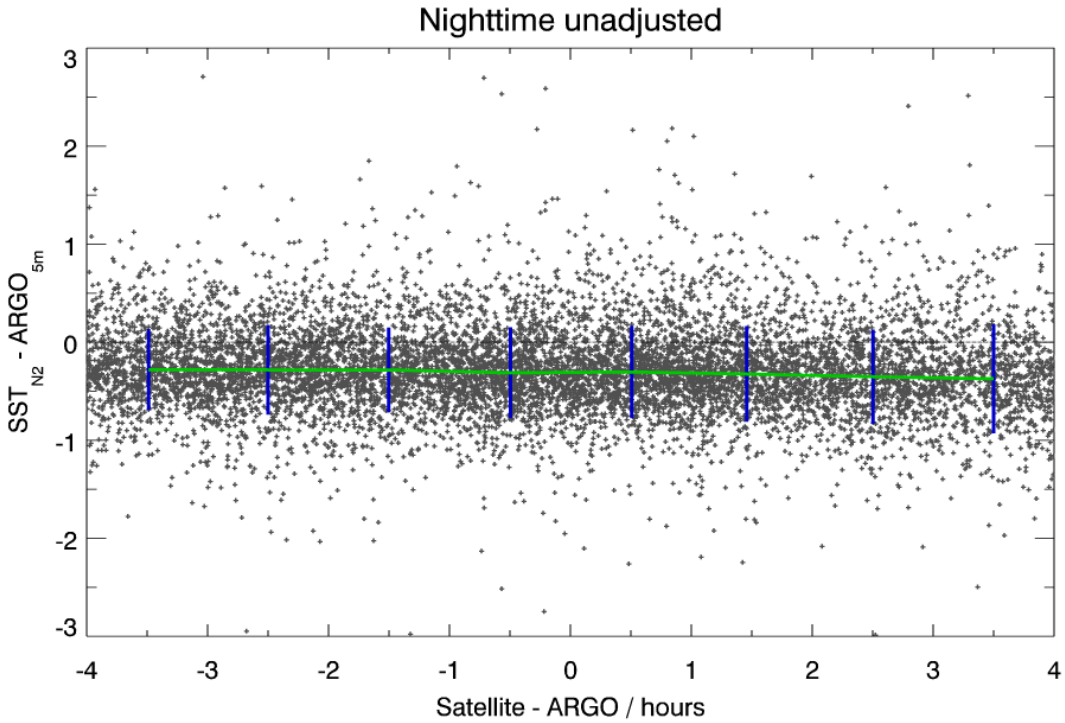
Daytime depth adjustment



Again, mostly negative (skin effect)

Some warming in a few cases

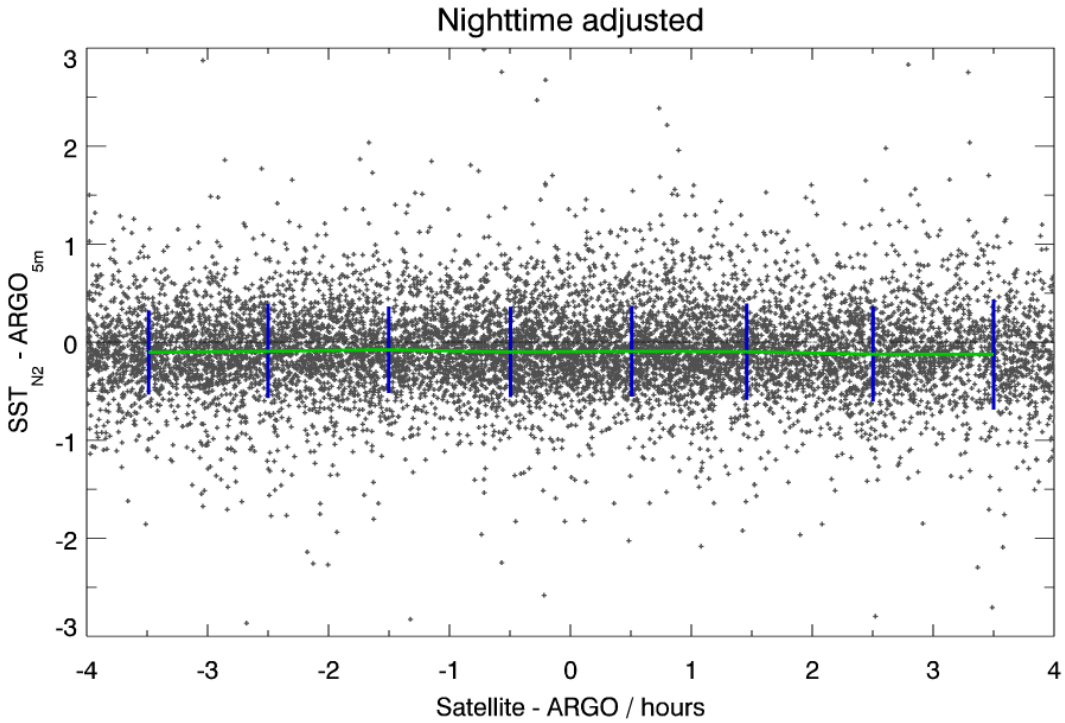
Effect of Depth Adjustment



Nightime 2-channel

Uncorrected has slight gradient w.r.t. time difference

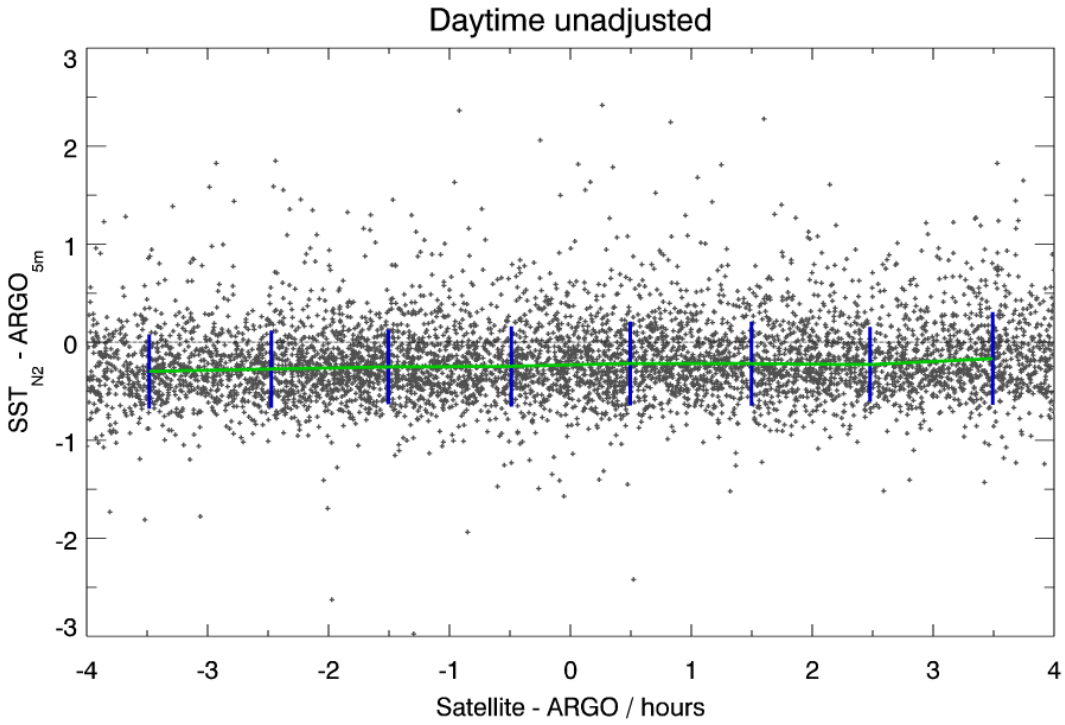
Effect of Depth Adjustment



Nightime 2-channel

Adjusted has ~no gradient w.r.t. time difference and close to zero bias

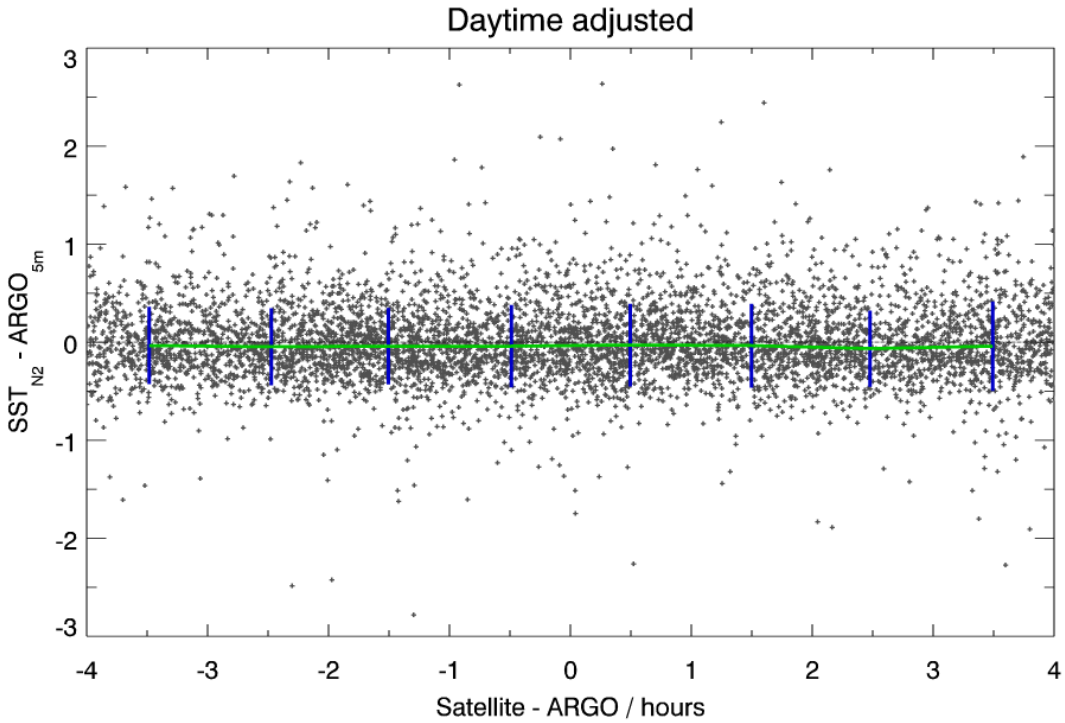
Effect of Depth Adjustment



Daytime 2-channel

Uncorrected has slight gradient w.r.t. time difference (opposite to nighttime)

