Bridging instrument and science capabilities and performance

IOCS 2023 SAT Meeting
14 November

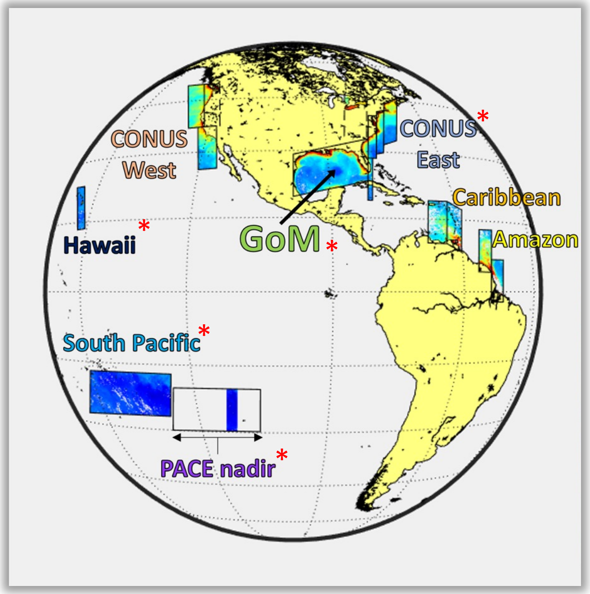
Antonio Mannino

Contributions from: Steve Persh, Ryan Vandermeulen, Sean Bailey & Boryana Efremova

Outline

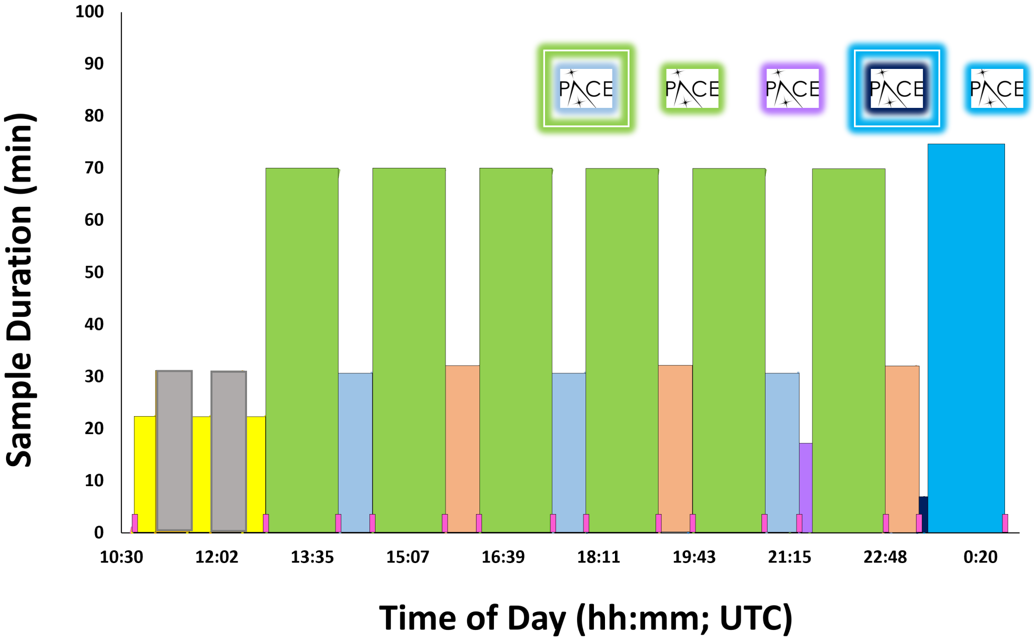
- Instrument capabilities and expected performance
  - Daily science operations and calibrations
  - Spectral
  - SNR
  - Radiometric uncertainties
- On-orbit calibration
- GLIMR Data Product Science Performance & Modeling (ρ_w)
- Validation of Science Data Products
- Peak into Cloud statistics
- Science Data Segment – Algorithm Tool

