

Quantifying uncertainties in phytoplankton
absorption coefficients for accurate validation
of the PACE ocean color sensor:
moving towards satellite retrieved
phytoplankton functional types (PFTs)

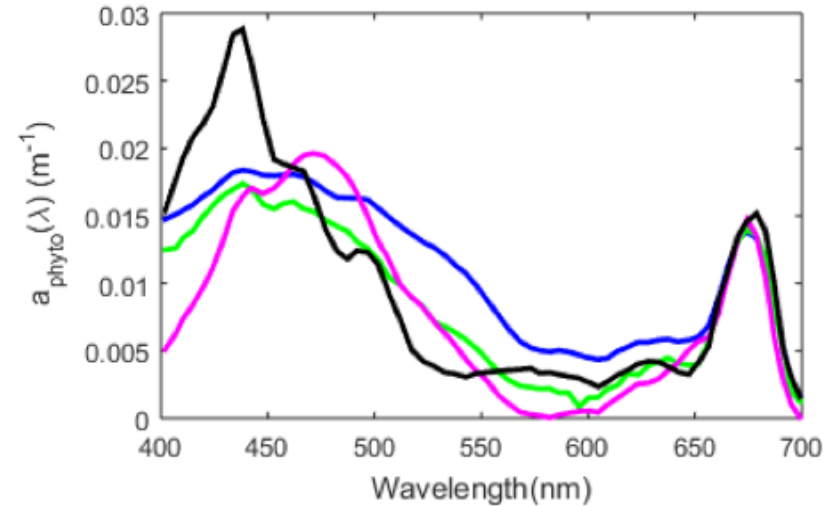
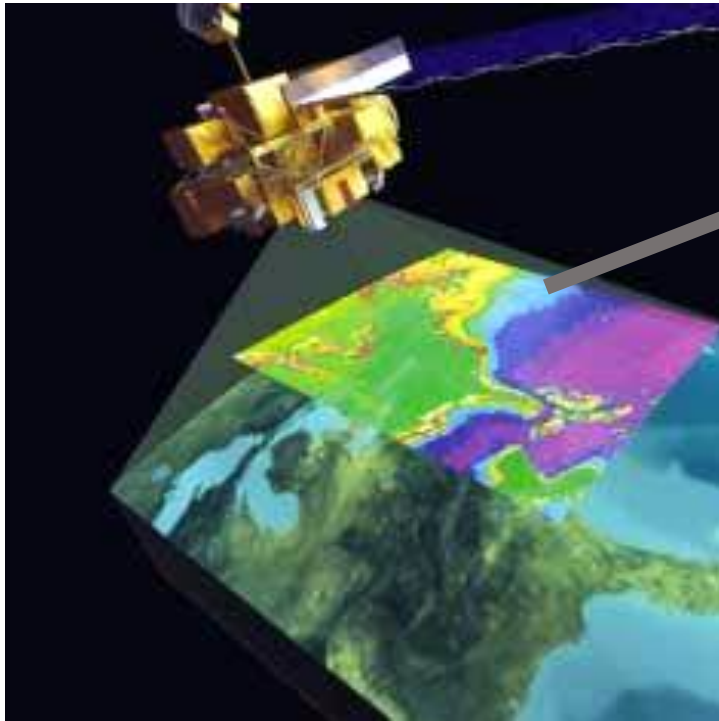
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One of the core PACE objectives is to support the estimation of IOPs in general, specifically optically-based Phytoplankton Functional Types



- Invert ocean color signal to retrieve hyperspectral phytoplankton absorption coefficients
→ key to PFT inversion
- Requires capability to **validate with uncertainties**



Approach to improved PFT validation

- $R_{rs}(\lambda)$ input to IOP inversion algorithm
- $a_{ph_sat}(\lambda)$ output from IOP inversion
- **Validate with *in situ* $a_{ph_sat}(\lambda)$**
- *in situ* $a_{ph_sat}(\lambda)$ derived from *in situ* $a_{ph}(\lambda, z)$
- *in situ* $a_{ph}(\lambda, z)$ derived from *in situ* $a_{p_acs}(\lambda, z)$
- *in situ* $a_{p_acs}(\lambda, z)$ derived from *in situ* total and filtered $a_{acs}(\lambda, z)$
- $a_{p_acs}(\lambda, z) = a_{T_acs}(\lambda, z) - a_{<0.2\mu m_acs}(\lambda, z)$
- $a_{acs}(\lambda, z)$ are temperature, salinity and scattering corrected
- *in situ* $a_{ph}(\lambda, z_{sample})$ validated with discrete $a_{ph}(\lambda, z_{sample})$
- Discrete $a_{ph}(\lambda, z_{sample})$ derived from spectrophotometric observations of $a_p(\lambda, z_{sample})$ and $a_{nap}(\lambda, z_{sample})$