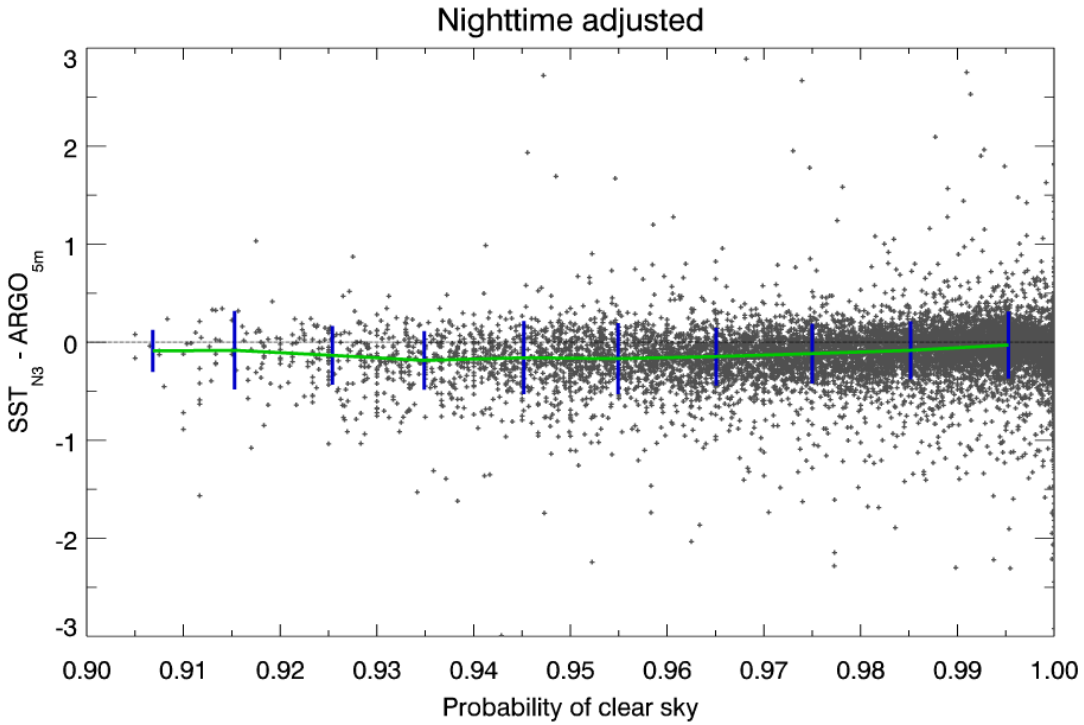
Effect of Depth Adjustment



Daytime 2-channel

Adjusted has ~no gradient and virtually no bias

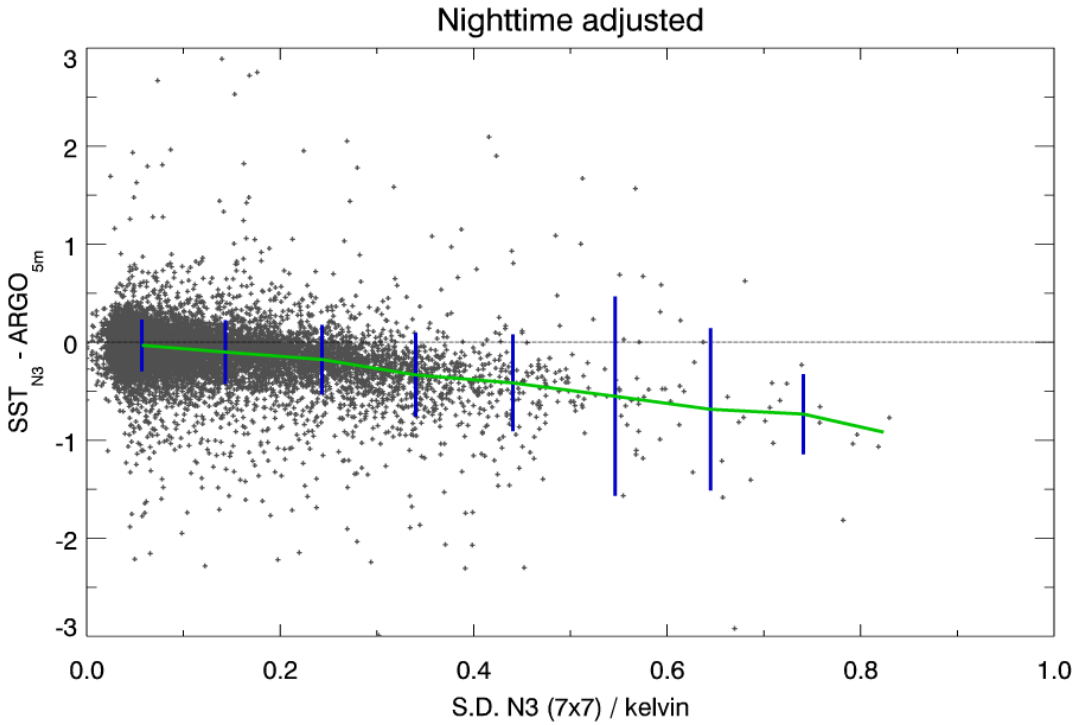
Dependence on Pclear



Nighttime 3-channel

Very slight trend with probability (to be expected)

Dependence on S.D. 7x7

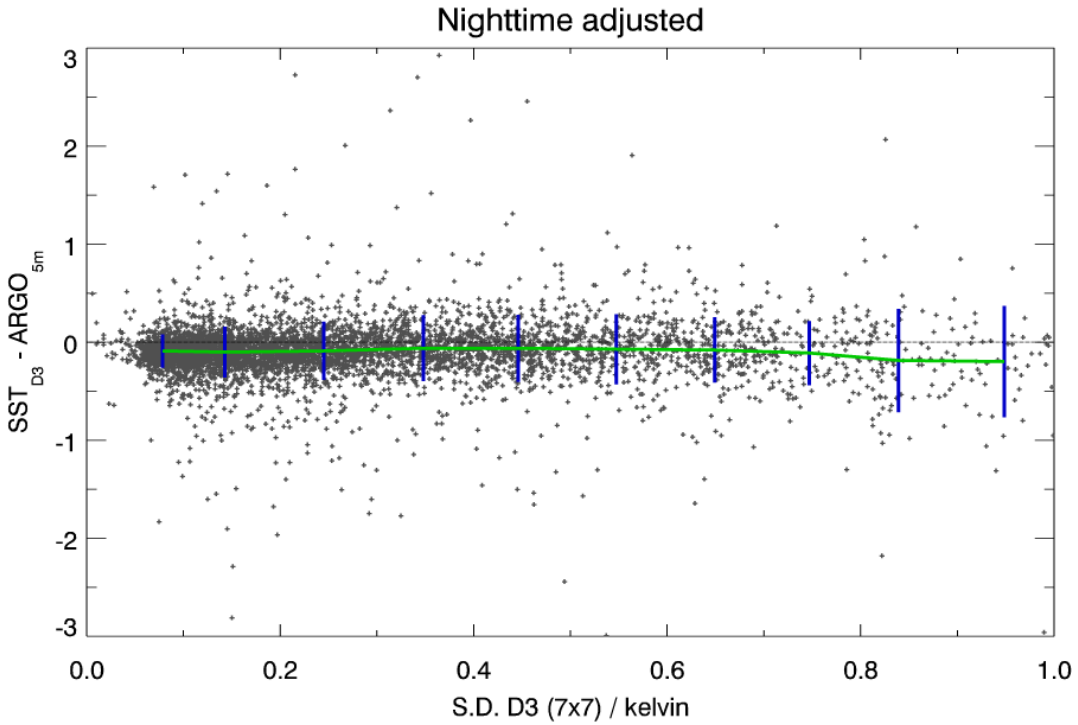


Nighttime 3-channel

Some trend w.r.t. S.D. in 7x7 box

Suggests residual cloud?

