PACE R_{rs} validation

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Requirements for R_{rs} ($\rho_w = \pi R_{rs}$)

Data Product	Baseline Uncertainty
Water-leaving reflectances centered on (±2.5 nm) 350, 360, and 385 nm (15 nm bandwidth)	0.0057 or 20%
Water-leaving reflectances centered on (±2.5 nm) 412, 425, 443, 460, 475, 490, 510, 532, 555, and 583 (15 nm bandwidth)	0.0020 or 5%
Water-leaving reflectances centered on (±2.5 nm) 617, 640, 655, 665 678, and 710 (15 nm bandwidth, except for 10 nm bandwidth for 665 and 678 nm)	0.0007 or 10%

these are required for mission success & drive OCI design

Additional required products to be generated
Chlorophyll concentration
Spectral diffuse attenuation coefficients
Spectral absorption coefficients (phytoplankton, CDOM+NAP)
Spectral backscattering coefficients
Fluorescence line height

Atmospheric Correction using OCI alone

*Better characterization of aerosols using MAP

Each uncertainty requirement is defined as the maximum absolute and relative values for Level-2 satellite data processing (geophysical values in the original satellite coordination system). These requirements are specified for **≥ 50% of the observable deep ocean** (≥ 1000 m).

Validation Rrs product

- Rrs product from satellite
- In-situ truth/independent measurements
- Match up process (aggregate data)
- Validation metrics (meet requirements?)

How do we validate operational products?

SeaBASS web-based search tools:

Users can filter validation results based on metadata date or location ranges, keywords, datasets, or exclusion quality criteria

Keyword Search Filters:

Search for affiliation, PI (principal investigator), experiment, or cruise name. Use the plus button to ad

Search String

CORAL

Any All

Products:

a, a_{dg}, angstrom, AOT, a_{ph}, b_{bp}, chl, K_d_490, PAR, PIC, POC, R_{rs}

Data Sources:

SeaBASS Only / SeaBASS + AERONET-OC* / AERONET-OC Only* / MOBY Only*

Sensor Selection:

MODIS-Aqua vs. In situ

MODIS-Aqua vs. MODIS-Aqua

Water Depth:

Minimum (in meters): 0.0 Maximum: 10000

Exclusion Criteria:

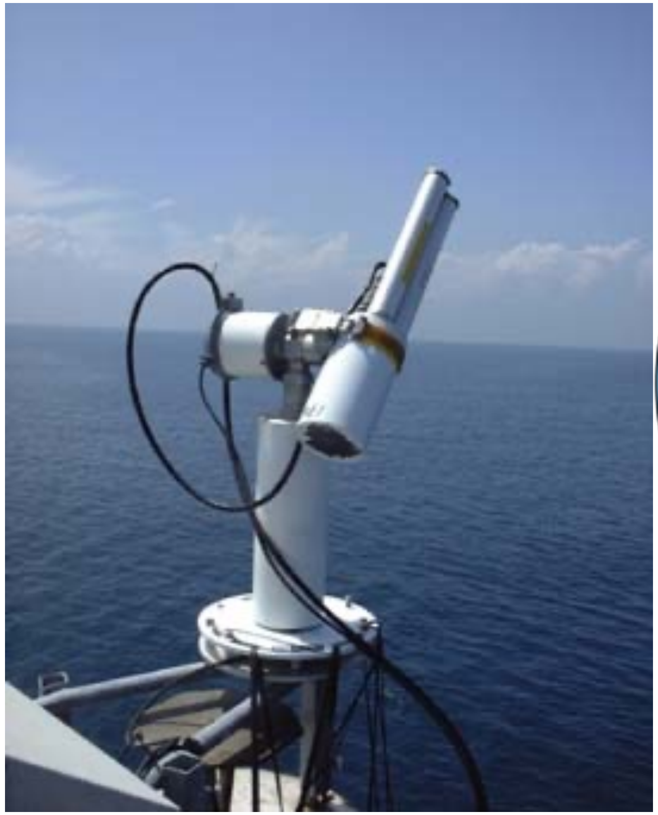
	MODIS-Aqua	
Minimum valid satellite pixels:	50	%
Maximum solar zenith angle:	75	degrees
Maximum satellite zenith angle:	60	degrees
Maximum time difference between satellite and in situ:	3	hours
Maximum coefficient of variation of satellite pixels:	0.15	
Maximum irradiance difference between measured and modeled:	20	%
Maximum windspeed:	35	m/s

Satellite Data Version(s):

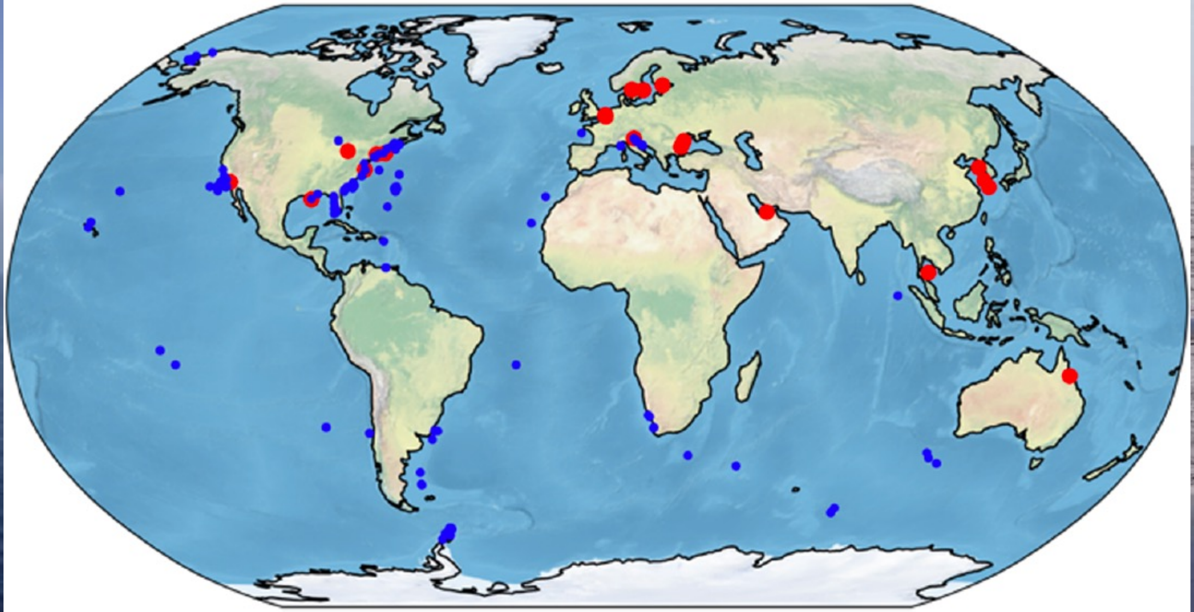
MODIS-Aqua: 2018.0

In-situ radiometry in AERONET-OC + SeaBASS

- ➢ AERONET-OC has about 27 sites, and all are coastal.
- ➢ SeaBASS shipborne measurements have a large dynamic range of waters