Approach to improved PFT validation – *in situ* measurement schema

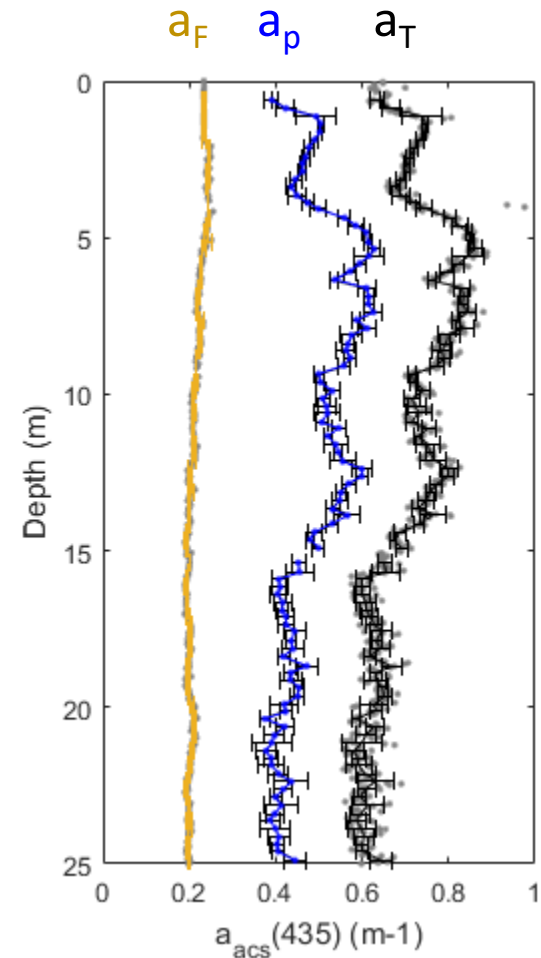
- Measured *in situ* total and filtered $a_{acs}(\lambda, z)$
- $a_{acs}(\lambda, z)$ temperature, salinity corrected
- $a_{p_acs}(\lambda, z) = a_{T_acs}(\lambda, z) - a_{<0.2\mu m_acs}(\lambda, z)$
- $a_{p_acs}(\lambda, z)$ scattering corrected
- *in situ* $a_{ph}(\lambda, z)$ derived from *in situ* $a_{p_acs}(\lambda, z)$
- *in situ* $a_{ph_sat}(\lambda)$ derived from *in situ* $a_{ph}(\lambda, z)$



Measured acs profiles

– binning and T, S correction

- Example raw profile
- 25-cm bin averaged
- Uncertainty associated with binning $\sim 2.6\%$
- Temperature and salinity correction using simultaneous SeaBird CTD measurements uncertainty $\sim 0.5\%$
- Subtract filtered profile to obtain particulate absorption, mathematical uncertainty propagation for $a_p(\lambda)$



Measured acs profiles

– Scattering Correction (proposed)

- Scattering correction

$$a(\lambda) = a_m(\lambda) - \varepsilon(\lambda)$$

- In situ sensors have poorly understood scattering error
 - acs - hyperspectral but has scattering errors, no UV
 - ICAM - “no” scattering error, 9 wavelengths, 1 UV
- Require merging the best of each sensor
 - Use ICAM to
 - determine scattering correction
 - extrapolate to UV
 - Interpolate to acs wavelengths

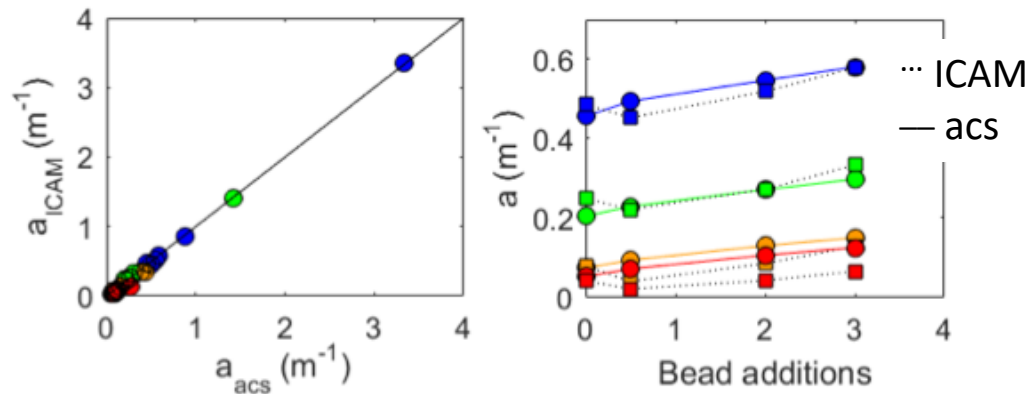


Measured acs profiles

- Scattering Correction (reality)

- In situ sensors have poorly understood scattering error
 - ICAM is **not** the solution
 - Same scattering error as acs but no NIR channel to assess error