Daily Observing & Calibration Science Operations



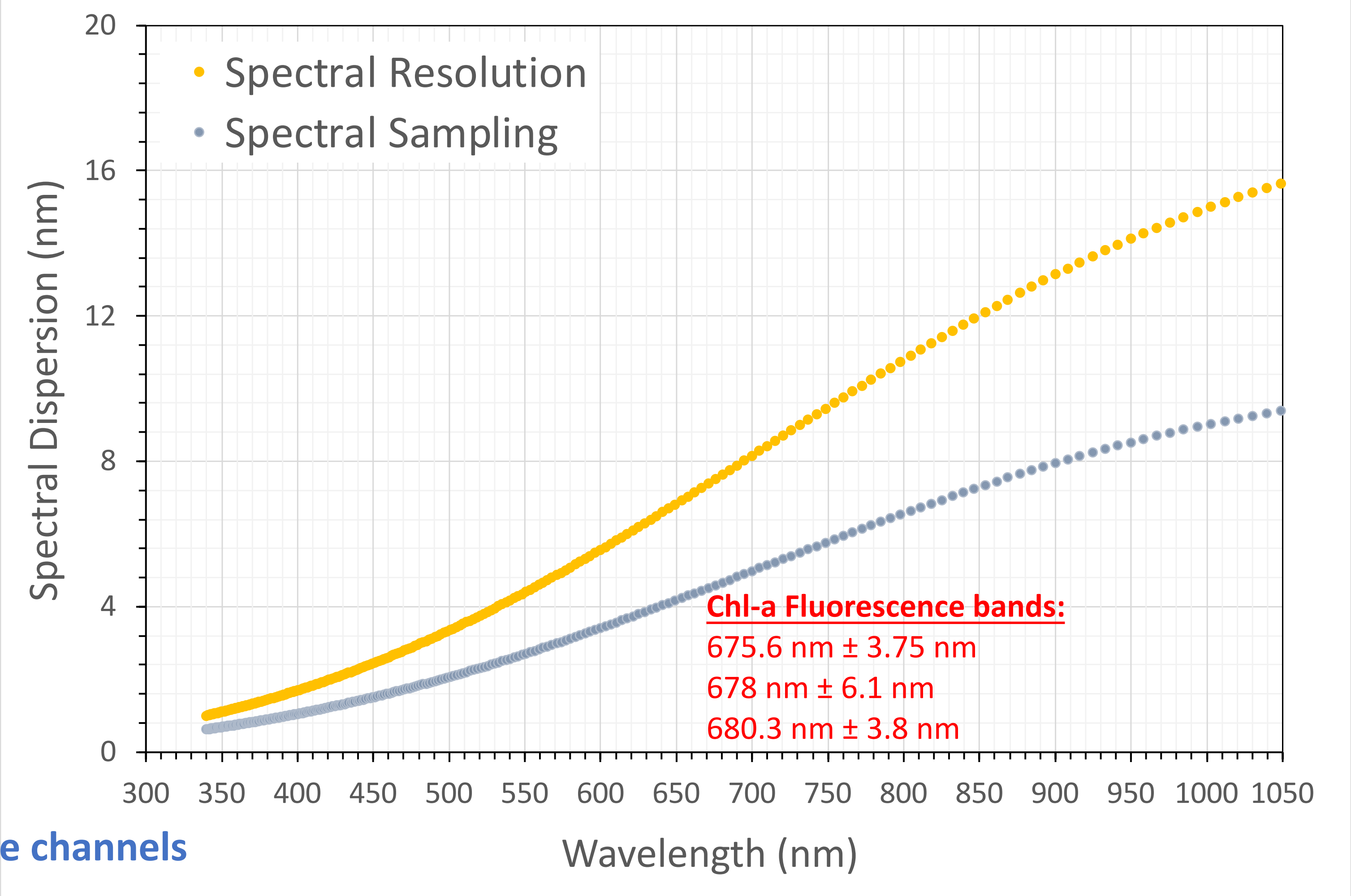
*Anticipated PACE overlap

Daily Fall/Spring schedule



Schedule affords up to 5-7 daily matchup areas with PACE OCI year-round

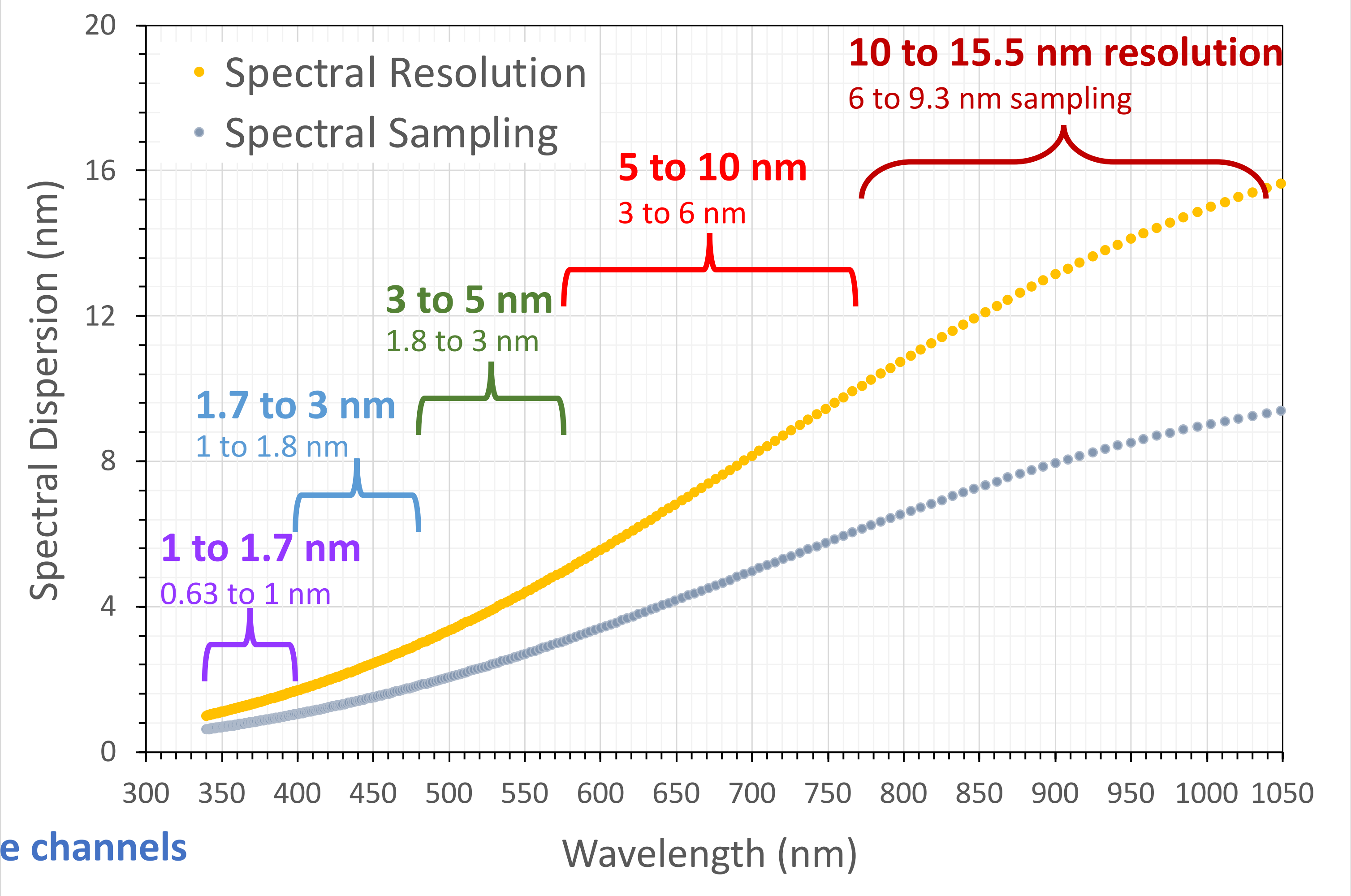
Modeled GLIMR Spectral Sampling and Resolution



Chl-a Fluorescence bands:
675.6 nm ± 3.75 nm
678 nm ± 6.1 nm
680.3 nm ± 3.8 nm

252+ discrete channels

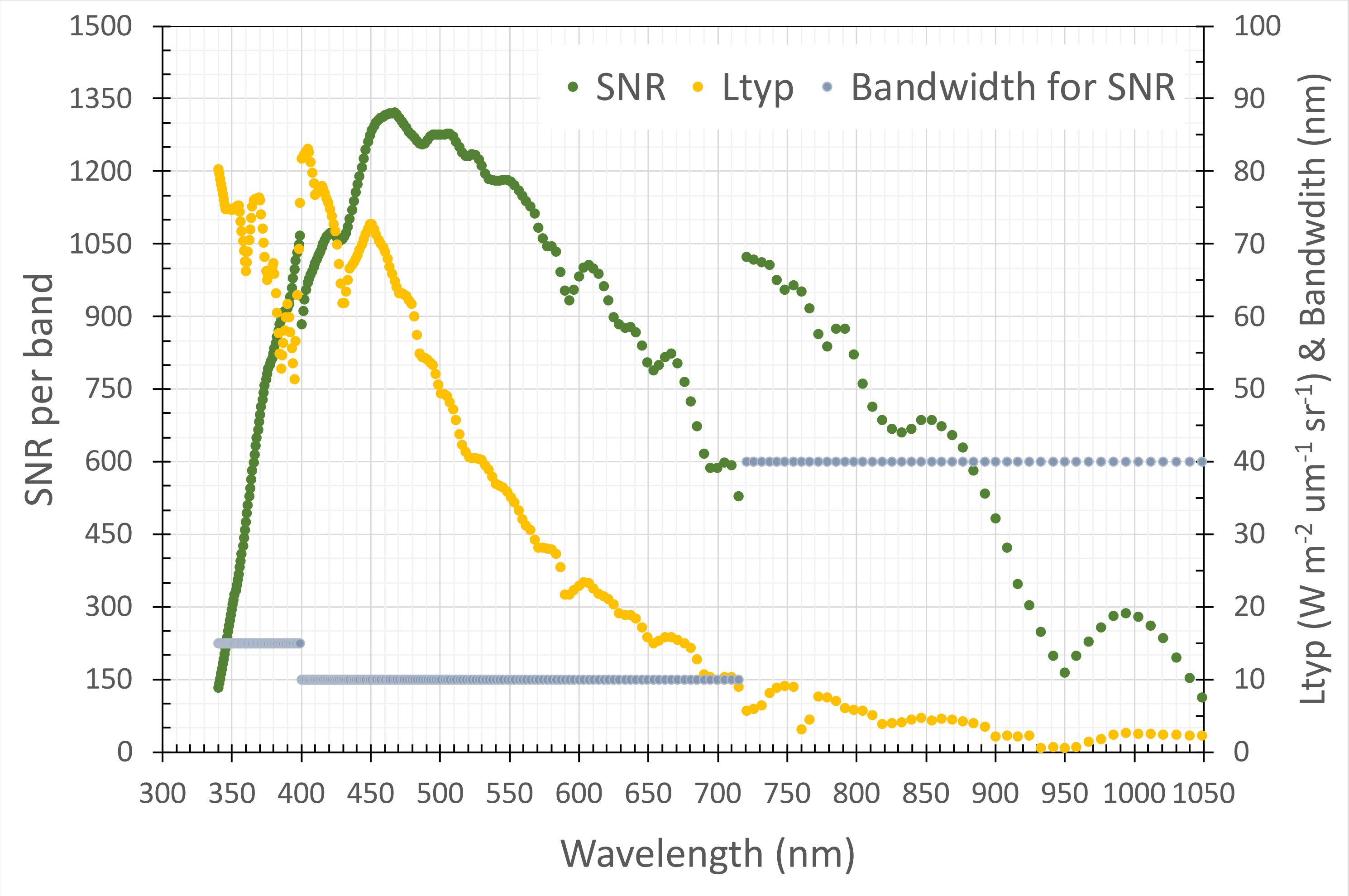
Modeled GLIMR Spectral Sampling and Resolution



252+ discrete channels

Bridging instrument and science capabilities and performance

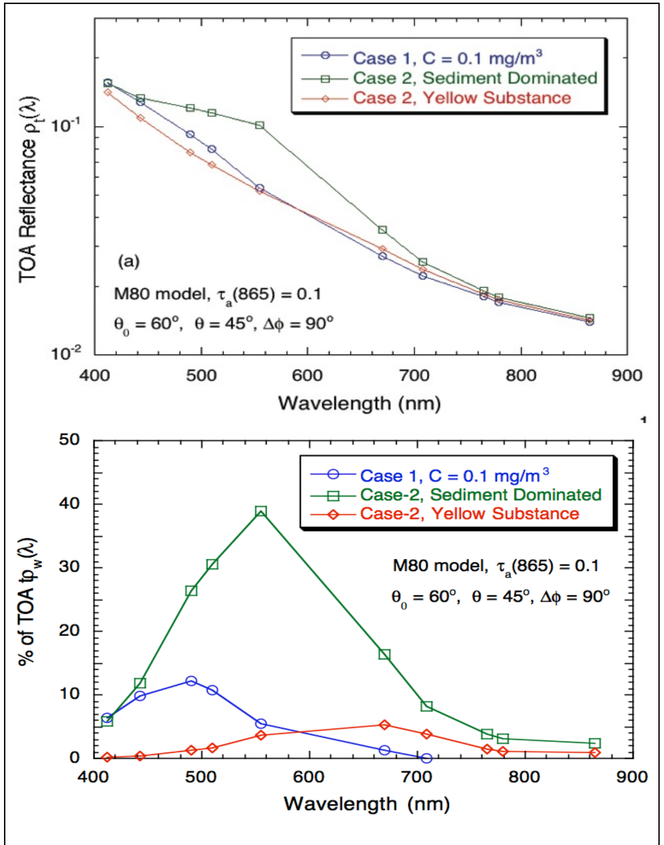
Modeled SNR as of June 2023



Bridging instrument and science capabilities and performance

Ocean Color Heritage Requirements

- Historically, the required performance goal for ocean color products (specifically, water-leaving radiance or reflectance) is 5% uncertainty.
  - Top-of-Atmosphere (TOA) radiance requirement ascribed to ocean color instruments is typically 0.5% uncertainty.
  - **Goal for GLIMR is to achieve ~0.5% uncertainty in TOA radiances in UV-Vis after vicarious calibration**