AERONET-OC site Venise

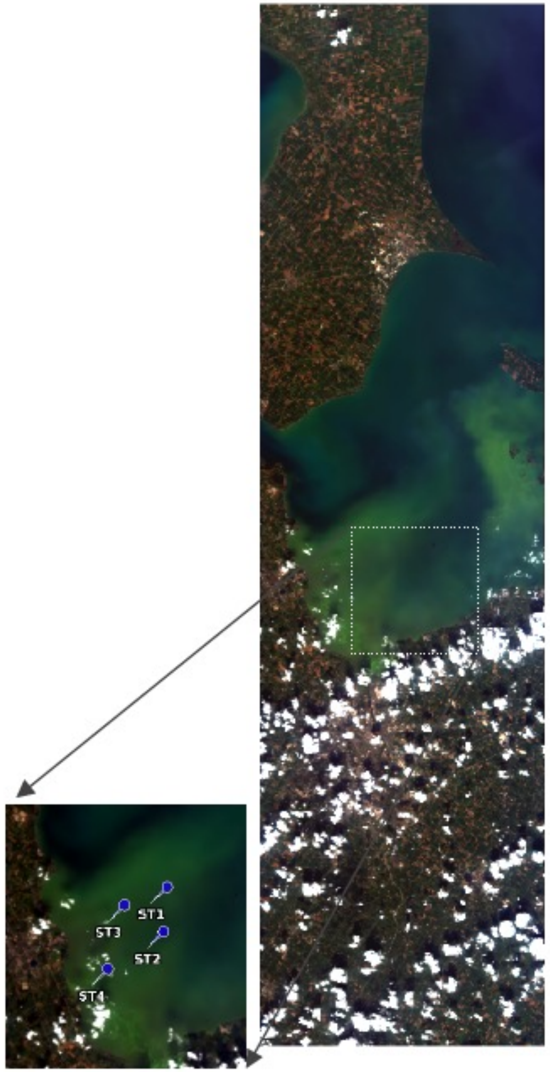


AERONET-OC
SeaBASS (matched with MODIS Aqua)