Raw acs, ICAM observations



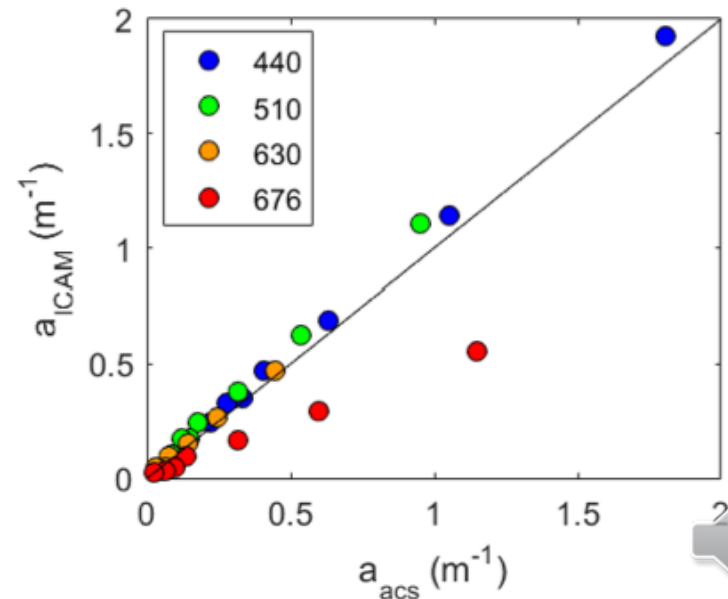
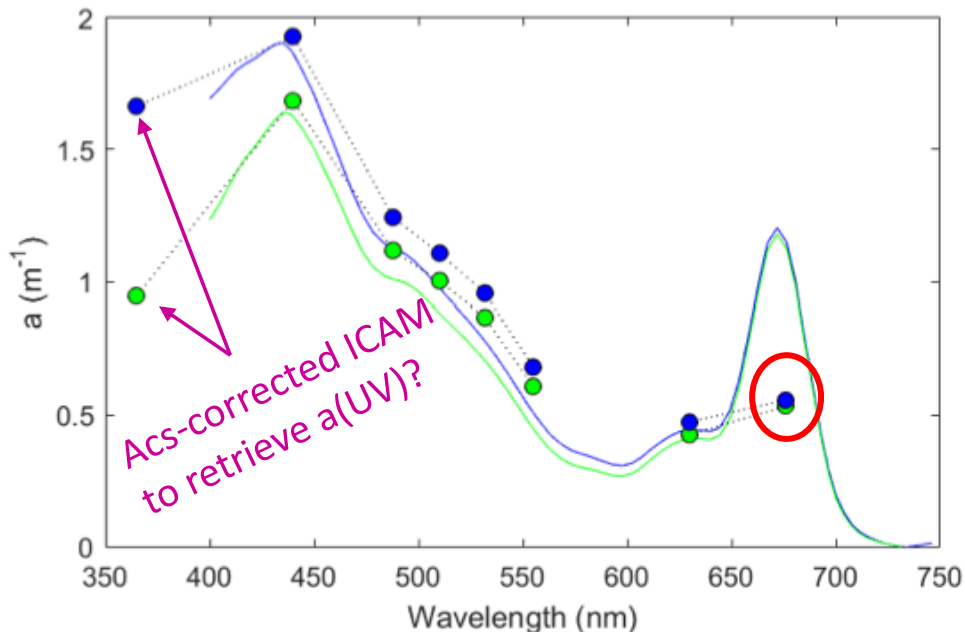
Scattering- corrected acs



Measured acs profiles

– Scattering Correction (reality)

- In situ sensors have poorly understood scattering error
 - ICAM is not the solution
 - Same scattering error as acs \rightarrow overestimates absorption 5 to 14% ± 3 to 11% ($r^2 > 0.99$, $p < 10^{-6}$) at all wavelengths
 - underestimates acs(676) by 55% $\pm 3\%$ ($r^2 > 0.99$, $p < 10^{-6}$)

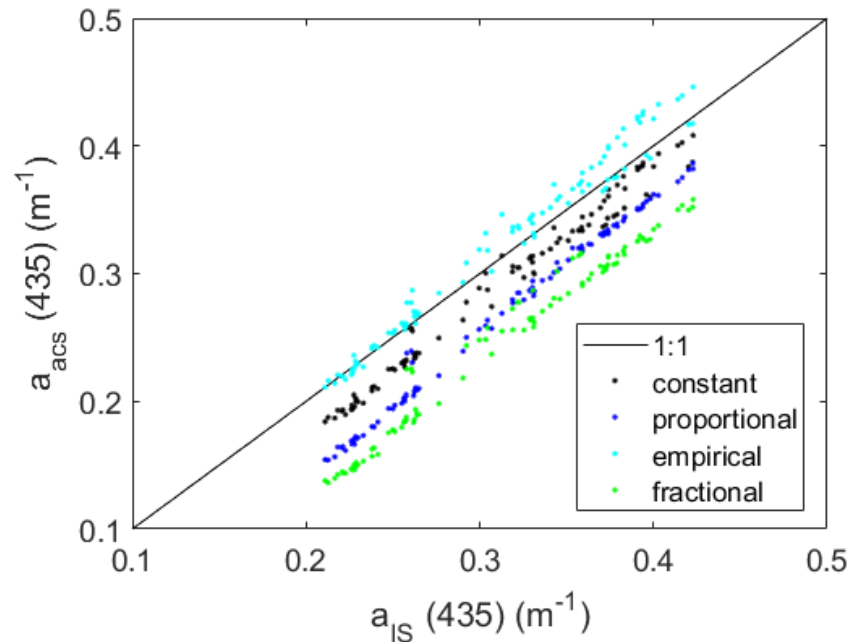


Measured acs profiles – Scattering Correction (models)