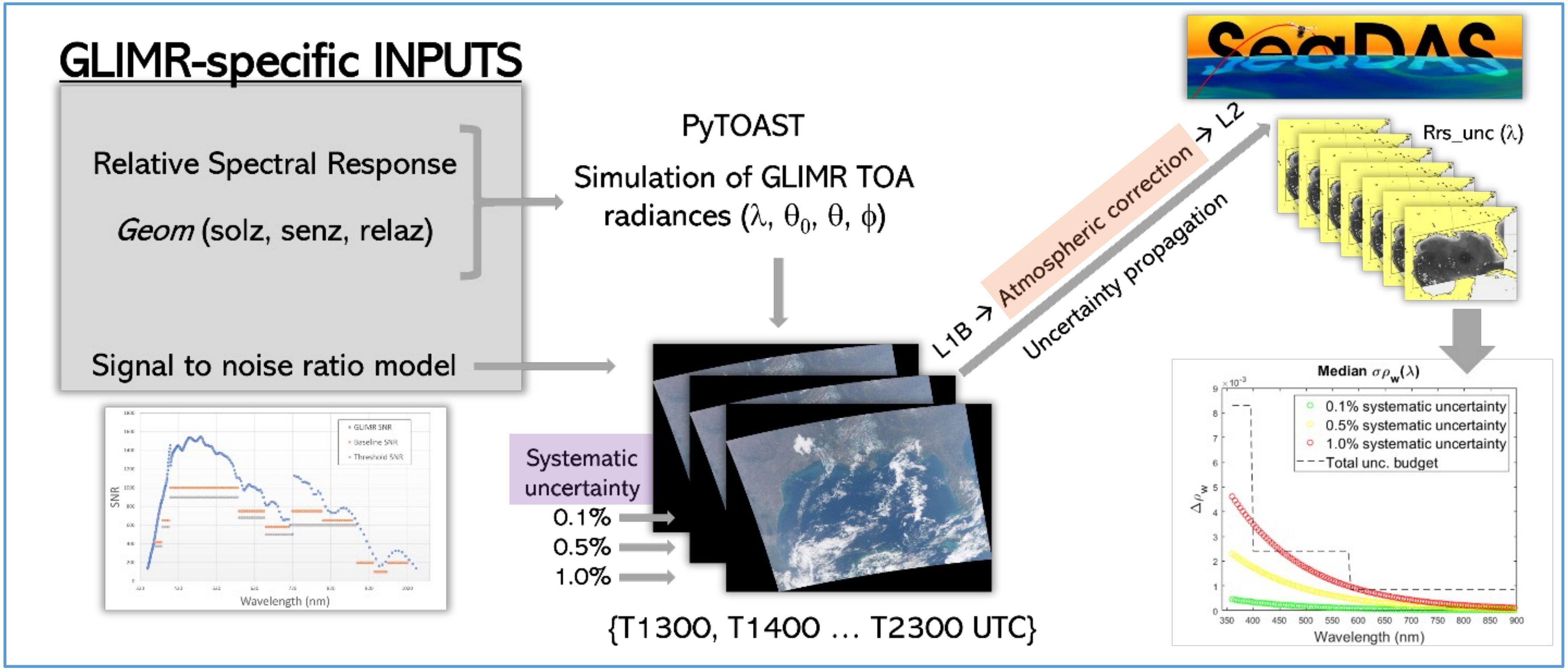
Menghua Wang, IOCCG Report 10

Small uncertainties at TOA have potentially large impacts on downstream products.

Modeled TOA Radiometric Uncertainties – End-Of-Life

	350-400	400-580	580-720	720-895	895-970	970-1040	Basis-of-Estimate
Goal uncertainty (%) – 1 sigma	**0.5**	**0.5**	**0.5**	**0.5 to 1.13**	**3.0**	**2.0**	Heritage ocean color for UV-Vis; NIR: from PACE OCI CBE + 20% as its EOL baseline
Instrument On-Orbit Radiometric Uncertainty Estimate (%)	**0.485**	**0.438**	**0.518**	**1.12**	**3.02**	**1.93**	Note: error terms summed by RSS for each header section (3 sections and at top level)
Gain and Linearity Uncertainties							RSS of K1, K2, K3, K5 and dn uncertainty terms; Radiometric stability, Temp., Linearity, dark counts
K1: Absolute/ Vicarious Gain	0.20	0.10	0.10	0.696	2.11	1.67	Heritage; best option; based on PACE OCI uncertainty of vicarious calibration (340-720 nm) and absolute solar calibration (>720 nm)
Image Artifact Uncertainties							RSS of unc. from Stray light, high-contrasts, crosstalk, OOB, non-uniformity
Polarization Sensitivity Residuals							

Science Data Product Performance Modeling Overview



GLIMR-specific INPUTS

Relative Spectral Response

Geom (solz, senz, relaz)

Signal to noise ratio model

PyTOAST

Simulation of GLIMR TOA radiances (λ, θ_0, θ, ϕ)

Systematic uncertainty

0.1%

0.5%

1.0%

{T1300, T1400 … T2300 UTC}

L1B → Atmospheric correction → L2

Uncertainty propagation

Systematic Uncertainty: instrument + vicarious calibration uncertainties

Science Data Product Modeling follows the approach implemented for PACE OCI

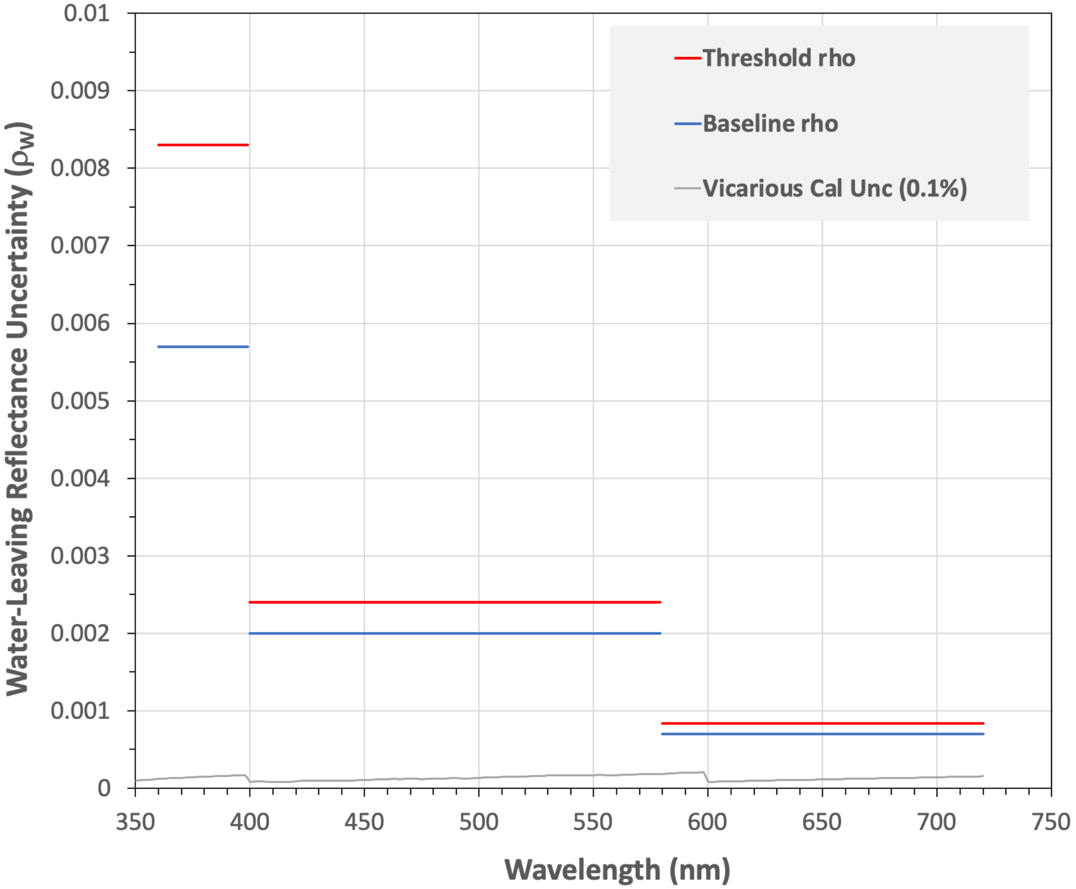
Science Data Product Performance ρ_w – Vicarious Calibr