Dependence on S.D. 7x7

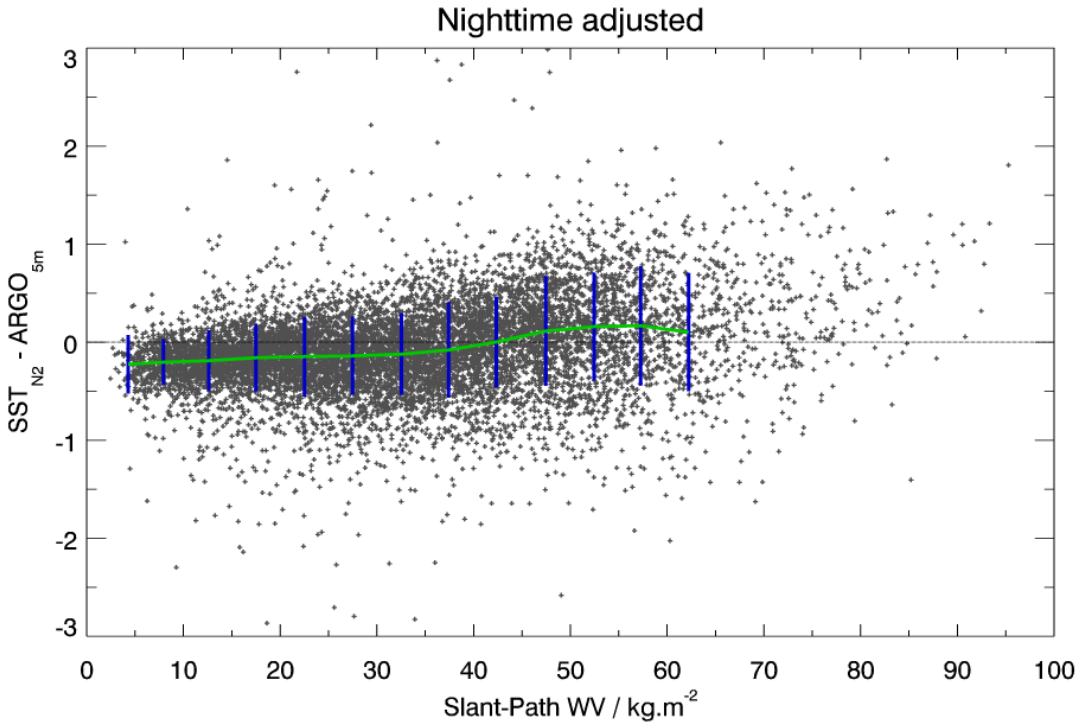


Nighttime Dual-3

Virtually no trend w.r.t. S.D. in 7x7 box

N.B. Residual cloud in oblique view will produce warm bias

Dependence on slant-path WV

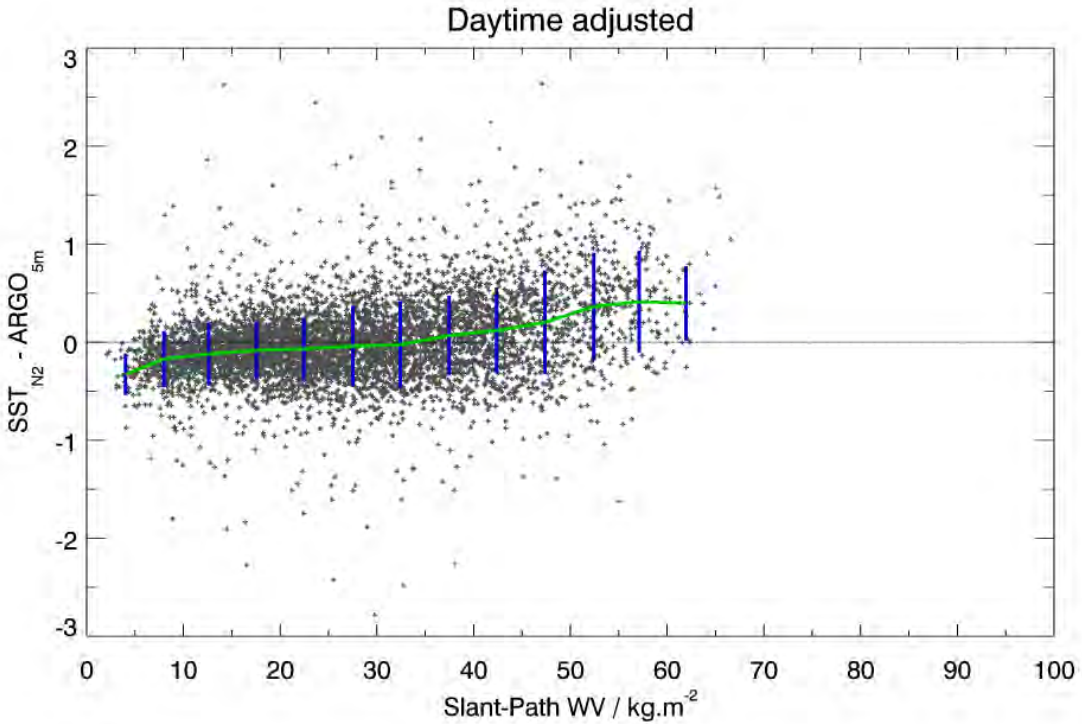


Nighttime 2-channel

Distinct trend with higher water vapour

N.B. Increase in scatter with WV is expected due to lower SNR

Dependence on slant-path WV



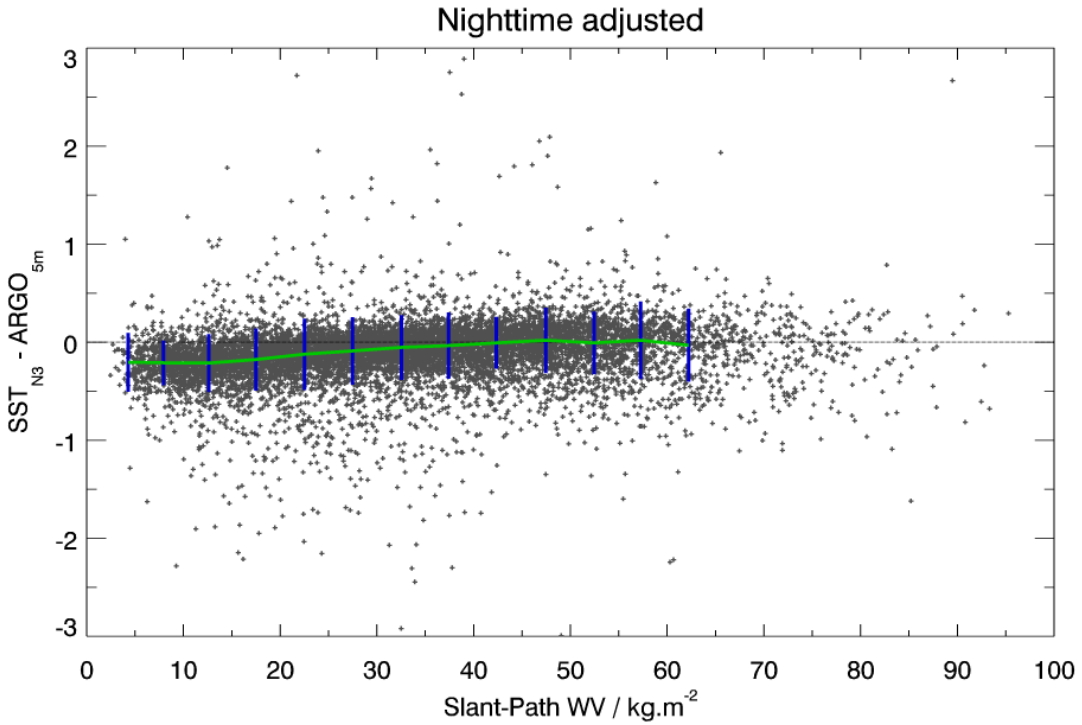
Daytime 2-channel

Again, distinct trend with higher water vapour

Fewer matches, less slant-path WV

N.B. Using WCT QL

Dependence on slant-path WV

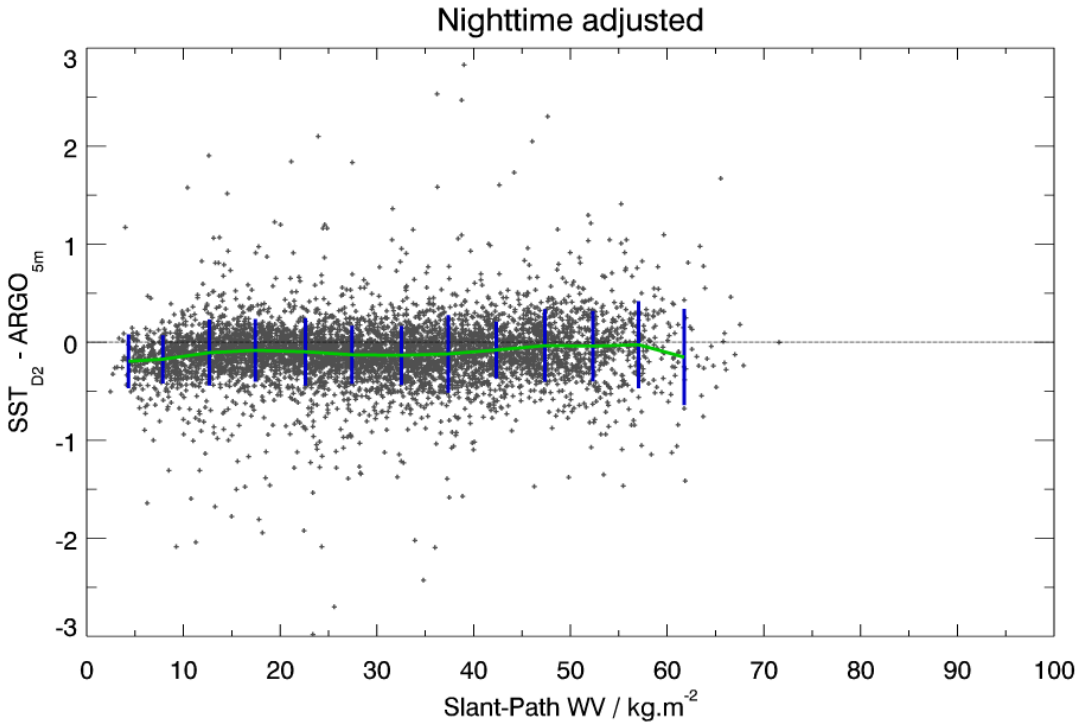


Nighttime 3-channel