- Scattering correction

$$a(\lambda) = a_m(\lambda) - \varepsilon(\lambda)$$

- $\varepsilon(\lambda) = a(NIR)$, (*constant*)
- $\varepsilon(\lambda) = a(NIR) * \frac{b(\lambda)}{b(NIR)}$ (*proportional*)
- $\varepsilon(\lambda) = C_1 * a(NIR)^{C_2}$ (*empirical*)
- $\varepsilon(\lambda) = F(a(NIR))$, (*fractional*)
- $\varepsilon(\lambda) = (a(NIR) - a_{IS}(NIR)) * \frac{b(\lambda)}{b(NIR)}$ (*integrating sphere*)



Measured acs profiles – Scattering Correction

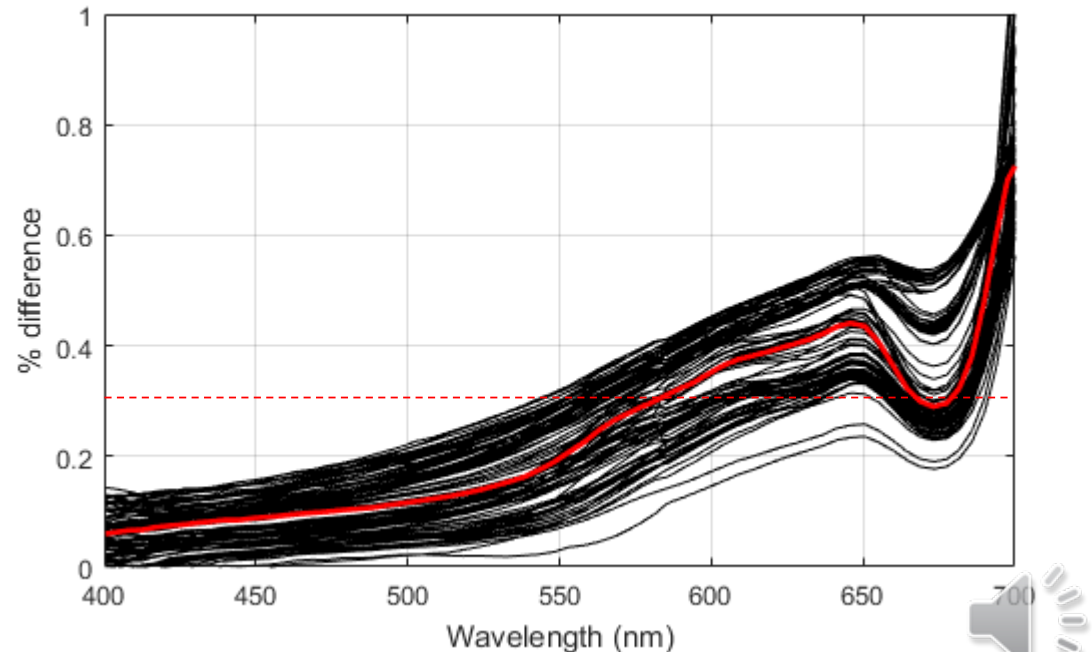
- Scattering uncertainty

$$a(\lambda) = a_m(\lambda) - \varepsilon(\lambda)$$

- $\varepsilon(\lambda) = a(NIR)$, (constant)

- $\varepsilon(\lambda) = (a(NIR) - a_{IS}(NIR)) * \frac{b(\lambda)}{b(NIR)}$ (integrating sphere)

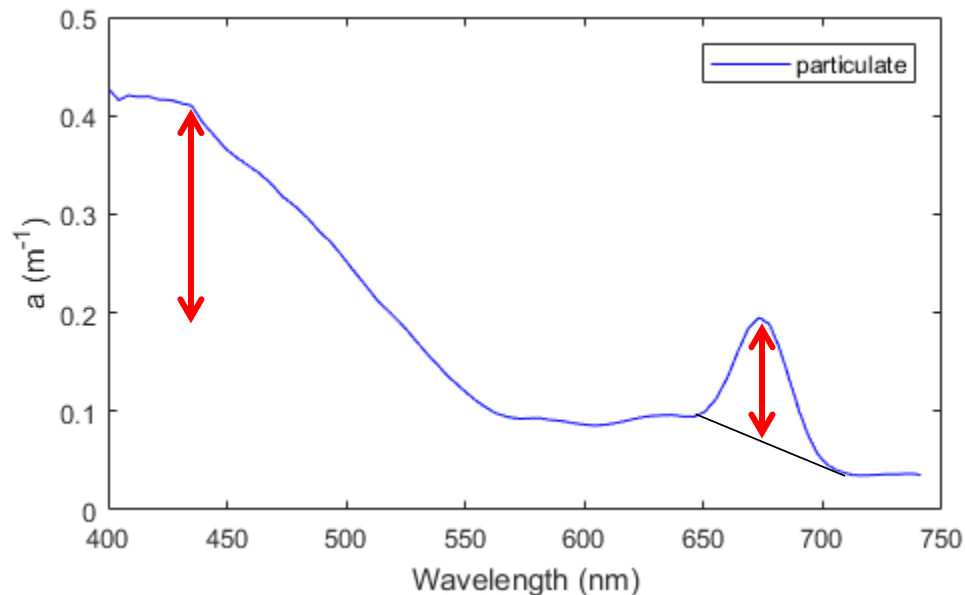
- <30% uncertainty
- 400 – 575 nm, 676 nm