Requirements

- Apply to bandwidths of 15 nm (or 10 nm over Fluorescence)

Assumptions

- Vic-Cal system(s) for PACE OCI adds 0.1% uncertainty
- Estimated at 0.2% for bands <400 nm

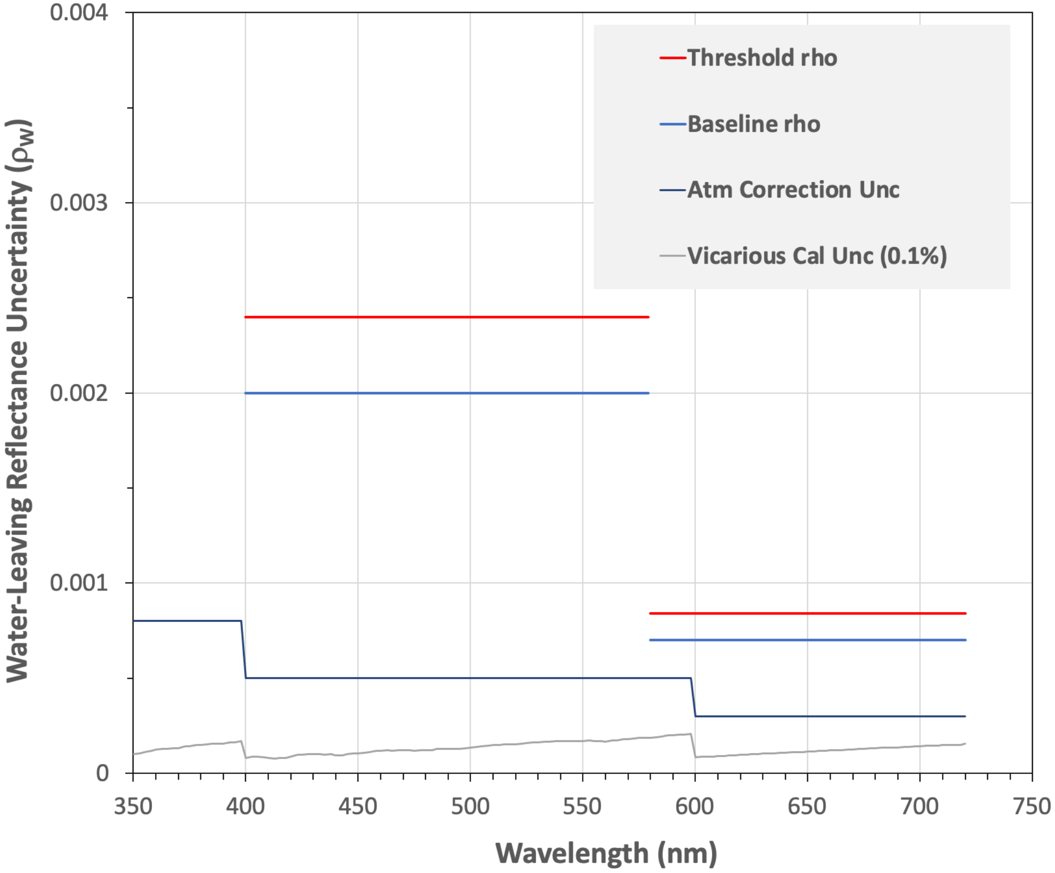


"rho" refers to ρ_w = water-leaving reflectance

Science Data Product Performance ρ_w – Atmos Corr

Assumptions

- Applying current heritage Atmospheric Correction Algorithm (MSEPS: Multi-Scattering Epsilon)

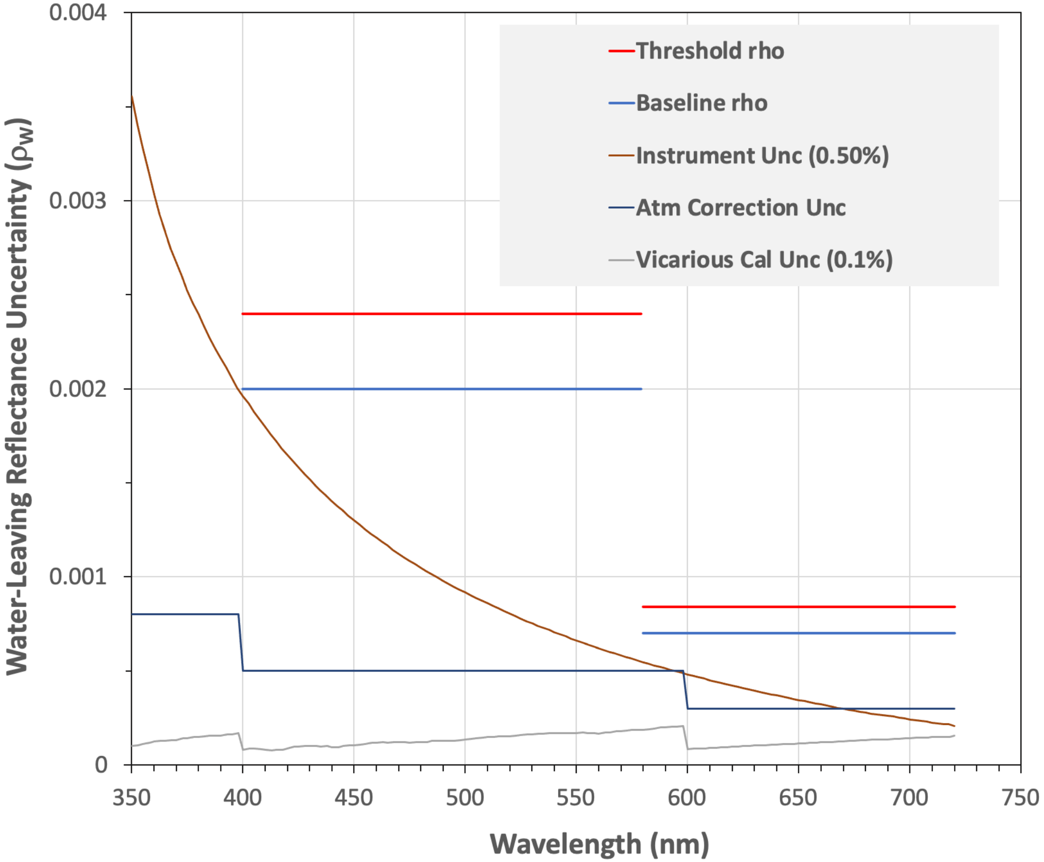


Bridging instrument and science capabilities and performance

Science Data Product Performance ρ_w – Instrument

Assumptions

- Instrument uncertainty modeling follows PACE OCI (PyTOAST) but adapted to GLIMR (geometries)
- GLIMR CBE SNR
- 0.5% Radiometric Systematic Uncertainty attributed to instrument only (Raytheon's precision requirement at EOL)
  - **Accounts for all instrument artifacts (T, polarization, stray light, non-linearity, crosstalk, drift, flat field uniformity, etc.)**
  - Scenario for entire Gulf of Mexico