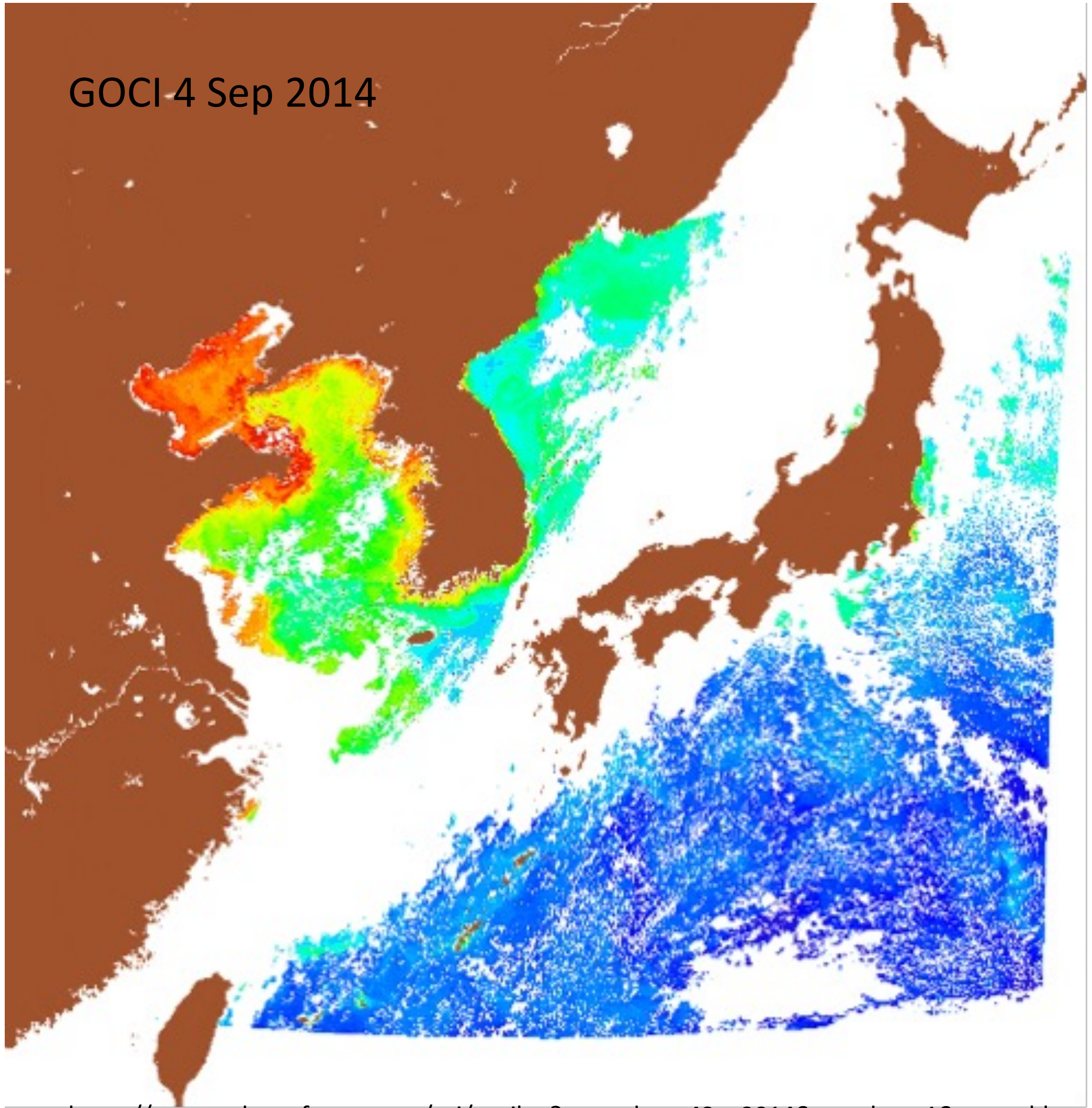
NOAA Cal/Val cruise 2014

Spatio-temporal variability

True color



HICO 90 meters pixel



https://oceancolor.gsfc.nasa.gov/cgi/gocibrs?start_date=4Sep2014&numdays=1&type=chl

SeaBASS web-based Level-2 Validation Search

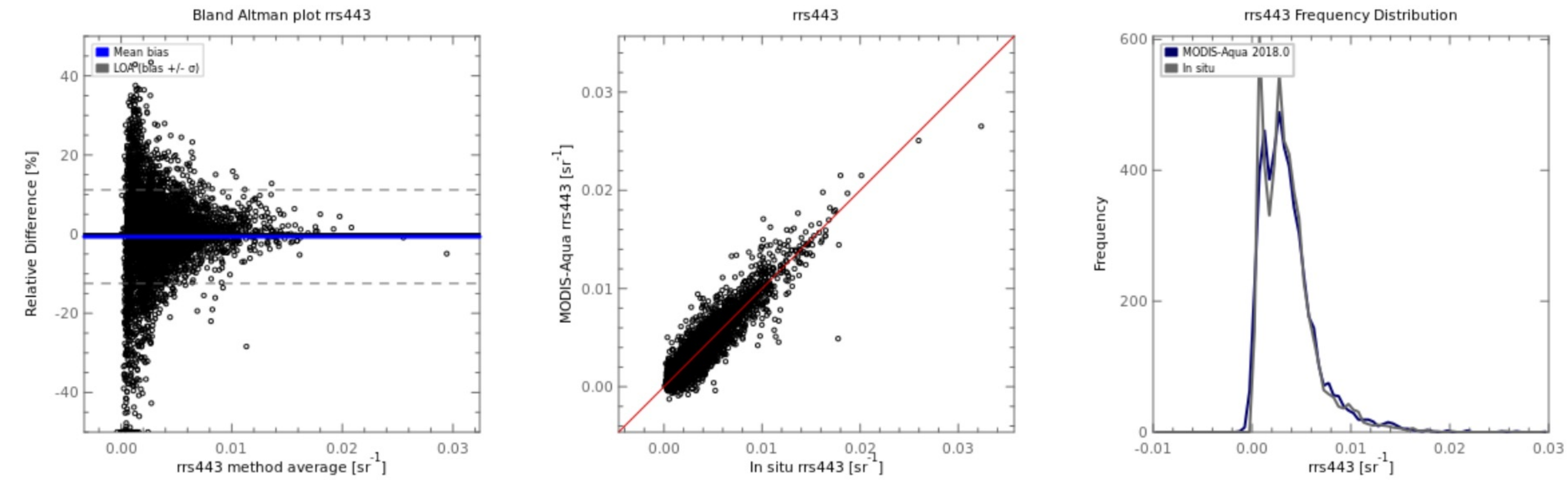
(https://seabass.gsfc.nasa.gov/search#val)

bias (mean bias)
accuracy (mean absolute error, MAE)

Data values and statistics for where successful coincident match-ups were calculated between *in situ* and satellite ocean color sensors measurements (Bailey and Werdell, 2006)