see also Stockley et al 2017

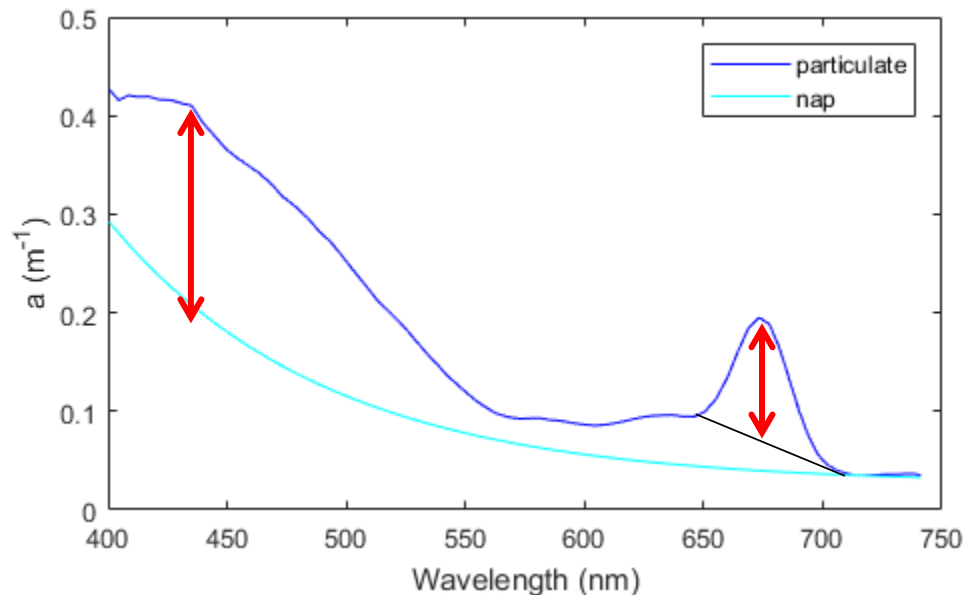
Modeled a_{ph} profiles

- Example model (Roesler et al. 1989)
 - $a_{ph}(676)$ from absorption line height (Roesler and Barnard 2013)
 - $a_{ph}(435)$ estimated from **blue to red peak ratio** (parameter)



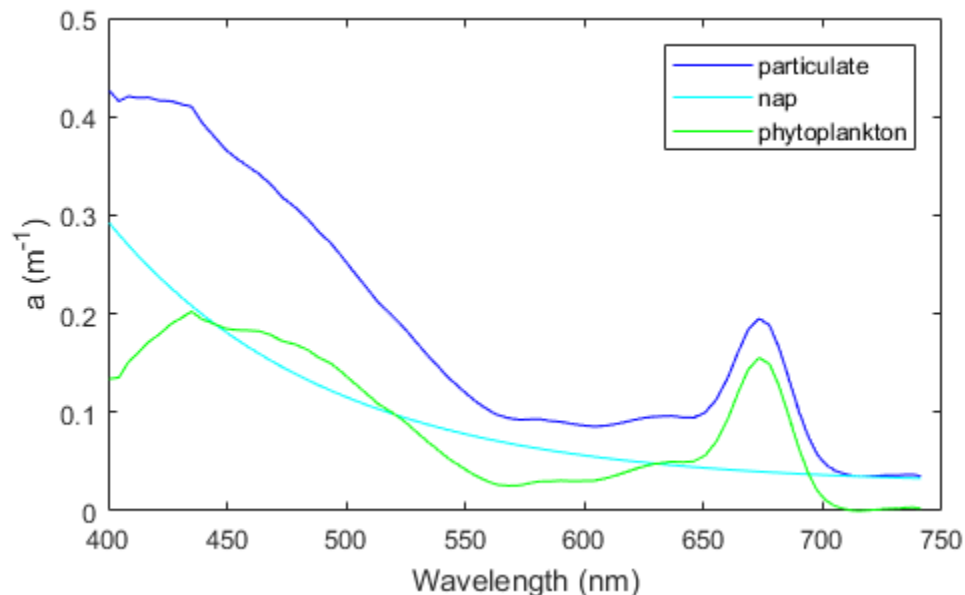
Modeled a_{ph} profiles

- Example model (Roesler et al. 1989)
 - $a_{ph}(676)$ from absorption line height (Roesler and Barnard 2013)
 - $a_{ph}(435)$ estimated from **blue to red peak ratio** (parameter)
 - $a_{nap}(435) = a_p(435) - a_{ph}(435)$
 - $a_{nap}(\lambda) = a_{nap}(435) \exp(\mathcal{S}_{nap}(\lambda - 435))$