Some trend with WV

N.B. Improved noise and linearity due to inclusion of 3.7 µm channel

Dependence on slant-path WV

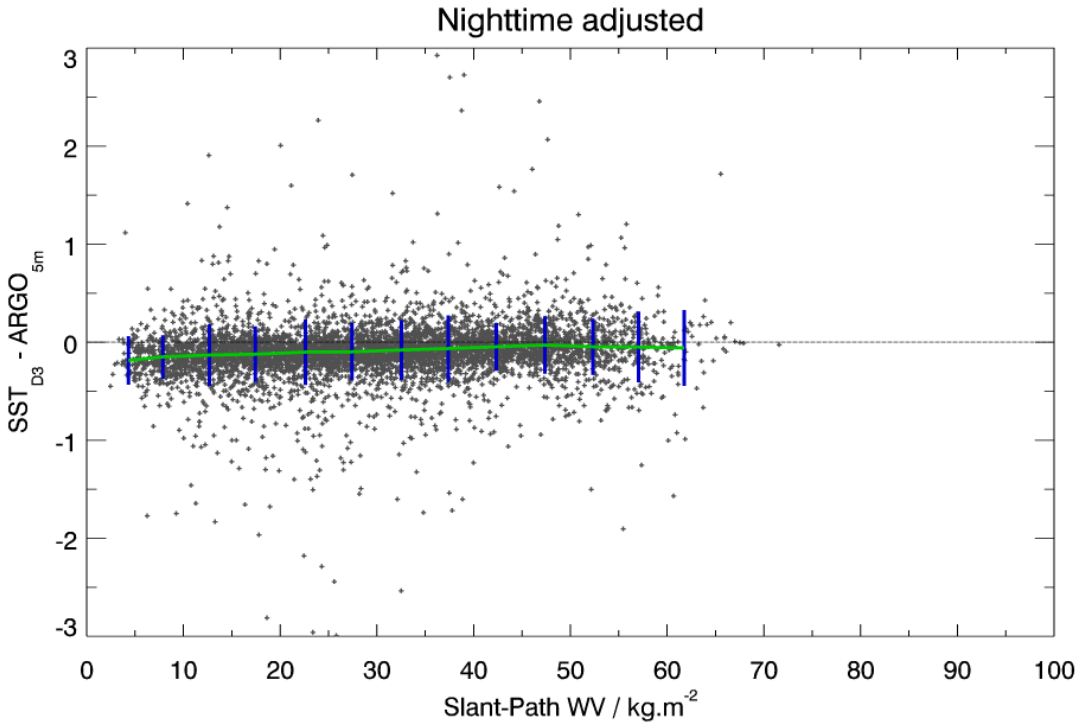


Nighttime Dual-2

Some structure due to WV (warmer at high values)

Note reduced range of slant-path WV

Dependence on slant-path WV



Nighttime Dual-3

About 0.2 K trend from low to high WV

Some checks using direct regression

Brightness temperatures have been added to the reprocessed MDB

- Opportunity to evaluate linearity characteristics

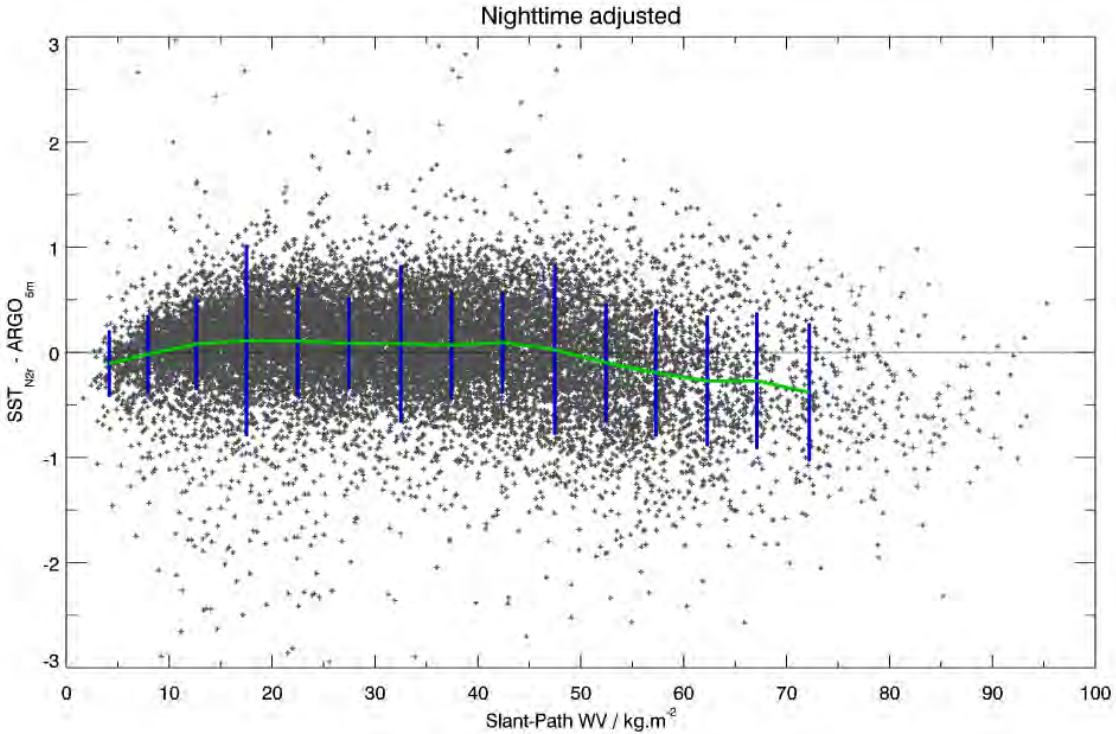
Use OSI-SAF style regression form

$$\mathrm{SST} = (a_0 + b_0.S) + \sum T_\mathrm{i}(a_\mathrm{i} + b_\mathrm{i}.S)$$