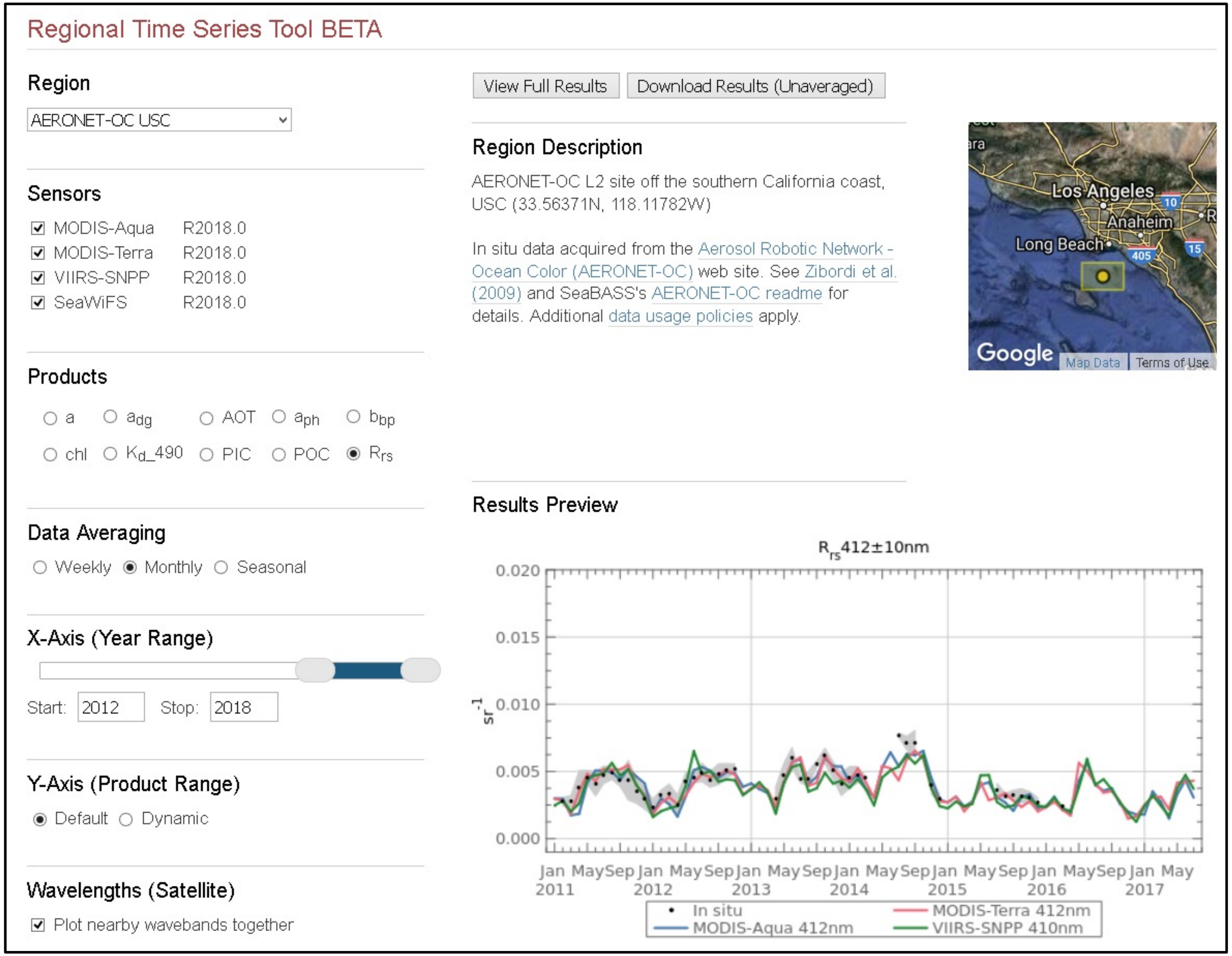
Statistics | Data

Product Name	#	Mean Bias	Mean Absolute Error (MAE)	MODIS-Aqua Range	In situ Range
rrs412	4932	0.00001	0.00102	-0.00310 - 0.02045	-0.00000 - 0.02771
rrs443	5135	0.00005	0.00077	-0.00126 - 0.02653	0.00007 - 0.03234
rrs488	4722	-0.00054	0.00079	0.00001 - 0.03311	0.00039 - 0.03952
rrs531	2904	-0.00055	0.00078	0.00087 - 0.02927	0.00113 - 0.03301
rrs547	4600	-0.00050	0.00078	0.00086 - 0.02854	0.00117 - 0.02885
rrs555	4399	-0.00079	0.00094	0.00058 - 0.02670	0.00102 - 0.02890
rrs667	4518	-0.00017	0.00029	-0.00053 - 0.01345	0.00000 - 0.01533
rrs678	538	-0.00016	0.00033	-0.00041 - 0.01008	0.00004 - 0.00904



Time Series Tool Features

Time series and percent frequency distributions of satellite and *in situ* data



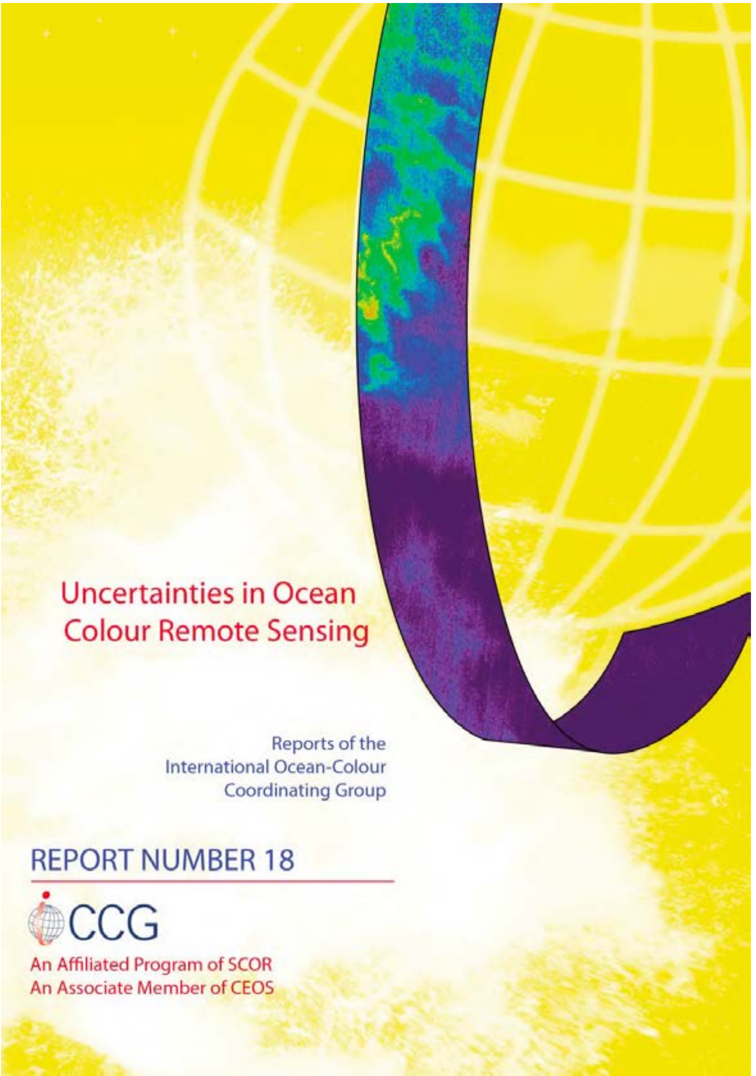
IOCCG validation metrics

Metric	Description
$\delta = \frac{1}{N} \times \sum_{i=1}^{N} y_i - x_i,$	Mean bias
$\lvert\delta\rvert = \frac{1}{N} \times \sum_{i=1}^{N} \lvert y_i - x_i \rvert$	Mean absolute error
$\Delta = \sqrt{\frac{1}{N} \times \sum_{i=1}^{N} (y_i - x_i)^2}$	Root mean square error
$\lvert\psi\rvert_m = 100 \times \frac{1}{N} \times \sum_{i=1}^{N} \frac{\lvert y_i - x_i \rvert}{x_i}.$	Mean absolute relative error