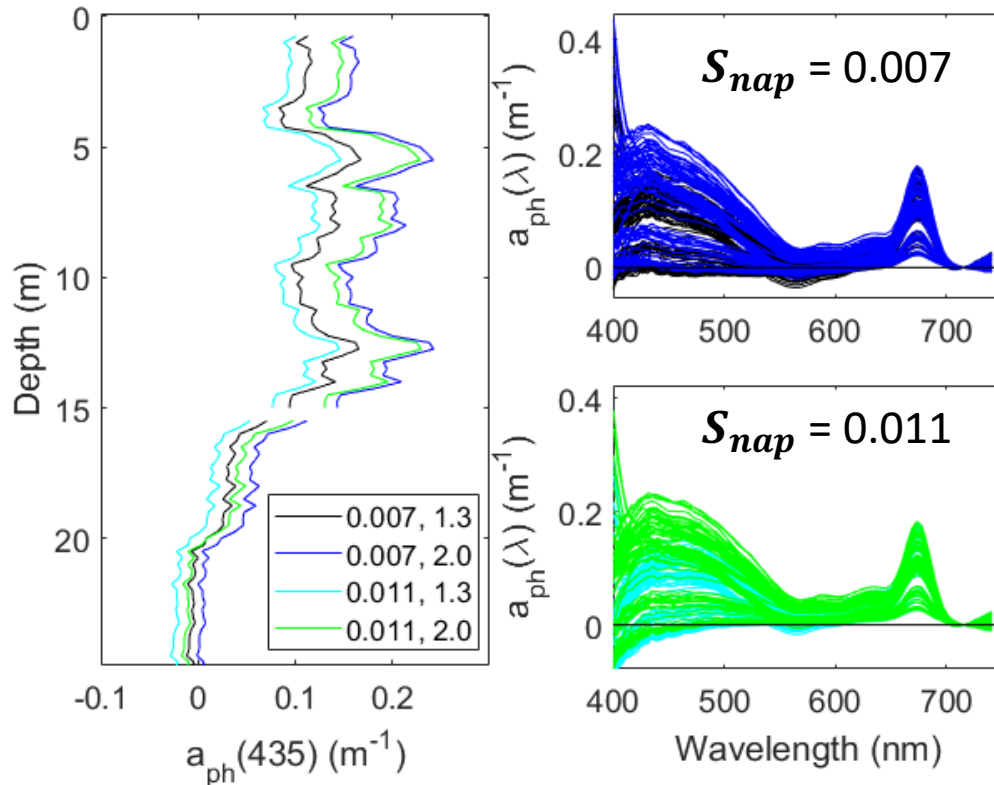


Modeled a_{ph} profiles

- Example model (Roesler et al. 1989)
 - $a_{ph}(\lambda) = a_p(\lambda) - (a_p(435) - R_{BR} * a_{ph}(676)) \exp(S_{nap}(\lambda - 435))$
 - Example output from single depth-binned acs measurement



Modeled a_{ph} profiles – parameter uncertainty



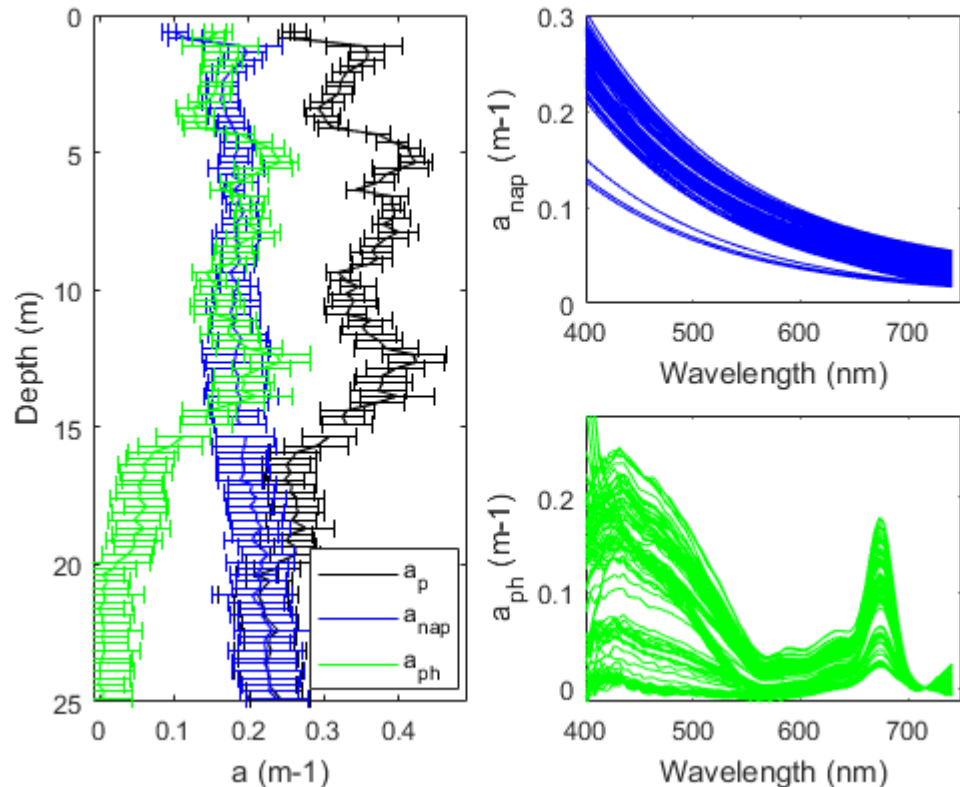
- $R_{BR} < 1.3 - 2.0 >$
 $a_{ph}(435)$ varies by 40%
- $S_{nap}, 0.007 - 0.011 >$
 $a_{ph}(435)$ varies by 15%
- Broad parameter ranges
yield unrealistic results
($a_{ph}(\lambda), a_{nap}(\lambda) < 0$)
- Uncertainty is reduced
within smaller
parameter ranges