$$S = sec(\mathrm{SZA}) - 1$$

Needed because *S* varies "continuously" in the matchup data

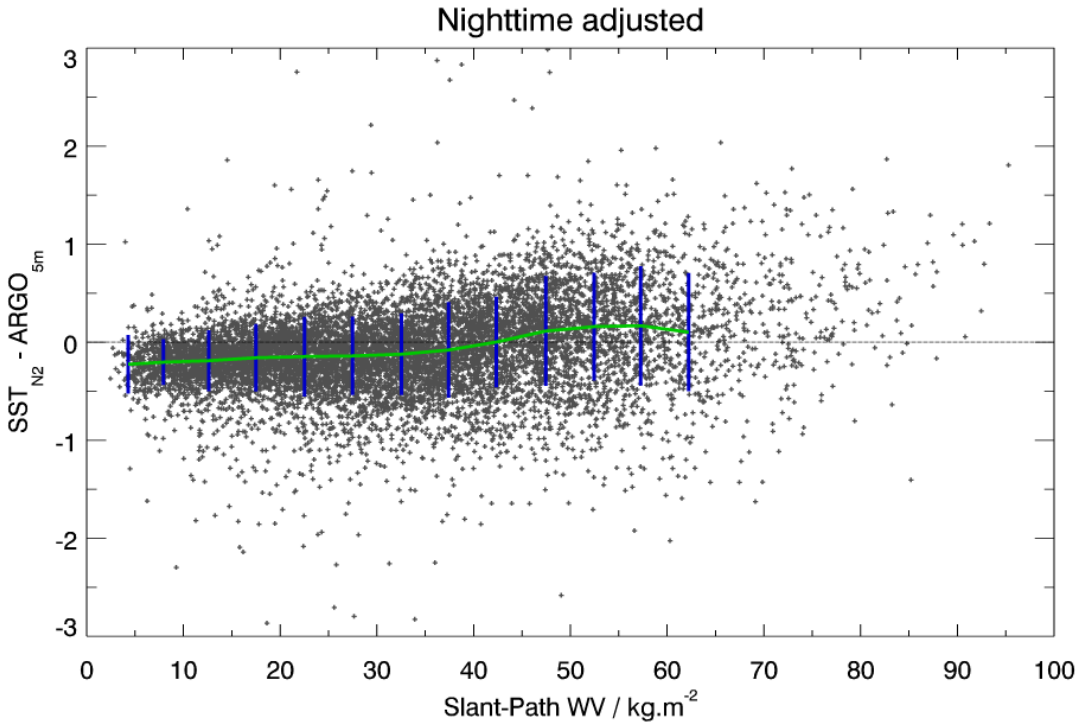
Direct regression vs slant-path WV



Nighttime 2-channel "Simple" split-window has curvature

N.B. The SLSTR algorithm is WV-dependent to flatten this out

Dependence on slant-path WV

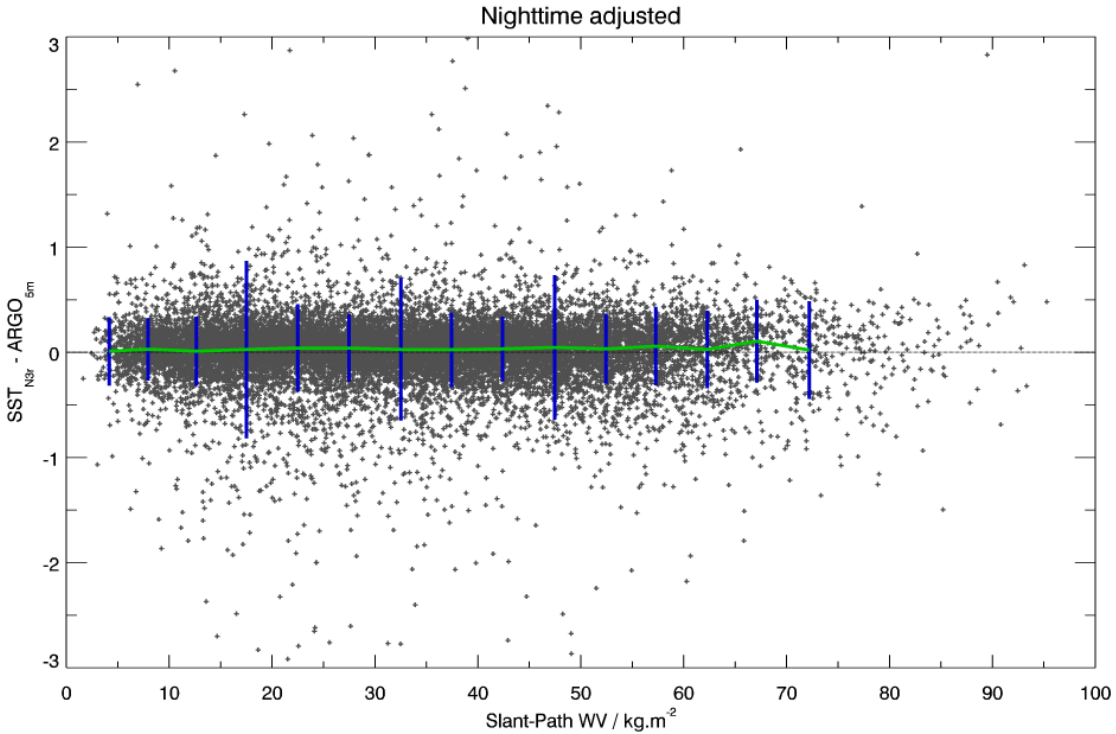


Nighttime 2-channel

…but seems to overdo it

Note improved scatter at low-mid WV cf. “simple” regression, but –ve bias

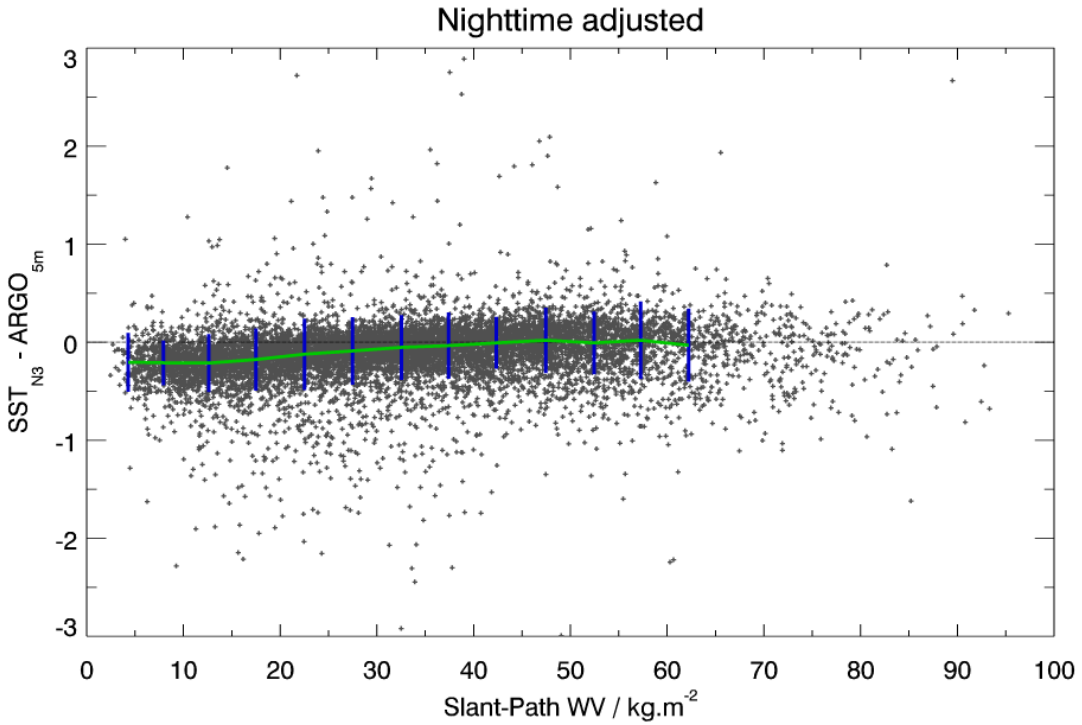
Direct regression vs slant-path WV



Nighttime 3-channel

3-channel regression shows ~no trend w.r.t. WV

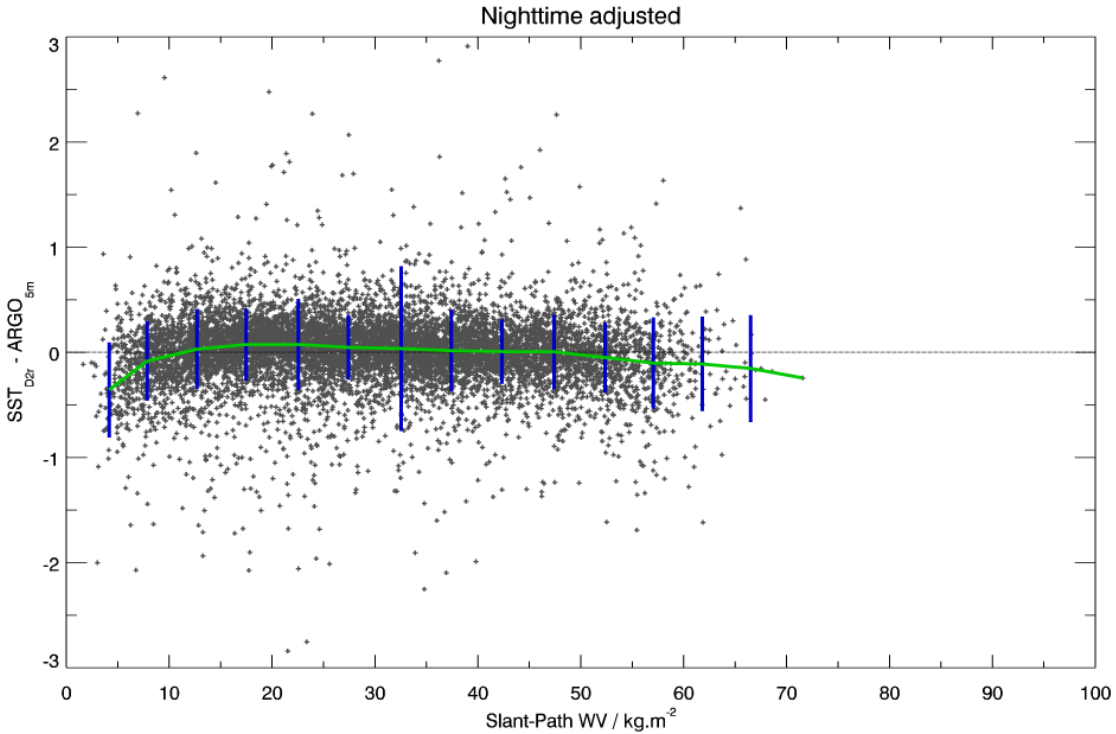
Dependence on slant-path WV



Nighttime 3-channel

3-channel regression shows ~no trend w.r.t. WV *cf.* production (~0.2 K gradient)

Direct regression vs slant-path WV

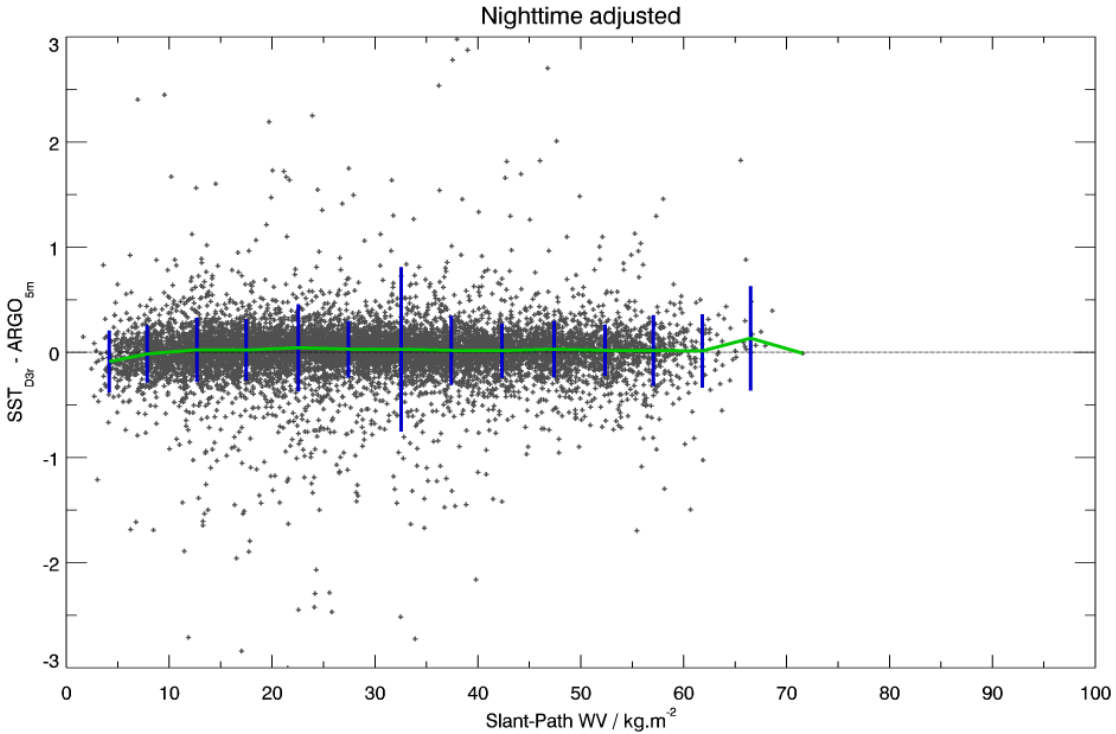


Nighttime Dual-2

Slight curvature in direct regression algorithm

Likely due to complexities of dual-view (RTM algorithms can be developed specifically)