$x_{i=1,N}$ Satellite

$y_{i=1,N}$ In-situ

Centered statistics

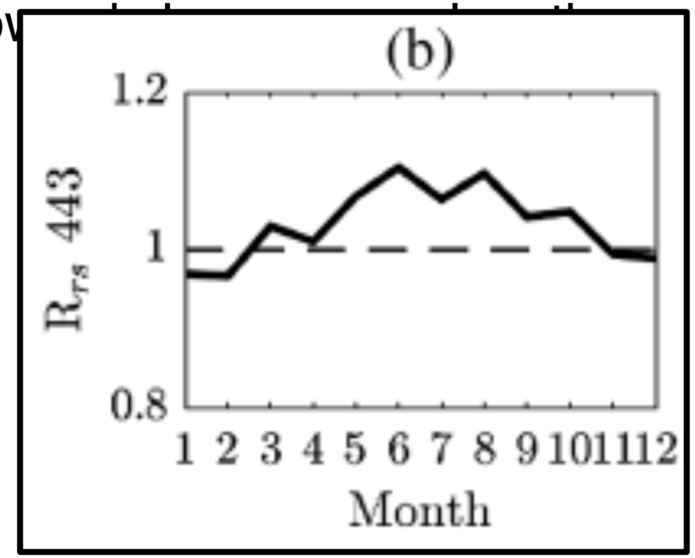


https://ioccg.org/wp-content/uploads/2020/01/ioccg-report-18-uncertainties-rr.pdf

Additional validation and diagnostic tools

Study summary

- Ocean color data are seasonally biased in low biomass regions.
- In terms of IOPs, bbp is the most affected as it's directly related to the magnitude of Rrs, while aph and adg are not.
- The bias in Rrs is more pronounced tow



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Seasonal bias in global ocean color observations

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In this study, we identify a seasonal bias in the ocean color satellite-derived remote sensing reflectances ($R_{rs}(\lambda)$; sr^{-1}) at the ocean color validation site, Marine Optical BuoY. The seasonal bias in $R_{rs}(\lambda)$ is present to varying degrees in all ocean color satellites examined, including the Visible Infrared Imaging Radiometer Suite, Sea-Viewing Wide Field-of-View Sensor, and Moderate Resolution Imaging Spectrometer. The relative bias in R_{rs} has spectral dependence. Products derived from $R_{rs}(\lambda)$ are affected by the bias to varying degrees, with particulate backscattering varying up to 50% over a year, chlorophyll varying up to 25% over a year, and absorption from phytoplankton or dissolved material varying by up to 15%. The propagation of $R_{rs}(\lambda)$ bias into derived products is broadly confirmed on regional and global scales using Argo floats and data from the cloud-aerosol lidar with orthogonal polarization instrument aboard the cloud-aerosol lidar and infrared pathfinder satellite. The artifactual seasonality in ocean color is prominent in areas of low biomass (i.e., subtropical gyres) and is not easily discerned in areas of high biomass. While we have eliminated several candidates that could cause the biases in $R_{rs}(\lambda)$, there are still outstanding questions regarding potential contributions from atmospheric corrections. Specifically, we provide evidence that the aquatic bidirectional reflectance distribution function may in part cause the observed seasonal bias, but this does not preclude an additional effect of the aerosol estimation. Our investigation highlights the contributions that atmospheric correction schemes can make in introducing biases in R_{rs} (λ), and we recommend more simulations to discern these influence R_{rs} (λ) biases. Community efforts are needed to find the root cause of the seasonal bias because all past, present, and future data are, or will be, affected until a solution is implemented.

Multiple linear regression

$$Rrs_{\text{aqua}} \sim \text{St}(\mu,\ \nu), \quad \textbf{(1)}$$

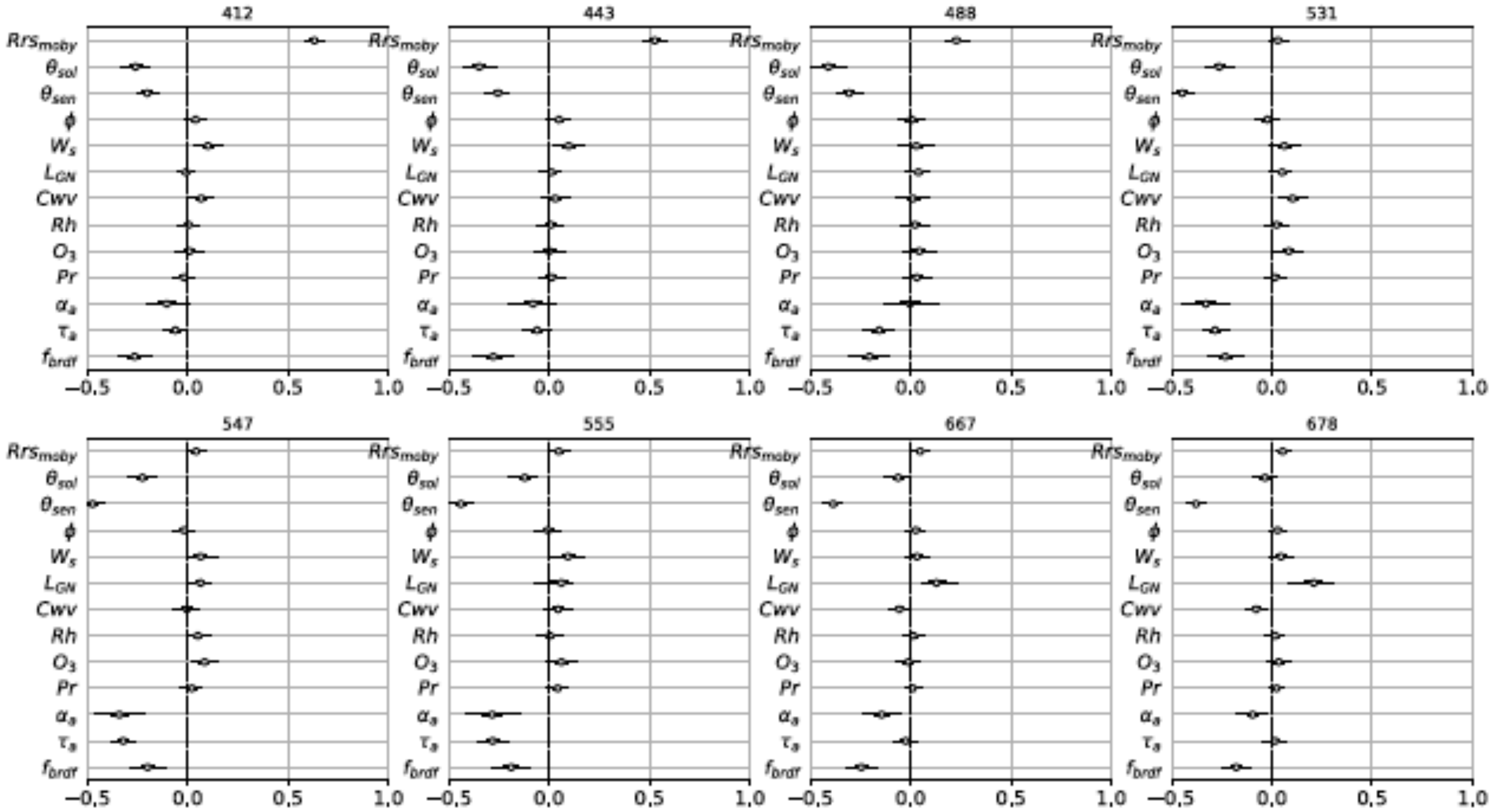
where μ and ν are the mean and degree of freedom of the Student's t distribution, respectively, and μ is modeled as