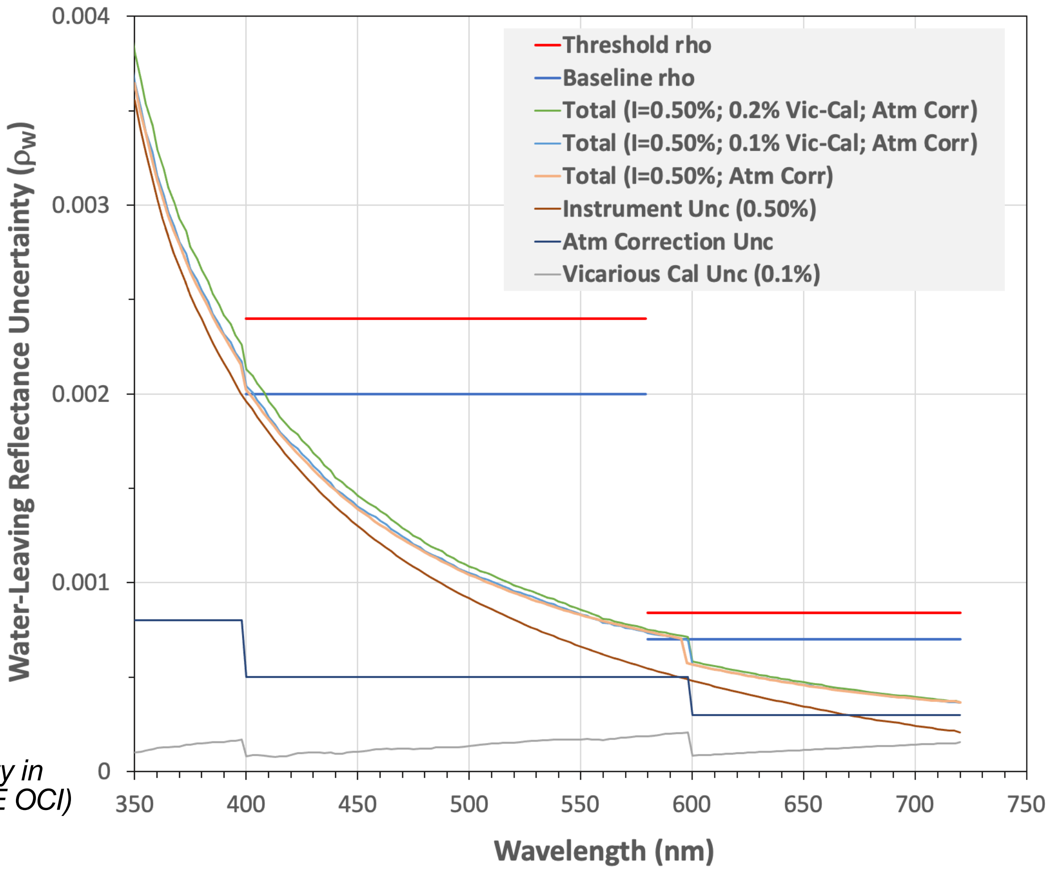
NOTE: (1) 0.69% Radiometric Systematic Uncertainty attributed for reference NIR band (870 nm) used to determine AOT as this band is not vicariously calibrated. (2) Approach follows PACE OCI's rigorously peer-reviewed (PRs, PDR, CDR, SIR, PSR) modeling and analysis

Science Data Product Performance ρ_w – Total

Assumptions

- Instrument uncertainty modeling follows PACE OCI (PyTOAST) but adapted to GLIMR (geometries)
- GLIMR CBE SNR
- 0.5% Radiometric Systematic Uncertainty attributed to instrument (Raytheon's precision requirement at EOL)
- Added Vicarious Calibration & Atmospheric Correction to instrument on top of instrument uncertainty
- Scenario for deep ocean subset of Gulf of Mexico

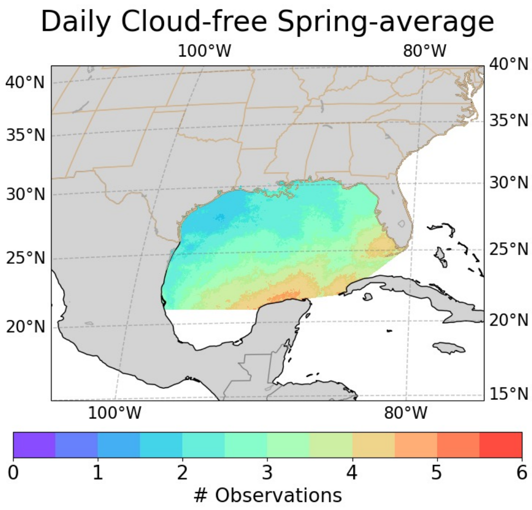
No change in performance when model with 2% uncertainty in NIR reference band (from 0.69% relative value from PACE OCI)

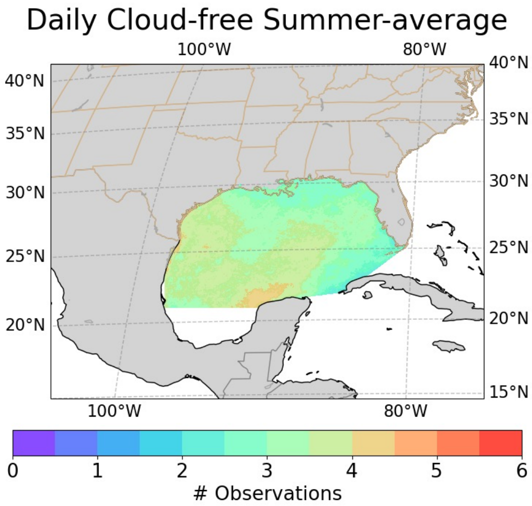


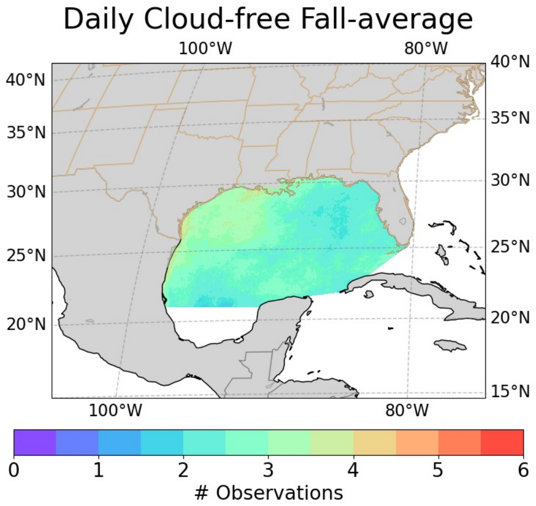
PLRA Threshold Requirements Fully Met and Baseline Met with Minor Exceptions

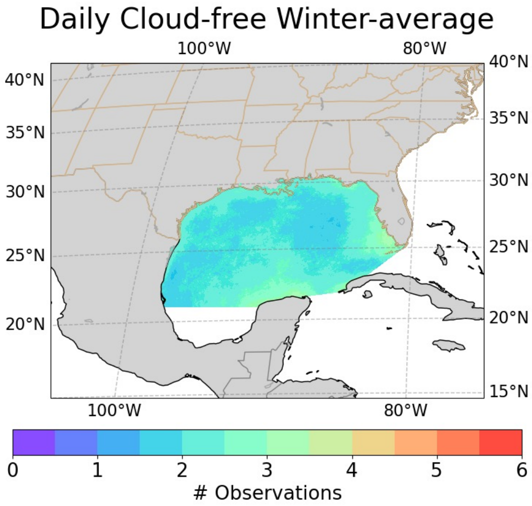
Daily Cloud-Free Observations by Season

- GOES-East ABI Cloud mask from 2020.
  - ✓Angular sampling distance: 56 microradia
  - ✓Time resolution: 30 mi
  - ✓Subsatellite longitude 75W


Daily Cloud-free Spring-average


Daily Cloud-free Summer-average


Daily Cloud-free Fall-average

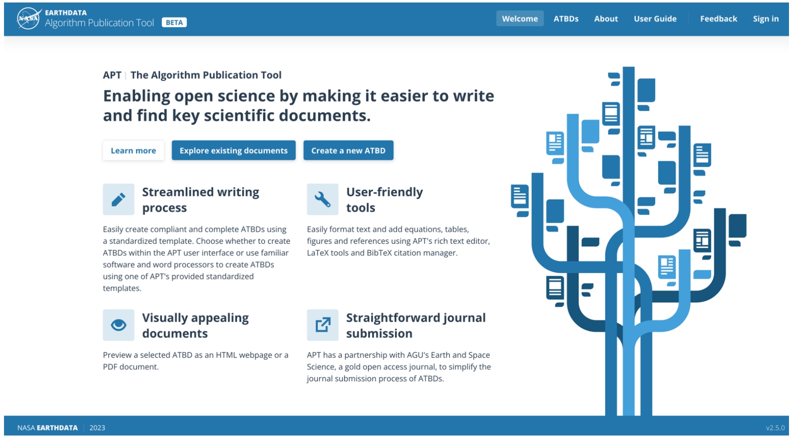

Daily Cloud-free Winter-average

The number of cloud-free observations per day are averaged over each season.

by Boryana Efremova

Science Data Segment “news”

- APT (Algorithm Publication Tool)
  - APT is the "new" ATBD. While still in beta, it is available and anyone considering an algorithm should get an account and use APT to satisfy the ATBD requirement.
  - https://www.earthdata.nasa.gov/apt/



APT | The Algorithm Publication Tool

Enabling open science by making it easier to write and find key scientific documents.

Streamlined writing process

Easily create compliant and complete ATBDs using a standardized template. Choose whether to create ATBDs within the APT user interface or use familiar software and word processors to create ATBDs using one of APT's provided standardized templates.

User-friendly tools

Easily format text and add equations, tables, figures and references using APT's rich text editor, LaTeX tools and BibTeX citation manager.

Visually appealing documents

Preview a selected ATBD as an HTML webpage or a PDF document.

Straightforward journal submission

APT has a partnership with AGU's Earth and Space Science, a gold open access journal, to simplify the journal submission process of ATBDs.

- SOT/SOB process (Science Operations Team/Board)
  - As the algorithms mature, we'll want the PIs to engage with the SOB/SOT process to get the algorithm into production.
  - The earlier the engagement the better.