Direct regression vs slant-path WV

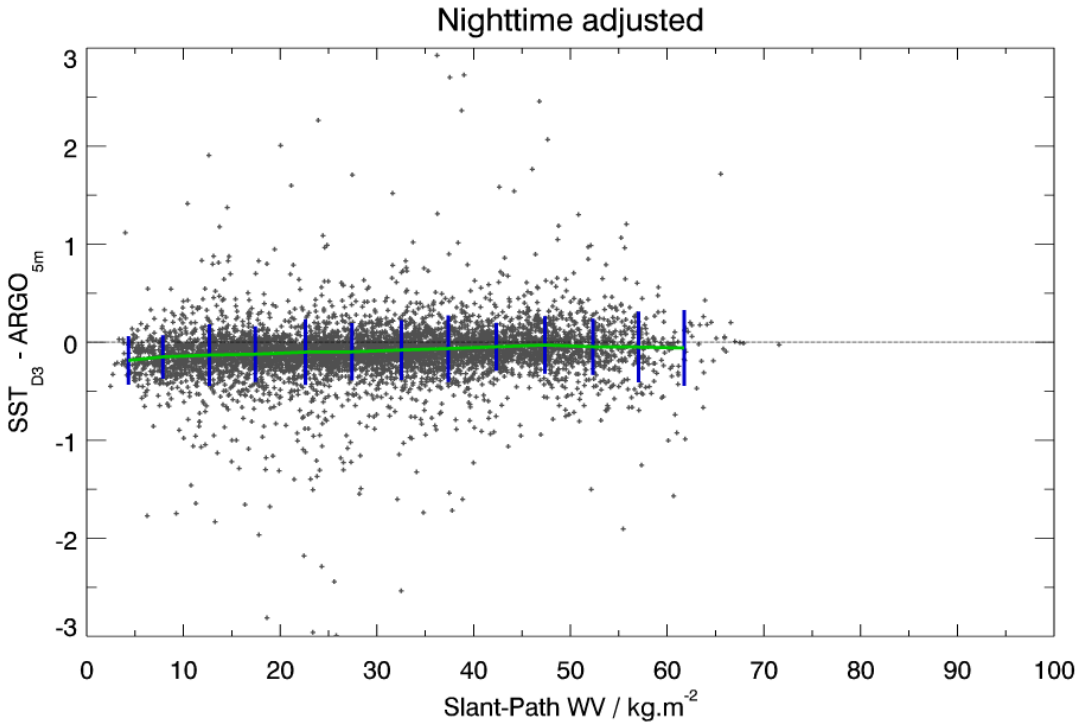


Nighttime Dual-3

Virtually flat w.r.t. WV

N.B. Dual-3 coefficients are generally smaller in magnitude than Dual-2

Dependence on slant-path WV



Nighttime Dual-3

Virtually flat w.r.t. WV

N.B. Dual-3 coefficients are generally smaller in magnitude than Dual-2

Again, production has ~0.2 K gradient

Physical retrieval methods

Principle

- Calculate top-of-atmosphere brightness temperatures from "initial guess" (a.k.a. *prior*) information
- Difference between modeled and observed brightness temperature is "measurement" $\Delta y = K\Delta x$
- So, we know Δy and want Δx
- *N.B.* x = (*e.g.*) [SST, TCWV]
- K is matrix of partial derivatives of channel BTs w.r.t. components of x

Least Squares

$$\Delta \boldsymbol{x} = (\mathbf{K}^T\mathbf{K})^{-1}\mathbf{K}^T\Delta \boldsymbol{y} \; [= \mathbf{G}\Delta \boldsymbol{y}]$$

Optimal Estimation

$$\mathbf{G} = (\mathbf{K}^T\mathbf{S_e}^{-1}\mathbf{K}+\mathbf{S_a}^{-1})^{-1}\mathbf{K}^T\mathbf{S_e}^{-1}$$

Modified Total Least Squares

$$\mathbf{G} = (\mathbf{K}^T\mathbf{K} + \lambda\, \mathbf{I})^{-1}\mathbf{K}^T$$

$$\lambda = (2\log(\kappa) / ||\Delta \boldsymbol{y}||)\, \sigma^2_{\text{end}}$$

σ_{end} = lowest singular value of $[\mathbf{K}\, \Delta \boldsymbol{y}]$

Physical retrieval methods

Revised version of MTLS

- I-matrix applies regularization evenly across retrieval space (SST & TCWV)
- Fletcher (1971) proposed modification to Levenberg-Marquardt – replace I with

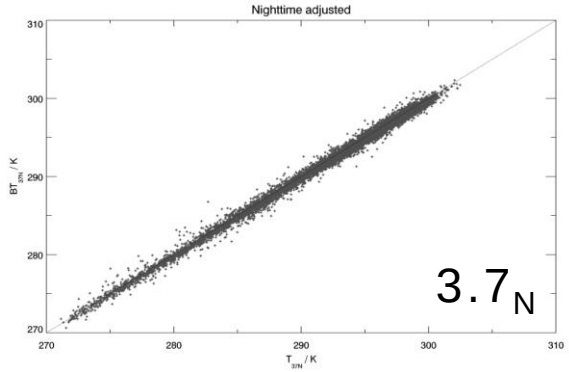
$$R = \mathrm{diag}\{K^T K\}$$

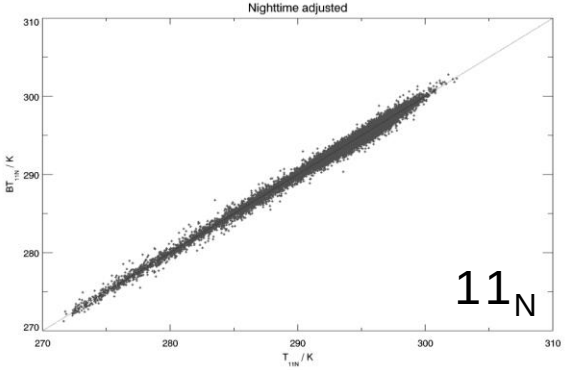
- Also normalize to preserve λ (*i.e.* sum to 2 in the case of 2-element retrieval)

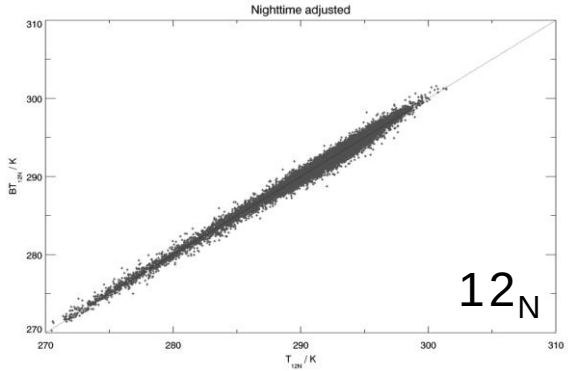
Other considerations

- RTTOV simulations do not include aerosol
- Note that the RTM is already being used in the Bayesian cloud detection
- *N.B.* Only using single-pixel information at this very preliminary stage
- Showing the Dual-3 results (*i.e.* 6 channels in retrieval)

RTTOV output

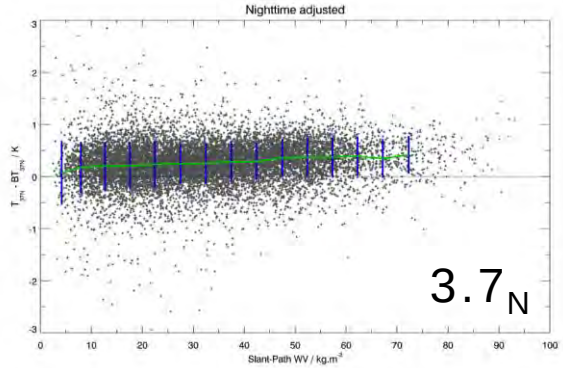


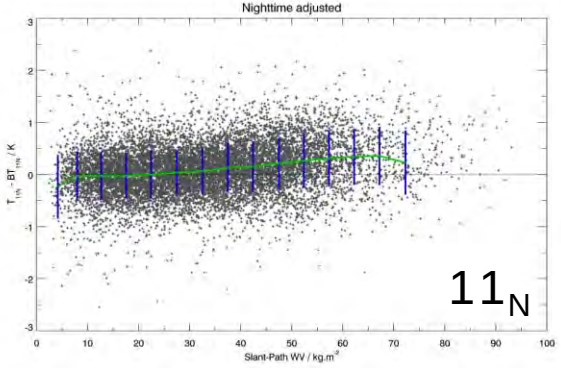


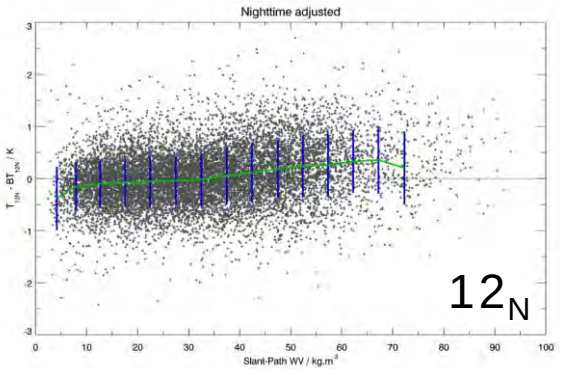


- Observed vs RTTOV modelled output looks “good”
- *N.B.* Physical retrieval algorithms function on Δy, so need to check for trends in this