$$\mu = \beta_0 \text{Rrs}_{\text{moby}} + \beta_1 \theta_{\text{sol}} + \beta_2 \theta_{\text{sen}} + \beta_3 \varphi + \beta_4 \text{W}_\text{s} + \beta_5 \text{L}_{\text{GN}} + \beta_6 \text{Cwv} + \beta_7 \text{Rh} + \beta_8 \text{O}_3 + \beta_9 \text{Pr} + \beta_{10} \alpha_\text{a} + \beta_{11} \tau_\text{a} + \beta_{12} f_{\text{brdf}} + \alpha.$$

Ideally all independent variables will have a slope of 0 and Rrs_moby of 1

Potential contributors to the bias:

1. BRDF
2. The aerosol type and optical depth

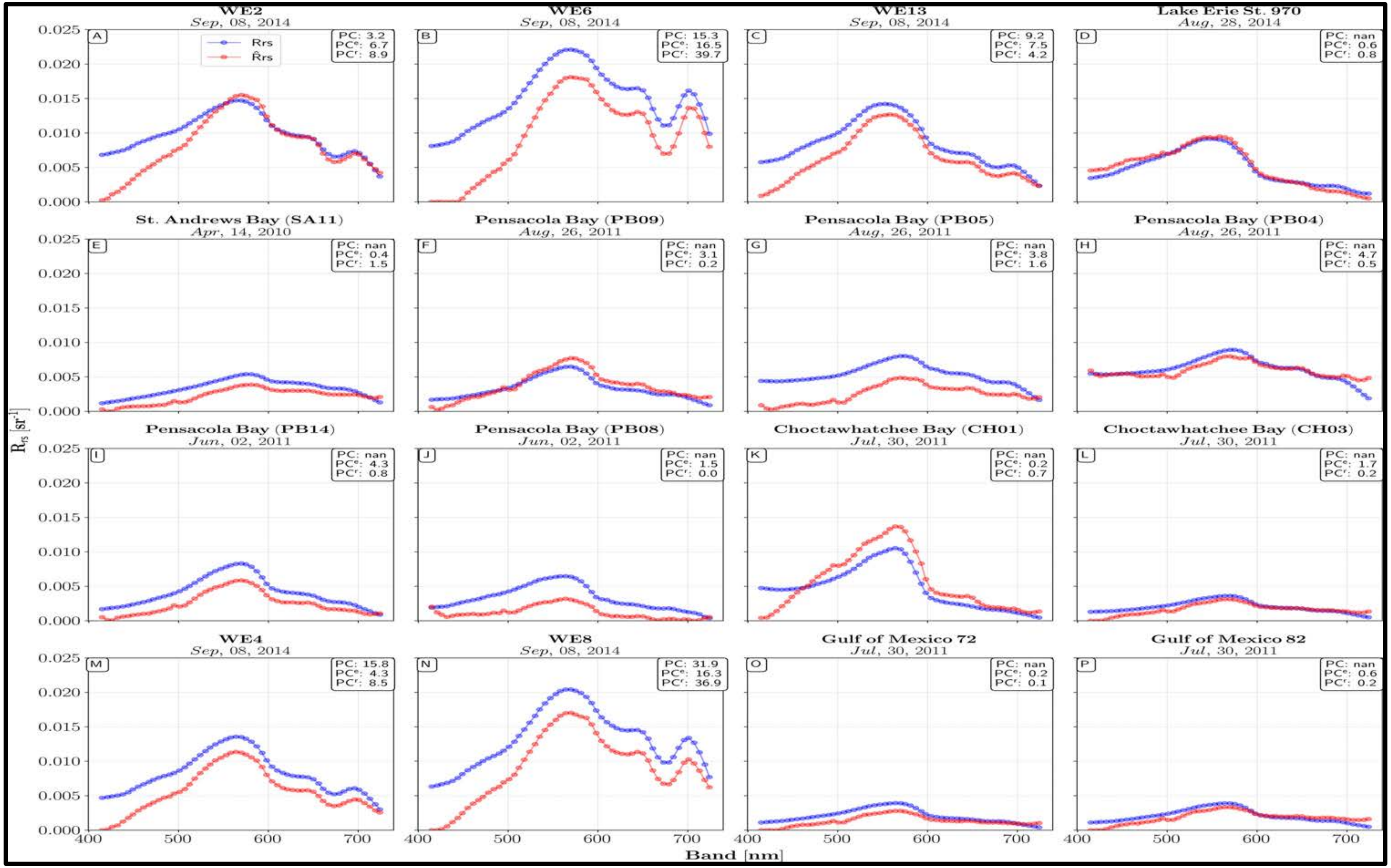


Challenges with validating PACE R_{rs}

- How do we validate Rrs at 239 wavelengths for full spectrum or 170 wavelengths from 400-700nm?
- What metrics do we use?
  - R2
  - RMSE
  - MAE
  - Mean bias
  - Spectral Angle (SA)
  - Euclidean Minimum Distance (EMD)
  - Apparent Visible Wavelength (AVW)
  - …
- How to visualize data? Scatter plots?
- How to include pixel-level uncertainties from satellite data in the validation?
- Do we have uncertainties in in-situ data?
- What about Flagging?
- If multiple algorithms produce the same product, how do we compare their relative performance?