Modeled a_{ph} profiles

- Example model (Roesler et al. 1989)
 - $a_{ph}(\lambda) = a_p(\lambda) - (a_p(435) - R_{BR} * a_{ph}(676)) \exp(S_{nap}(\lambda - 435))$
 - Example output from profile depth-binned acs measurement

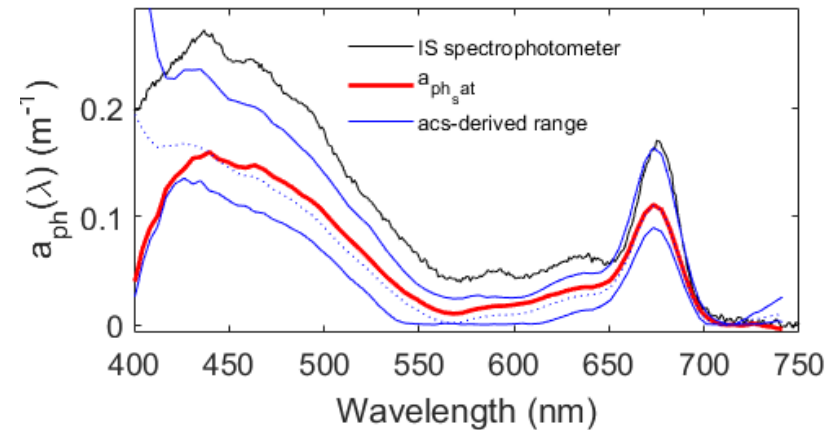
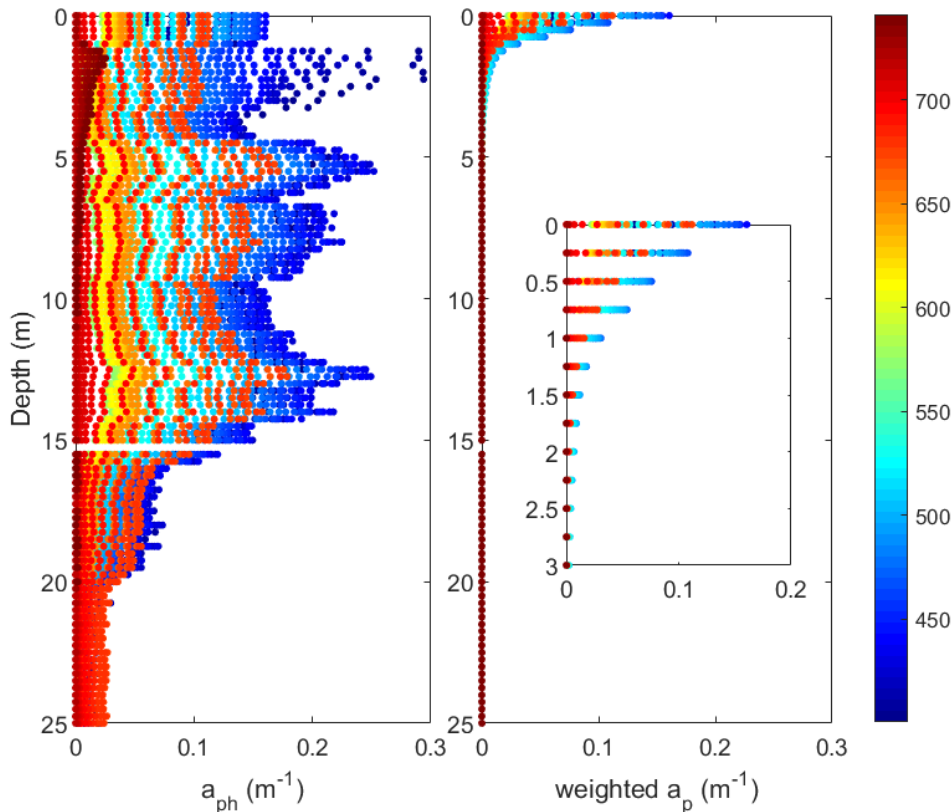
- $R_{BR} = 2.0$
- $S_{nap} = 0.007 \text{ nm}^{-1}$
- Uncertainty propagated