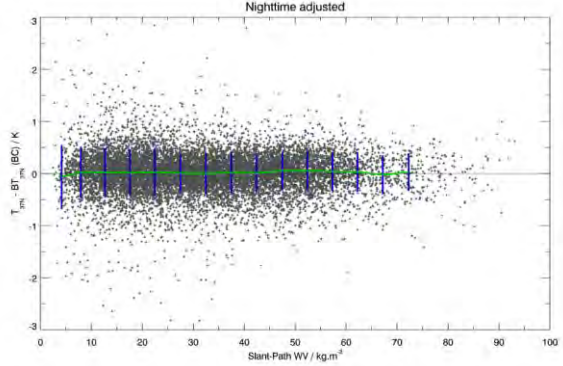
Simple bias correction w.r.t. WV

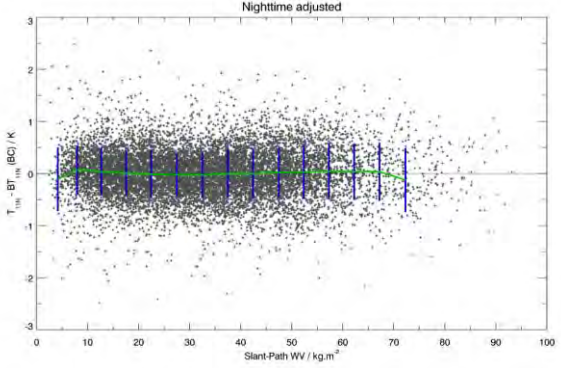


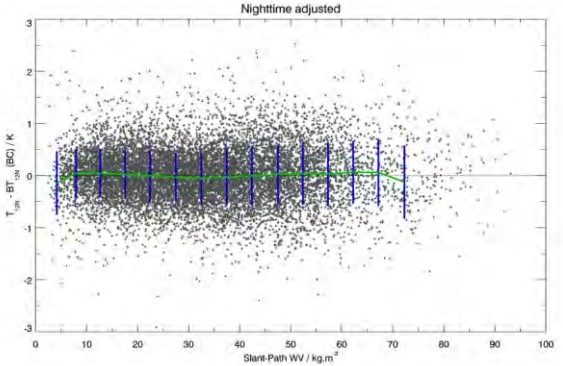




Uncorrected

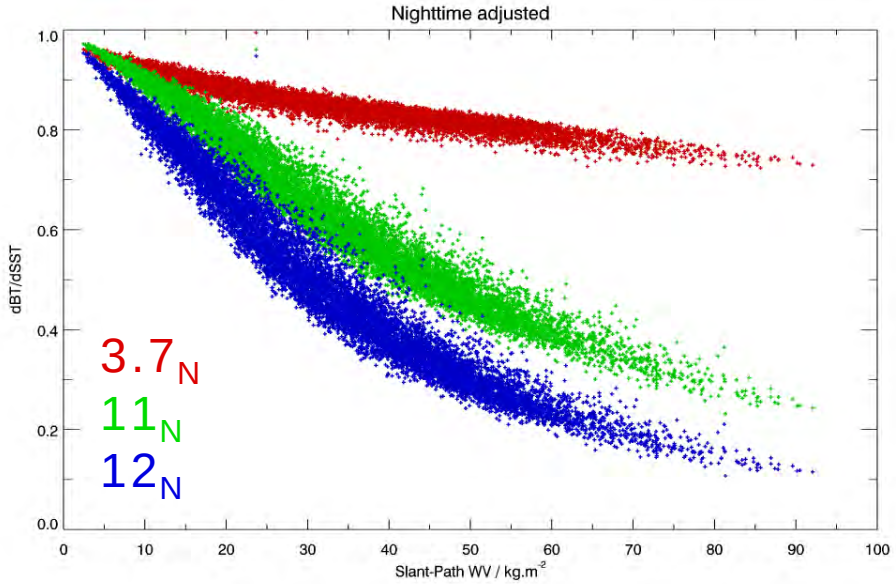


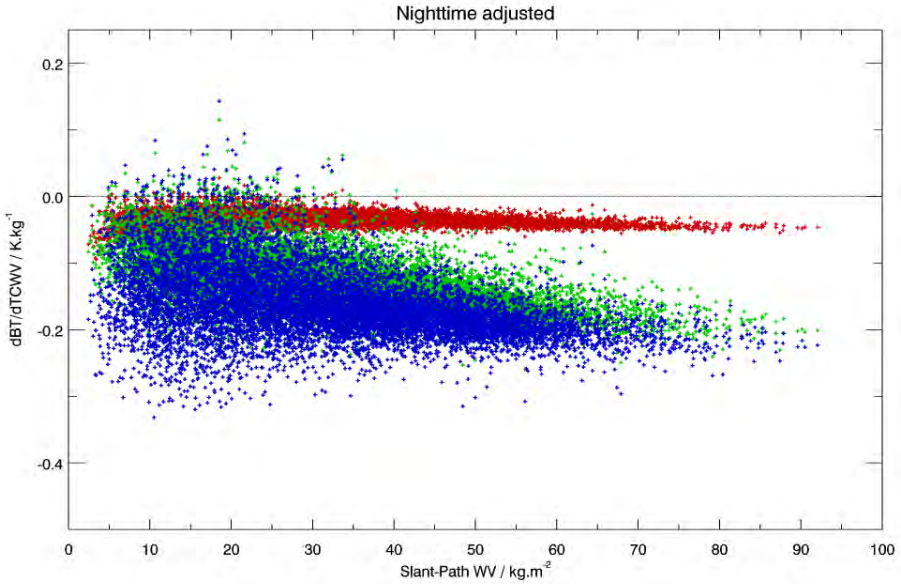




Corrected

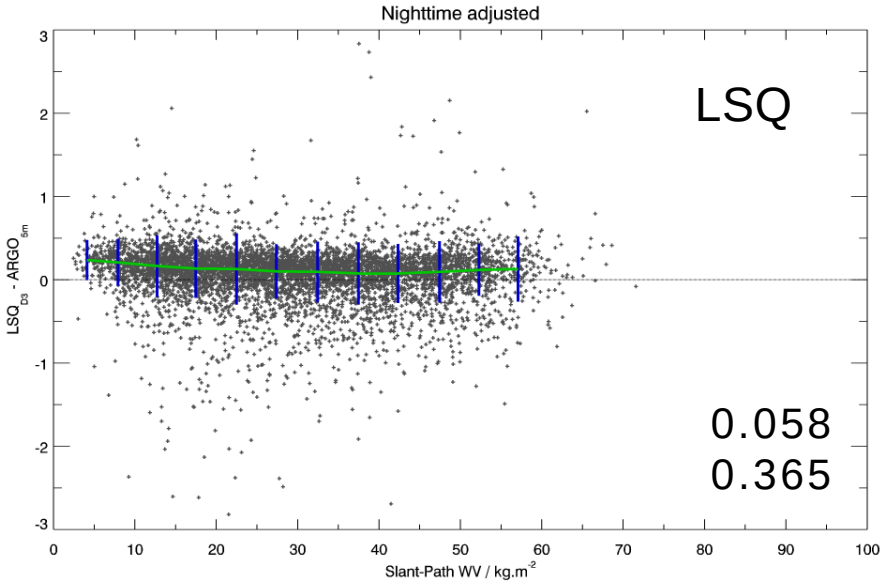
Jacobian behaviour

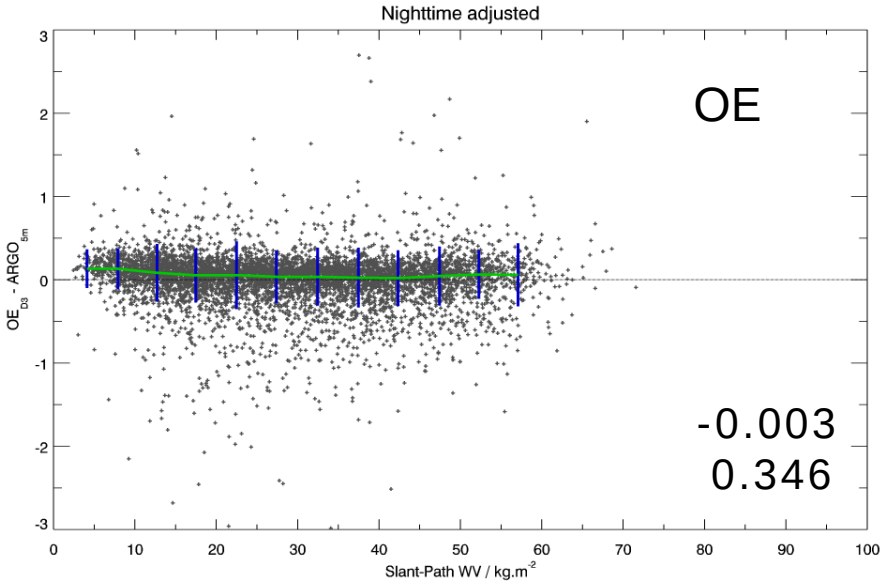




- SST jacobian shows how useful the 3.7 μm channel is
- N.B. Units of WV jacobian are $K.kg^{-1}$

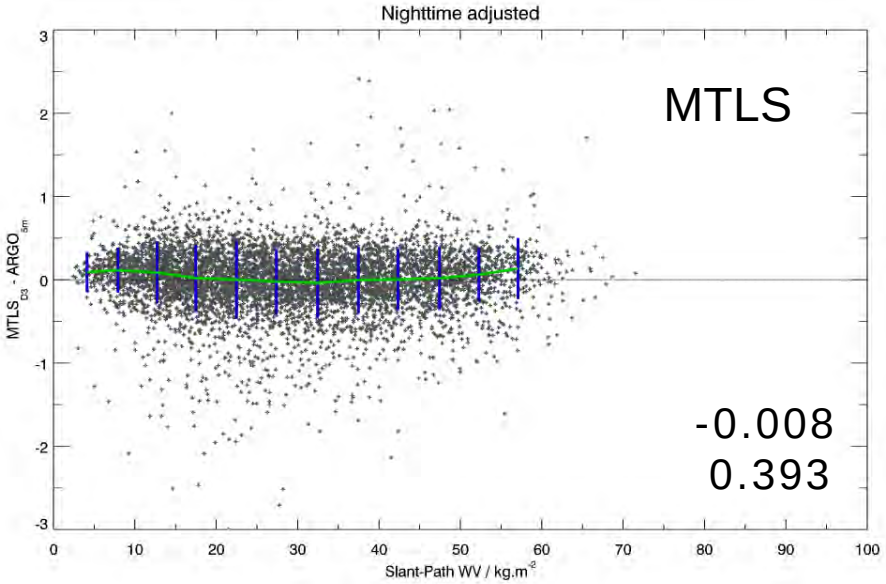
Dual-3 results: LSQ & OE

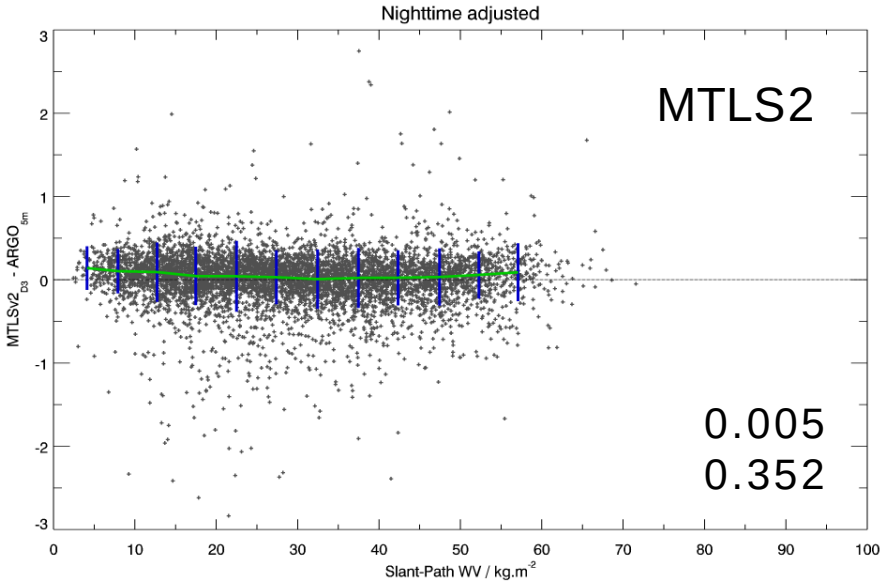




- LSQ performs quite well, although slight curve & warm bias
- OE has slightly reduced error & bias