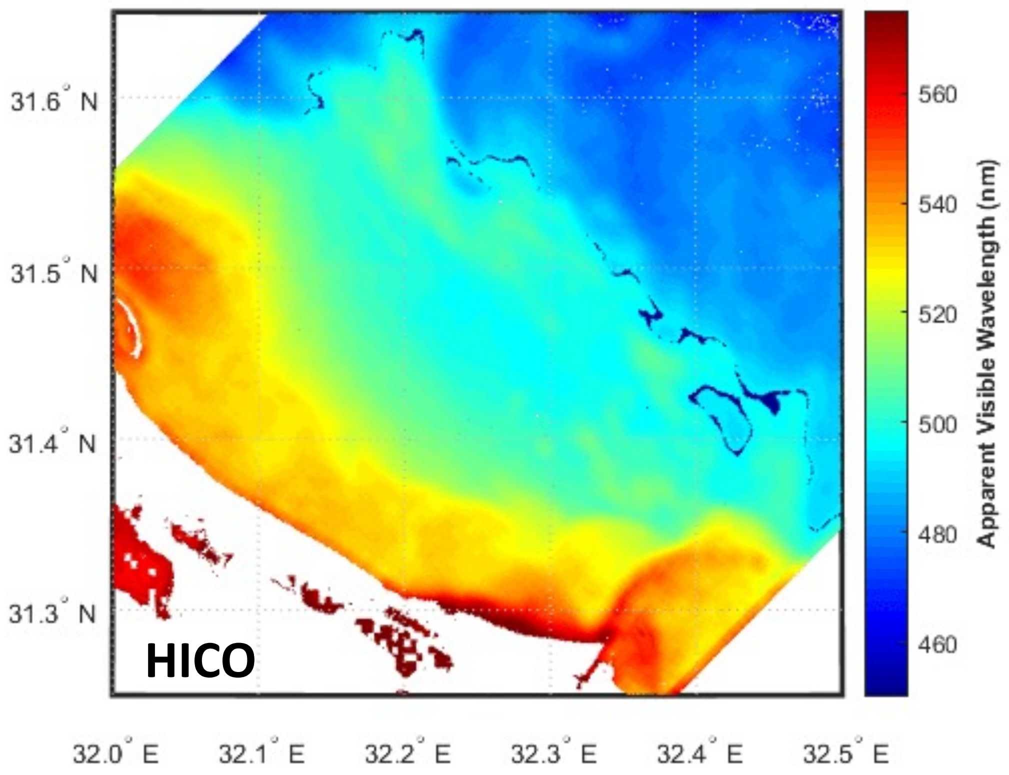
Going Hyperspectral

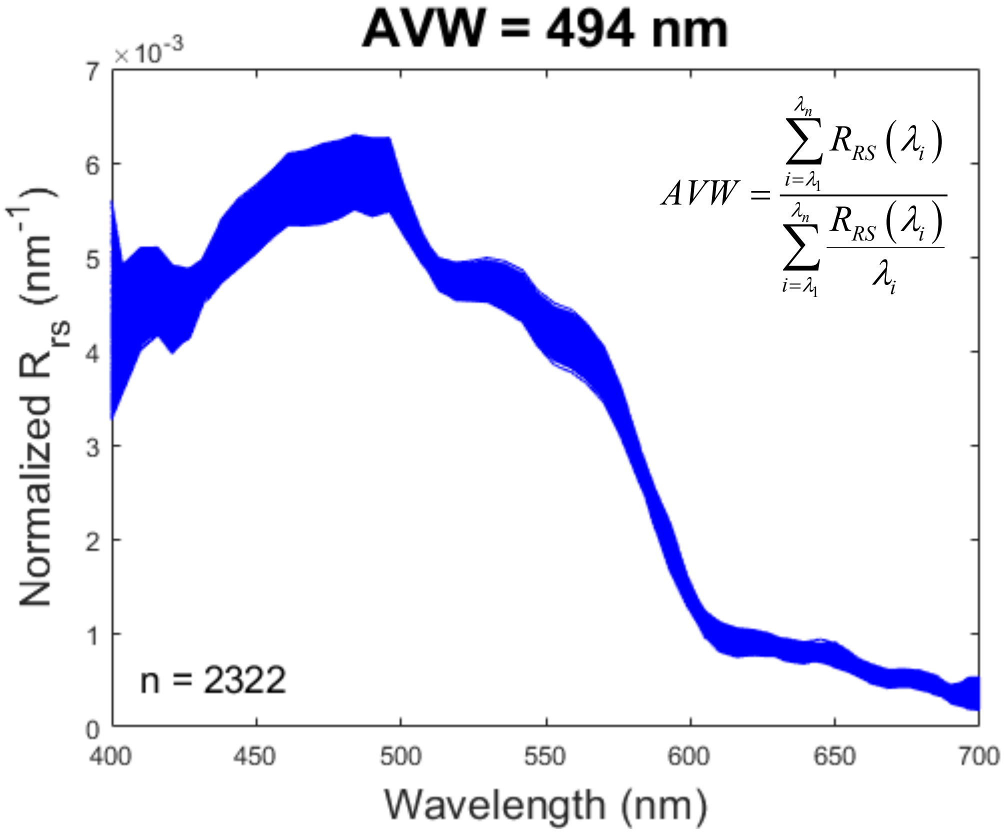
HICO processed with SeaDAS



O'Shea et al.,2021

New tools to investigate full spectral behavior

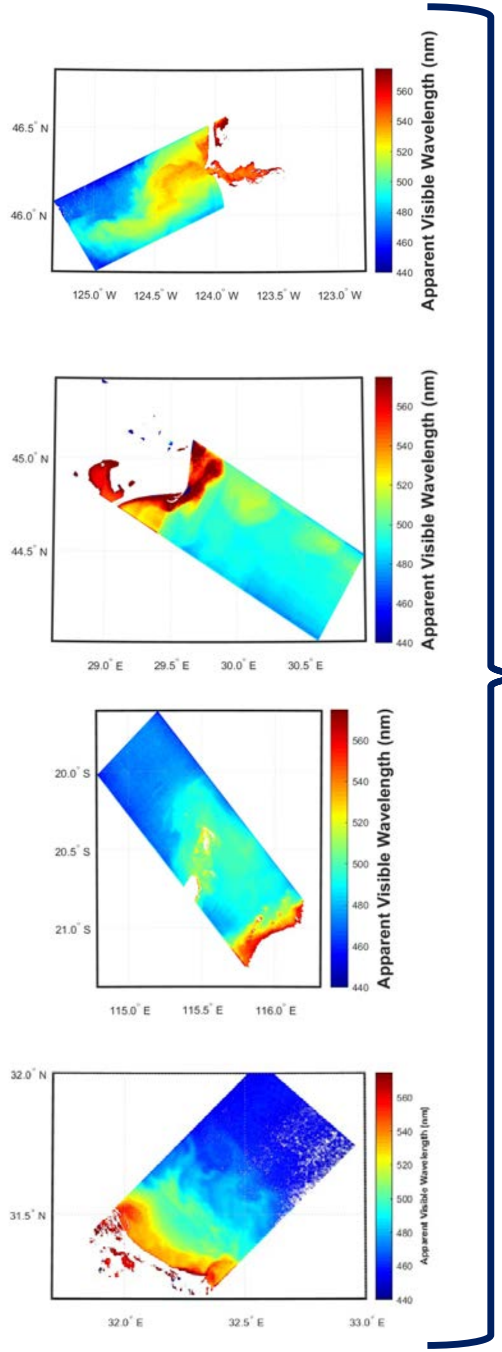




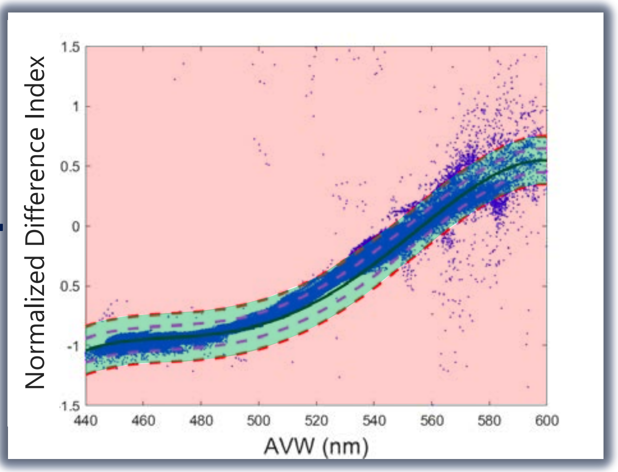
$$AVW = \frac{\sum_{i=\lambda_1}^{\lambda_n} R_{RS}(\lambda_i)}{\sum_{i=\lambda_1}^{\lambda_n} \frac{R_{RS}(\lambda_i)}{\lambda_i}}$$

Using full spectral information represents a more holistic approach to unraveling spectral variability, ensuring that any diagnostic signals present are