BACKUP

Science Data Product Validation

- Validation with data products from other satellite missions
  - PACE OCI, Sentinel 3A/3B/3C/3D OLCI, NOAA-20/21 VIIRS, etc.
- AERONET-OC (SeaPRISM) - https://aeronet.gsfc.nasa.gov/new_web/ocean_color.html
- NASA SeaBASS - https://seabass.gsfc.nasa.gov/ (ESDS-supported)
  - NASA and other field data collections
    - e.g., NASA supports collection of up to 3000 pigment samples annually
  - **Perform GLIMR validation matchups and uncertainty estimation**
- HYPERNETS - http://www.hypernets.eu/from_cms/summary
- Other federal/state/local government agencies; universities; etc.

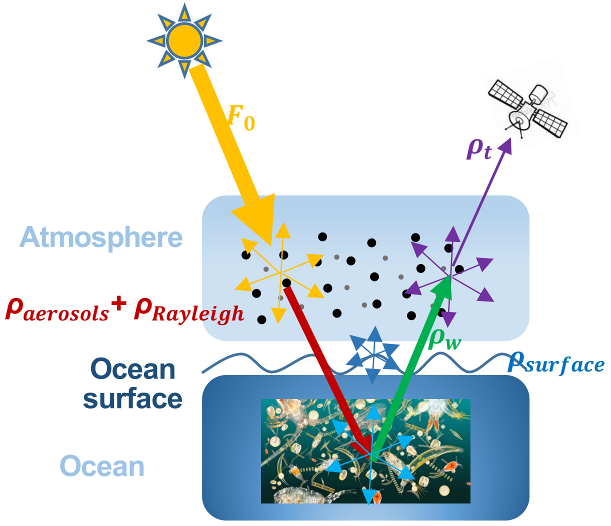
VALIDATION APPROACH – Follow heritage and PACE methodologies

GLIMR must rely on other sources of in situ data as field validation efforts were descoped at KDP-C

Cross-(Vicarious) Calibration with OCI

Following methods for polarization sensitive instrument*

- Daily matching of GLIMR pixels with OCI normalized water-leaving radiance (nL_w)
  - e.g., 3x3 OCI pixel bins (~3.6x3.6 km)
  - Case 1 waters with depths greater than 1000 m; low AOT and Chl-*a*; homogeneous AOT and Chl-*a*
- Inverse processing of GLIMR (L2 to L1B) to bring OCI nL_w to the TOA and output modeled pixel Stokes vectors, $[L_t, Q_t, U_t, 0]^T$, at GLIMR wavelengths and GLIMR solar and viewing geometries.
  - Band radiances adjusted to match GLIMR bands
  - BRDF effects are accounted for in the propagation of the radiances from OCI to GLIMR viewing and path geometries
- Screen TOA pixels (following quality criteria) and generate datasets of radiance pairs $[L_t, Q_t, U_t, 0]^T$; L_m^G) and ancillary information, detector element and time, geographic coordinates, solar and viewing geometries, and glint reflectance.
- Derive M_{11}, M_{12}, and M_{13} per band and detector element.
- Compute ratio L_t / L_m^G to derive the cross-/vicarious gain coefficients (K1) per band

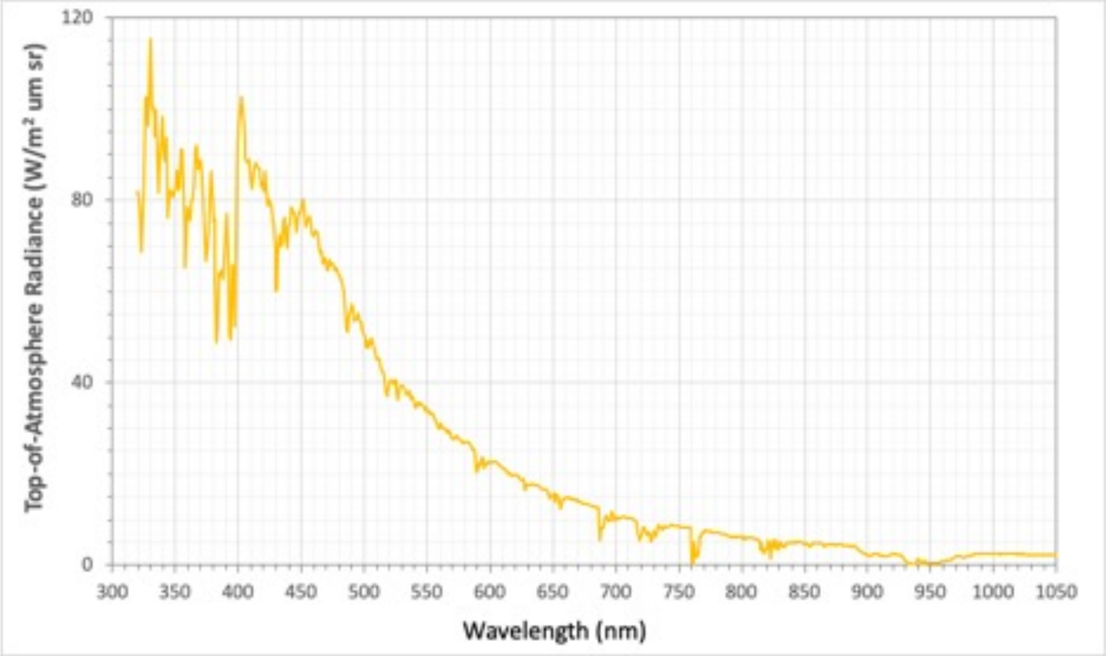


* *Kwiatkowska, Franz, Meister, McClain, & Xiong (2008). Cross calibration of ocean-color bands from Moderate Resolution Imaging Spectroradiometer on Terra platform," Appl. Opt. 47, 6796-6810.*

L_m^G = actual GLIMR TOA radiances

On-Orbit Calibration approach with OCI understood and mature

Spectral Response Trending



- Potential change in dispersion over time on orbit. Use emission and absorption lines to track any changes

1. Fraunhofer solar emission lines:
    - Will use at least two lines
    - 434.048 nm (Hg), 588.997 nm (Na D_2), 656.281 nm (Ha), 866.217 nm (Ca II)
2. Atmospheric absorption lines:
    - 686.719 nm (O_2 B), 759.370 nm (O_2 A), 822.696 nm (O_2 Z), 898.765 nm (O_2 y)

Multi-Scattering Epsilon (MSEPS)

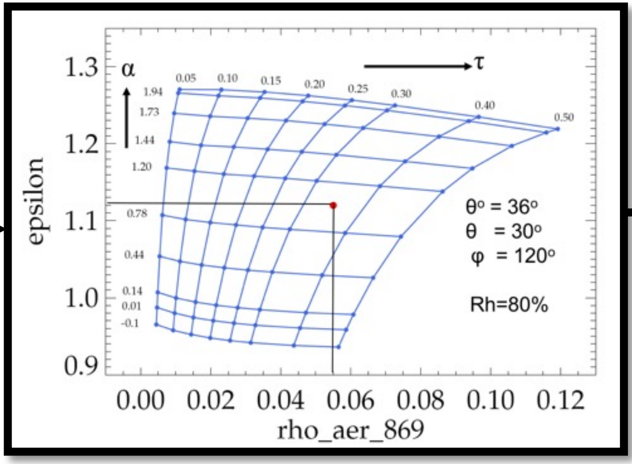
TOA reflectance

Step 1

Rayleigh, gas, and glint correction

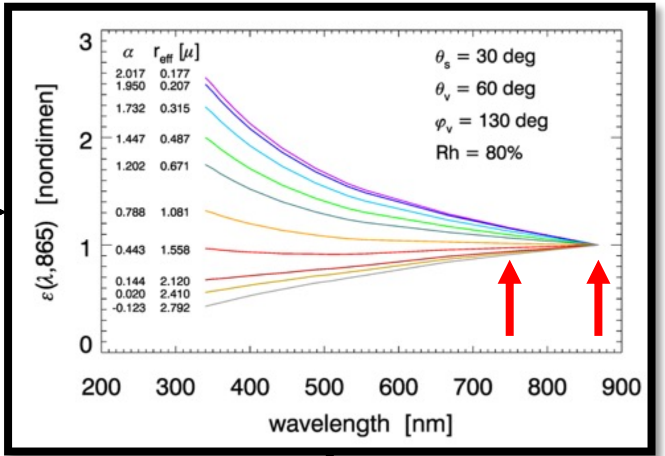
Step 2

Estimate the optical depth at the longest high radiometric quality band for each relative humidity aerosol model set



Step 3

From (multi-scattering) Epsilon, find the closest aerosol fine mode fractions (FMF).