Modeled a_{ph_sat} profiles

- Satellite sees exponentially-weighted absorption

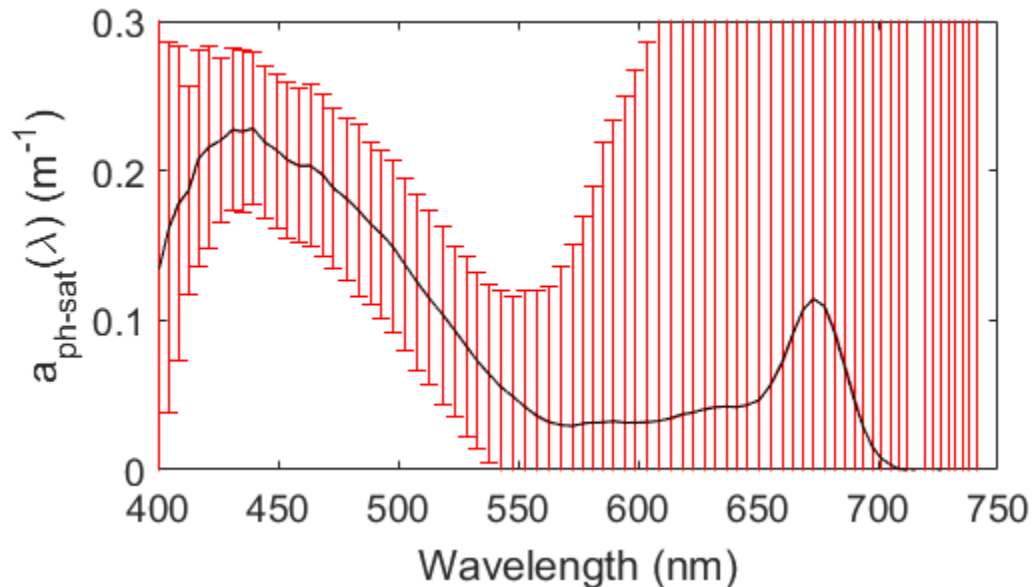
- Morel and Berthon (1989) $\bar{a}_{sat}(\lambda) = \frac{\int_0^{Z_{pd}} a(z) \exp(-2k(\lambda) z) dz}{\int_0^{Z_{pd}} \exp(-2k(\lambda) z) dz}$



Modeled $a_{\text{ph_sat}}$ profiles – uncertainty budget

0.0	Depth binning	Scattering correction	Model parameters	Sum of uncertainties	Depth weighting*
Color	Black	Blue	Cyan	Green	Red
U (m^{-1})	0.0105	0.0202	0.0045	0.0262	0.0667
%CV	12%	23%	5%	30%	44%

* 400 – 550 nm



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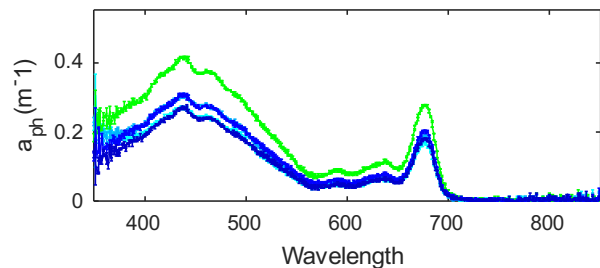
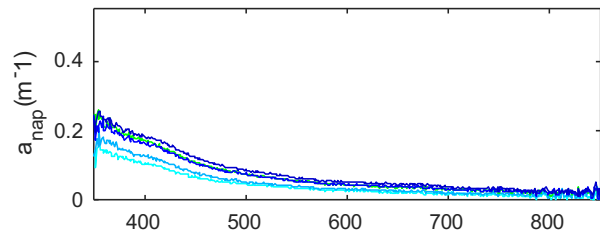
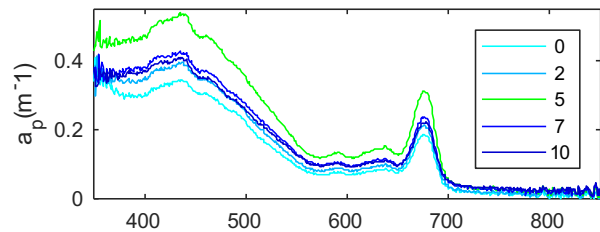
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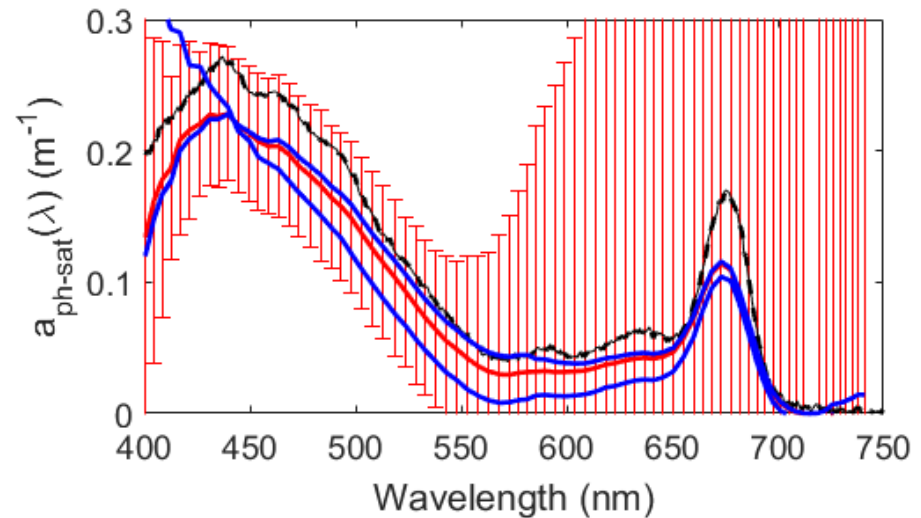


Measured a_{ph} spectra – discrete samples

- Filter pad measurements in integrating sphere



Uncertainty	Absolute (m^{-1})	CV %
Experimental	0.0026- 0.0027	1.2 - 1.9
Replication	0.0040 - 0.020	1.1 - 5.3
Null	0.0100- 0.0240	7.2 - 14.2



Conclusions

- Protocol for obtaining in situ optical depth-weighted hyperspectral phytoplankton absorption coefficients to validation PFT inversion products
- Uncertainty budget for validation product