considered, and thus can help maximize the potential of spectral information embedded in remote sensing data.

Vandermeulen et al. (2020)

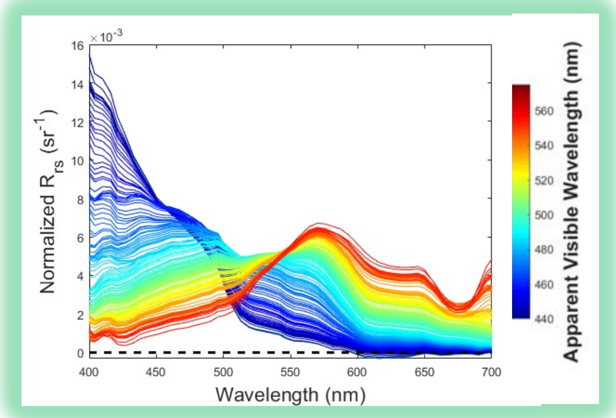


Quality Water Index Polynomial (QWIP)



Comparing full spectral information against empirical indices enables a quick and efficient means of assessing the relative quality of hyperspectral satellite and/or in situ data

Accept



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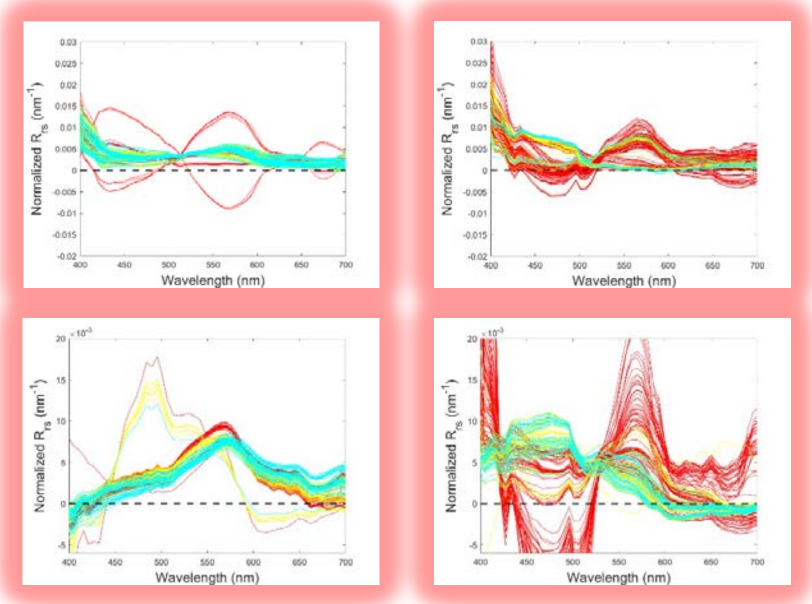

Deviation score | 0.2 – 0.25 | 0.25 – 0.35 | > 0.35

Dierssen et al. (2022)