Dual-3 results: MTLS & MTLS2

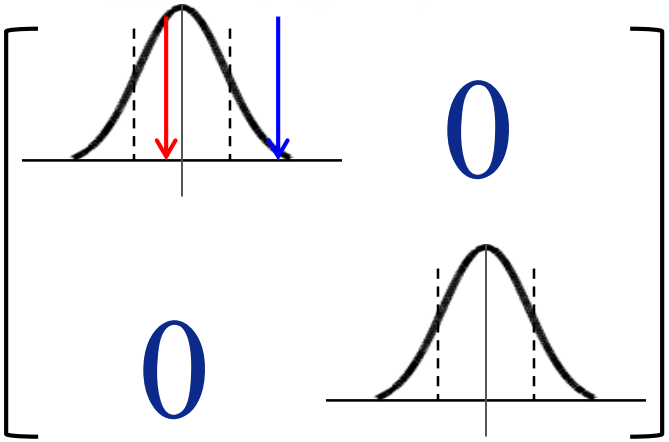




- MTLS has curvature & increased scatter
- Revised version with Fletcher regularization shape is better

"Optimized" OE

$[S_e]$, S_a =



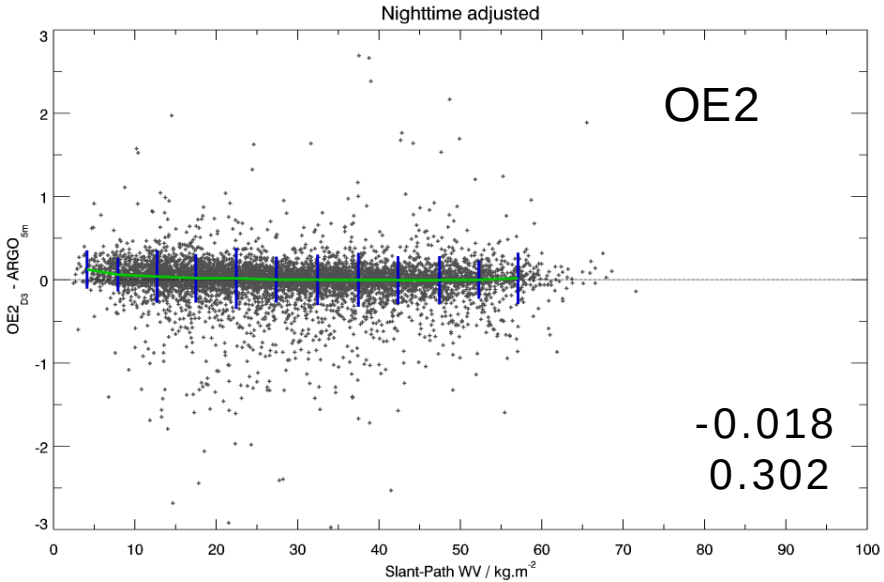
σ^2 is an overestimate…

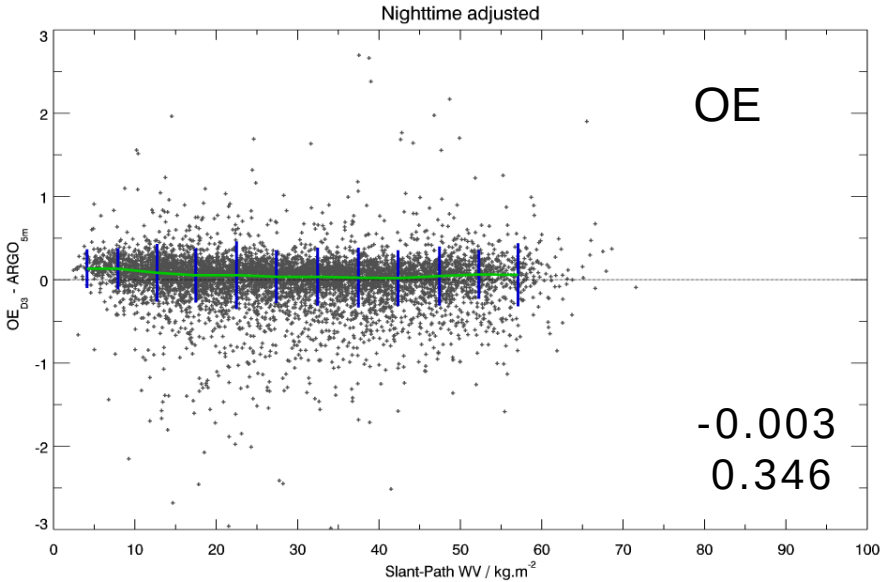
…or an underestimate

Perform experiment – insert "true" SST error into S_a^{-1}

Can only be done when truth is known, *e.g.* with matchup data

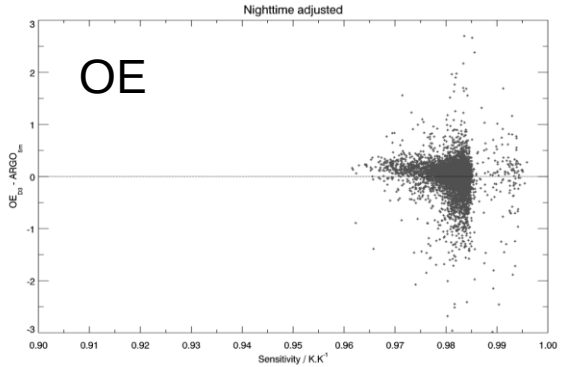
Dual-3 results: OE2 *cf.* OE

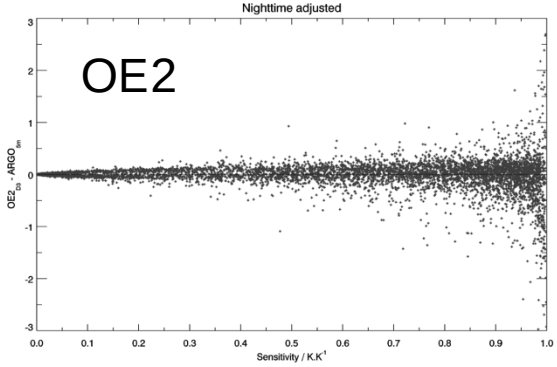


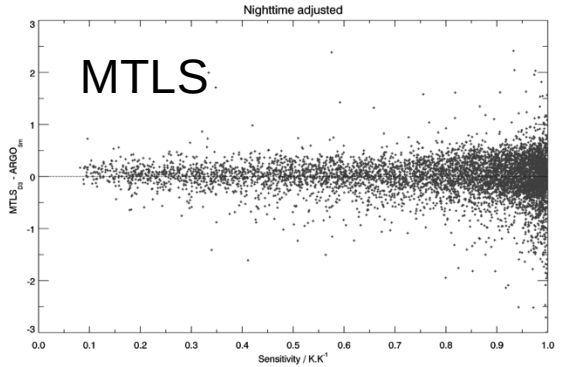


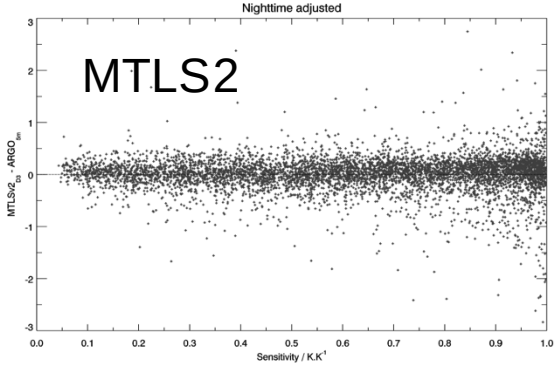
- "Optimized" OE shows notably reduced scatter and is virtually flat
- Improved accuracy is great, but what about sensitivity?

Error vs. Sensitivity









Substantial range in Sensitivities

- OE has highest sensitivity by far (except LSQ) but some trend
- MTLS & MTLS2 may have very low sensitivity
- Most accurate result (OE2) has lowest sensitivity
- Note general trend of less error with lower sensitivity

Summary: Operational SLSTR SSTs

Argo is a powerful validation source **for assessing "climate quality"**

- Critical to apply diurnal and skin adjustments
- Requires full 1-d model to allow correction to specific depth and also subsequent temporal adjustment at depth

Biases <0.1 K, S.D. <0.3 K (dual-3)

- Impressive for independent RTM-based algorithms

Some issues remain

- Although Nadir-2 algorithm is least accurate, there are residual biases
- These are probably due to RTM and affect other algorithms
    - Flagging N2 above 35 $kg.m^{-2}$ does not address the problem

Summary: Physical retrieval

RTM BTs + Jacobians needed for physical retrieval

- Biases w.r.t. WV in all channels
- "Simple" bias correction allows some tests to be performed
- More sophisticated bias correction may help, but better to fix at source

Could also use IASI matches

- However, need to cover high WV regions

N.B. Fast RTM generally introduces "noise"

- "Better" fast RTM (OSS, PC-RTM) may help

Summary: Physical retrieval

Physical retrieval results show promise

- LSQ works quite well
- OE works well "out-of-the-box"
- MTLS may not be configured correctly
- Fletcher regularization shape shows benefit
- "Optimized" OE shows notably better results, but illustrates issue with sensitivity

Many more things to try, e.g.

- Extended OE (can be applied to MTLS & LSQ as well)
- MTLS configuration needs to be examined more closely
- Aerosol information should be incorporated into RTM and retrieval, as it is a factor (and reason for dual-view)
- *N.B.* Bayesian cloud detection means validation dataset well-matched for OE