Step 4

Calculate the spectral aerosol reflectance for the closest models in relative humidity and FMF space

Step 5

Calculate the weighted mean of the models to get the final aerosol reflectance and diffuse transmittance

R_{rs}, τ_a, Ångström

Ahmad, Z. and B. Franz (2018), Uncertainty in aerosol model characterization and its impact on ocean color retrievals, in PACE Technical Report Series, Volume 6: Data Product Requirements and Error Budgets (NASA/TM-2018 - 2018-219027/ Vol. 6)

Multi-Band Atmospheric Correction (MBAC)

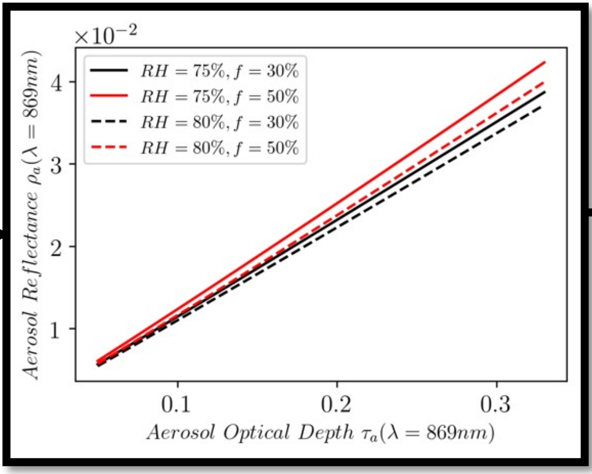
TOA reflectance

Step 1

Rayleigh, gas, and glint correction

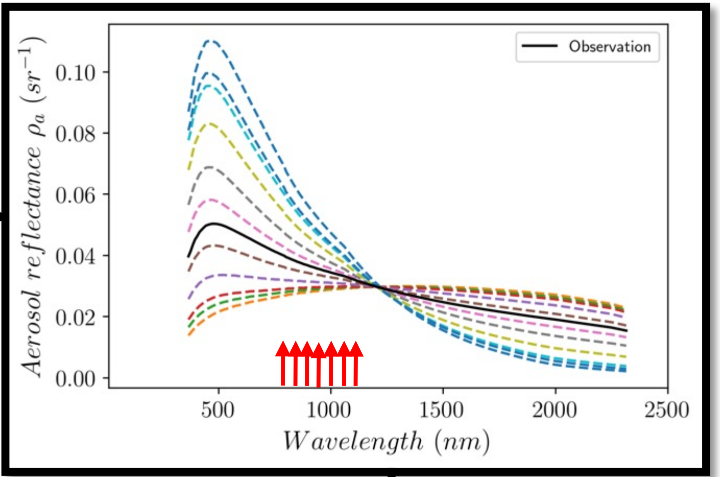
Step 2

Estimate the optical depth at the longest high radiometric quality band for each relative humidity aerosol model set



Step 3

Calculate the aerosol reflectance for all candidate models



Step 4:
$\nabla\chi^2$
minimization

$$\chi^2(RH,f) = \frac{1}{DOF} \times \sum_{\lambda=\lambda_s}^{\lambda_l} \frac{[\rho_{obs}(\lambda) - \rho_a(\lambda, RH, f)]^2}{\sigma^2(\lambda)} \times SW(\lambda)$$

Step 5

Calculate the weighted mean of the models to get the final aerosol reflectance and diffuse transmittance

R_{rs}, τ_a, Ångström

Ibrahim, A., Franz, B. A., Ahmad, Z., & Bailey, S. W. (2019). Multiband atmospheric correction algorithm for ocean color retrievals. Frontiers in Earth Science, 7, 116.

Future Directions for PACE and GLIMR AC

- extend MBAC to utilize UV spectral range in UV-dark waters
- include gas absorption in Rayleigh/aerosol LUTs to capture coupling
- include wind speed-dependent glint model in Rayleigh/aerosol LUTs
- improve correction for bi-directional reflectance (BRDF)

  Twardowski M, Tonizzo A. Ocean Color Analytical Model Explicitly Dependent on the Volume Scattering Function. Applied Sciences. 2018; 8(12):2684. https://doi.org/10.3390/app8122684.

- implement ocean-atmosphere simultaneous retrieval (UV-VIS-NIR-SWIR)

  Ibrahim, A., B.A. Franz, A.M. Sayer, K. Knobelspiesse, M. Zhang, S.W. Bailey, L.I.W. McKinna, M. Gao, and P. J. Werdell, "Optimal estimation framework for ocean color atmospheric correction and pixel-level uncertainty quantification," Appl. Opt. ***61****, 6453-6475 (2022).*

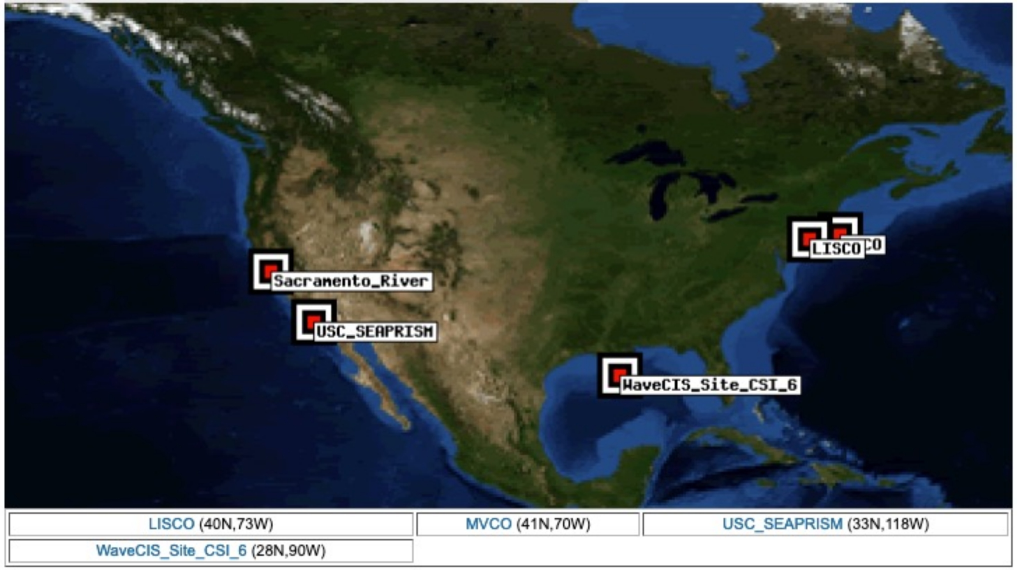
Approaches to Accomplish Vicarious Calibration (K1)

- Heritage MOBY approach - *in situ* instrumentation at appropriate field site(s) (e.g., Eplee et al. 2001; Franz et al. 2007; Zibordi & Melin 2017)
  - PACE vicarious calibration site or instrumentation (MarONet; HyperNAV)
- Alternate field site/instrumentation (e.g., Bailey et al. 2008; Zibordi et al. 2015)
  - AERONET-OC data; extrapolate spectrally
  - Hyperspectral sensors: in-water or above-water
    - HypSTAR in development at Tartu with ESA funding
    - Existing COTS with more extensive lab and field calibration
- Ocean surface reflectance model (Werdell et al. 2007)
- Ocean color satellite climatology of South Pacific waters (Franz et al. 2007; Concha et al. 2019)

Many options available to vicariously calibrate GLIMR

AERONET-OC – radiometric calibration alternative

- AERONET and –OC are NASA-funded programs
- Bands: 400, 412.5, 442.5, 490, 510, 560, 620, 665, and 667 nm
- Additional bands at 709, 865, and 1020 nm for quality checks, turbid water flagging, and for the application of alternative above-water methods (Zibordi et al. 2002).
- Most useful sites for GLIMR
  - WaveCIS in Gulf of Mexico
  - USC off southern California
  - MVCO – Cape Cod



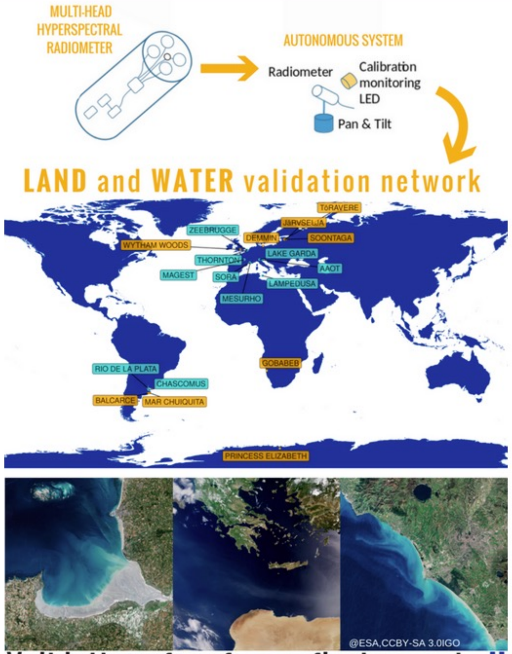
https://aeronet.gsfc.nasa.gov/new_web/ocean_color.html

HYPERNETS – on-orbit calibration/validation alternative

- Planned "new hyperspectral radiometer integrated in automated networks of water and land bidirectional reflectance measurements for satellite validation"
- Consortium of institutions coordinated by RBINS (Royal Belgian Institute for Natural Sciences)
- Funded by EU Horizon 2020

http://www.hypernets.eu/from_cms/summary

Embedding of the HYPERNETS sites into water and land surface reflectance validation networks based closely on the existing AERONET-OC and RadCalNet networks.

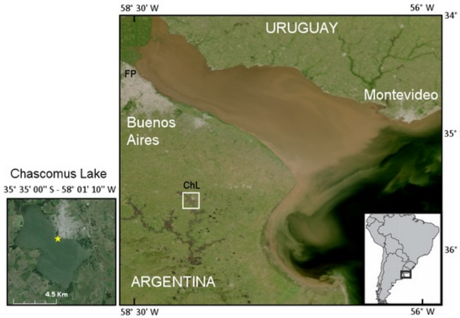


LAND and WATER validation network

Validation of surface reflectance at **all spectral bands** of **all optical missions**

SENTINE-2, SENTINEL-3, LANDSAT, MODIS AQUA AND TERRA, VIIRS, LANDMAPPER, PROBA-V, SABIAMAR, GOCI, GIDAT, AVHRR, SHALOM ENMAP, FLEX, GCOM, HYPXIM, PRISMA CHRIS, HIMAWARI, SKYSAT, GOESS, PACE/OCI, PLANET-SCOPE, WORDVIEW, NANOSATELLITES, ...

WATER SITE - Chascomus Lake



Shallow extremely turbid inland water site.

Coordinator: CONICET

Coordinates: 35.58281326 S and 58.02024078 W

WATER SITE - Rio de la Plata

Fishermen pier in extremely turbid waters.

Coordinator: CONICET

Coordinates: 34.560865 S and 58.39881167 W.

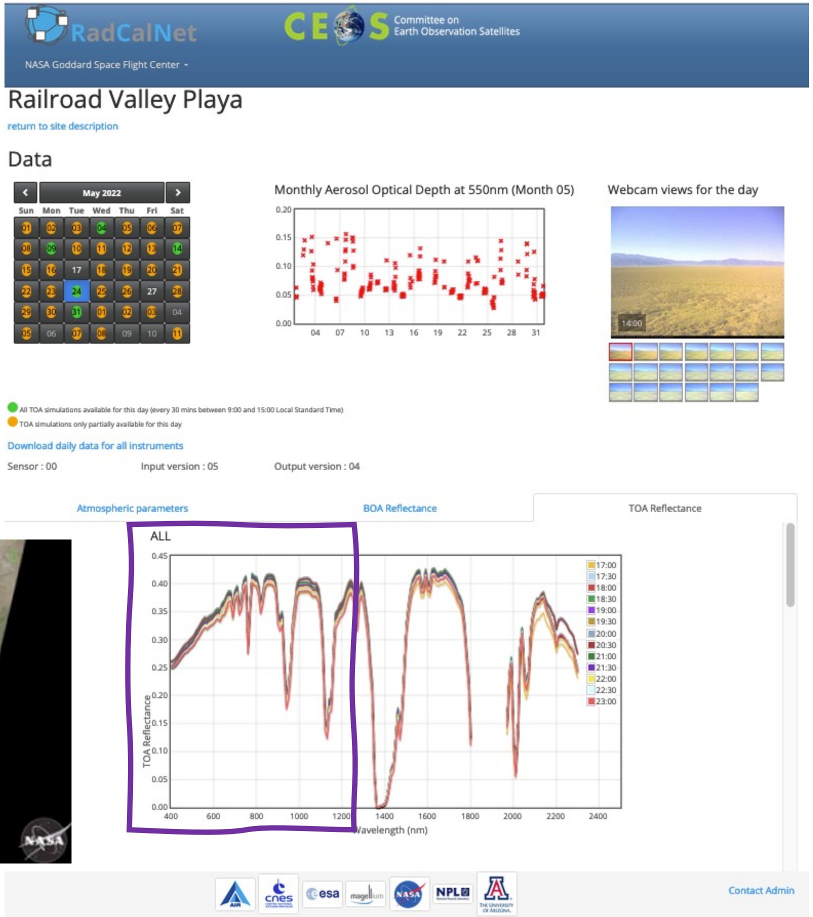
Terrestrial Calibration Sites

- **Radiometric Characterization and Calibration of Landsat and portable to GLIMR**
  - Derive surface spectral reflectance following established methodology
- **Pseudo Invariant Calibration Sites (PICS)**
  - Essentially invariant over time
  - Are spatially very uniform, have stable spectral responses over time
  - Atmospheric effects on upwelling radiance is minimal due to high surface reflectance
  - Are in regions where rainfall is extremely limited:
    - Prevents vegetative growth
    - Very sparse human populations

RadCalNet – source of TOA radiances for calibration

- ➢ TOA reflectance
  - at 30 min intervals from 9 am to 3 pm local time
  - Hyperspectral at 10 nm steps from 400 nm to 2500 nm
- ➢ Railroad Valley Playa
  - 15 x 15 km useable area
  - 38.50° N, 115.69° W
  - AERONET & RadCalNet

Source: https://calval.cr.usgs.gov/apps/railroad-valley



Railroad Valley Playa

return to site description

Data

● All TOA simulations available for this day (every 30 mins between 9:00 and 15:00 Local Standard Time)

● TOA simulations only partially available for this day

Download daily data for all instruments

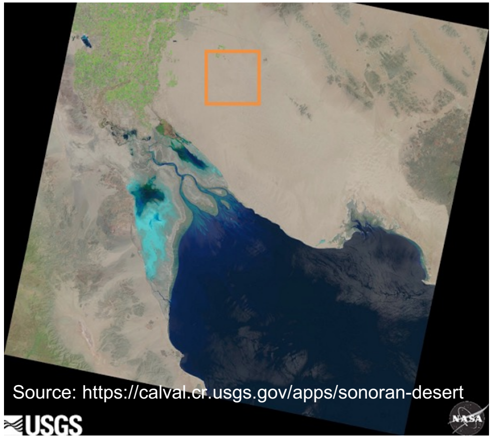
Sensor : 00 Input version : 05 Output version : 04

https://www.radcalnet.org/#!/

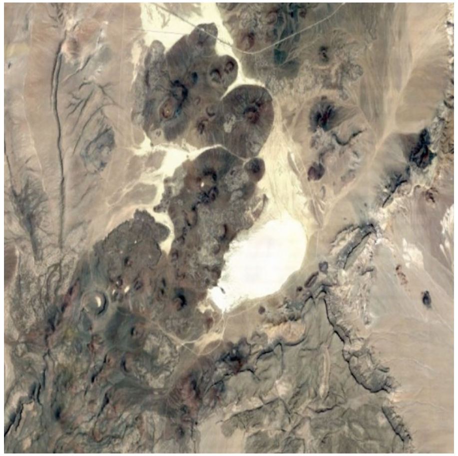
Bouvet et al. 2019 Rem Sens; https://doi.org/10.3390/rs11202401

USGS ECCOE Radiometric Calibration Sites

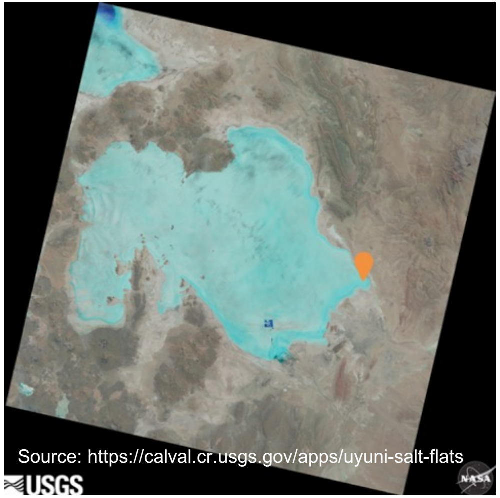
- Landsat; AERONET systems
- Lunar Lake Playa, Nevada
  - Dry lake bed; <0.5% reflectance variance
  - 1.5 x 2.5 km usable area
  - 38.4° N, 115.99° W
- Sonoran Desert, Mexico
  - spatially uniform
  - 15 x 15 km usable area
  - 32.35° N, 114.65° W



Source: https://calval.cr.usgs.gov/apps/sonoran-desert



- Uyuni Salt Flats, Potosi, Bolivia
  - 25 x 25 km usable area
  - 20.38° N, 66.95 W



Source: https://calval.cr.usgs.gov/apps/uyuni-salt-flats