



近海海洋环境科学国家重点实验室（厦门大学）

State Key Laboratory of Marine Environmental Science
(Xiamen University)



Optical
Oceanography
Laboratory

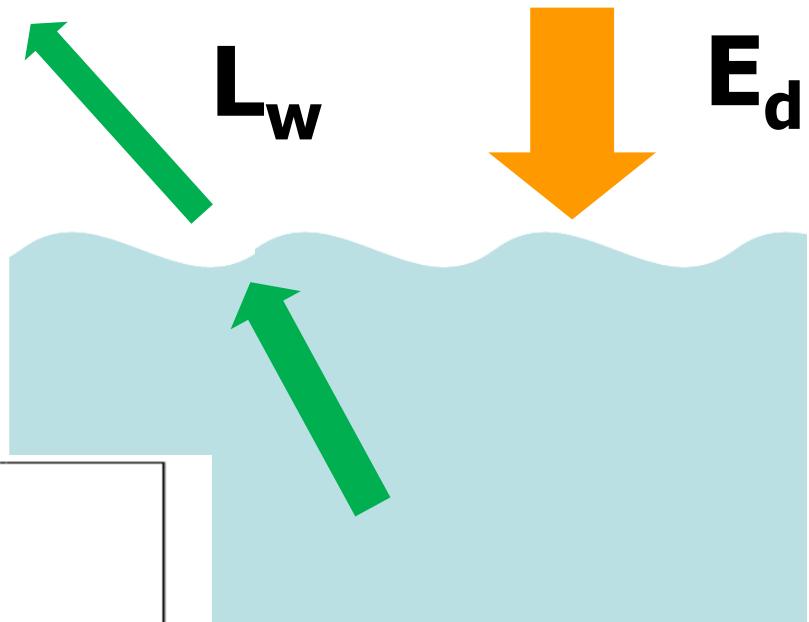
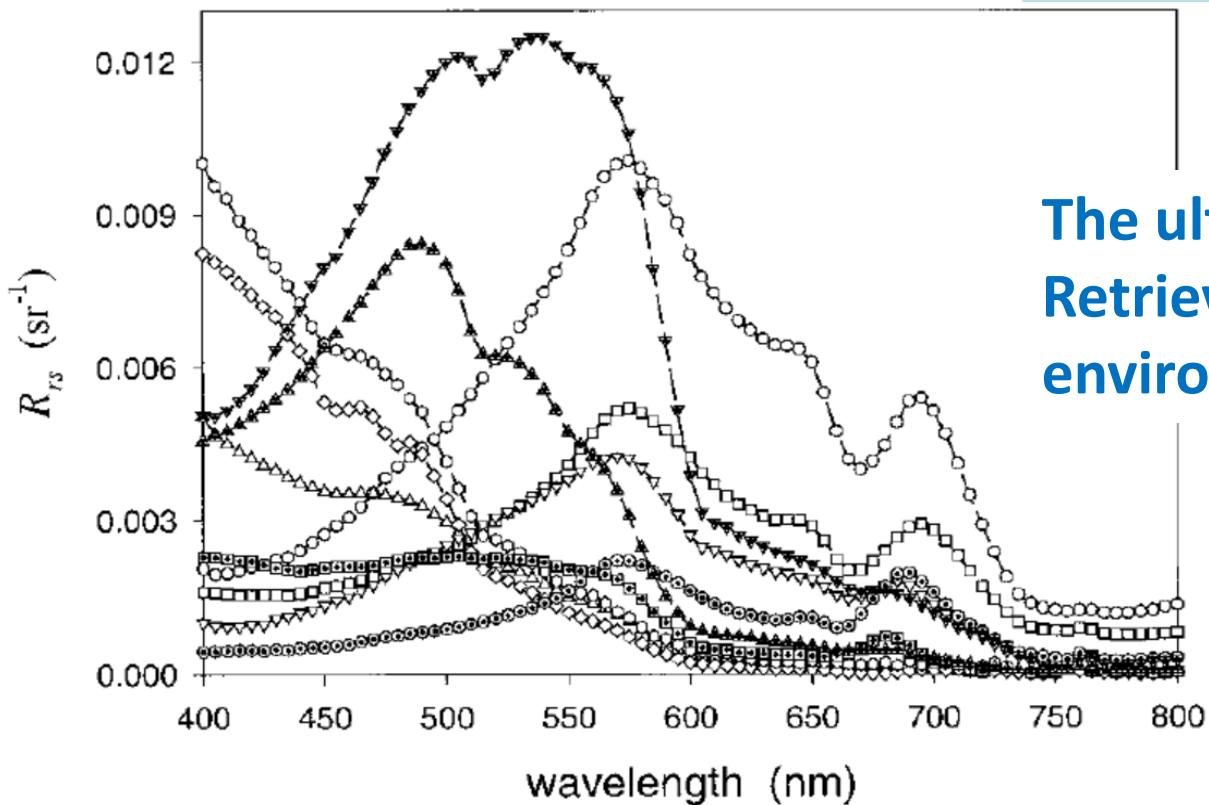
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Xiamen University

Inherent Optical Properties (IOPs)

Lecture 2: Inversion algorithms

Remote-sensing reflectance (sr^{-1}):

$$R_{rs}(\lambda) = \frac{L_w(\lambda, 0^+)}{E_d(\lambda, 0^+)}$$

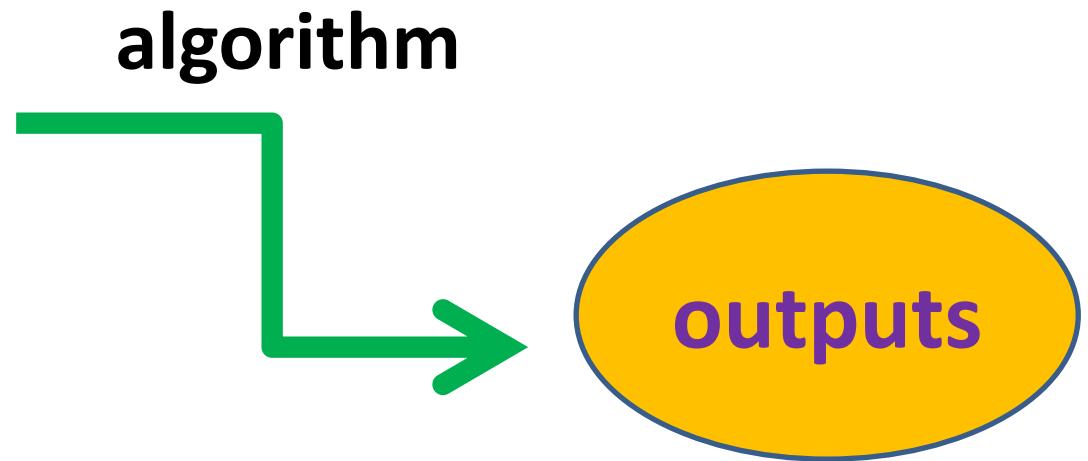


The ultimate objective of RS:
Retrieval useful/important
environmental information

How?
algorithm!

inputs

(L_w or R_{rs})



(IOPs or
[Chl] etc)

**Empirical
(explicit or implicit)**

Bio-optical models: No need

**Semi-analytical
(algebraic, LUT, optimization)**

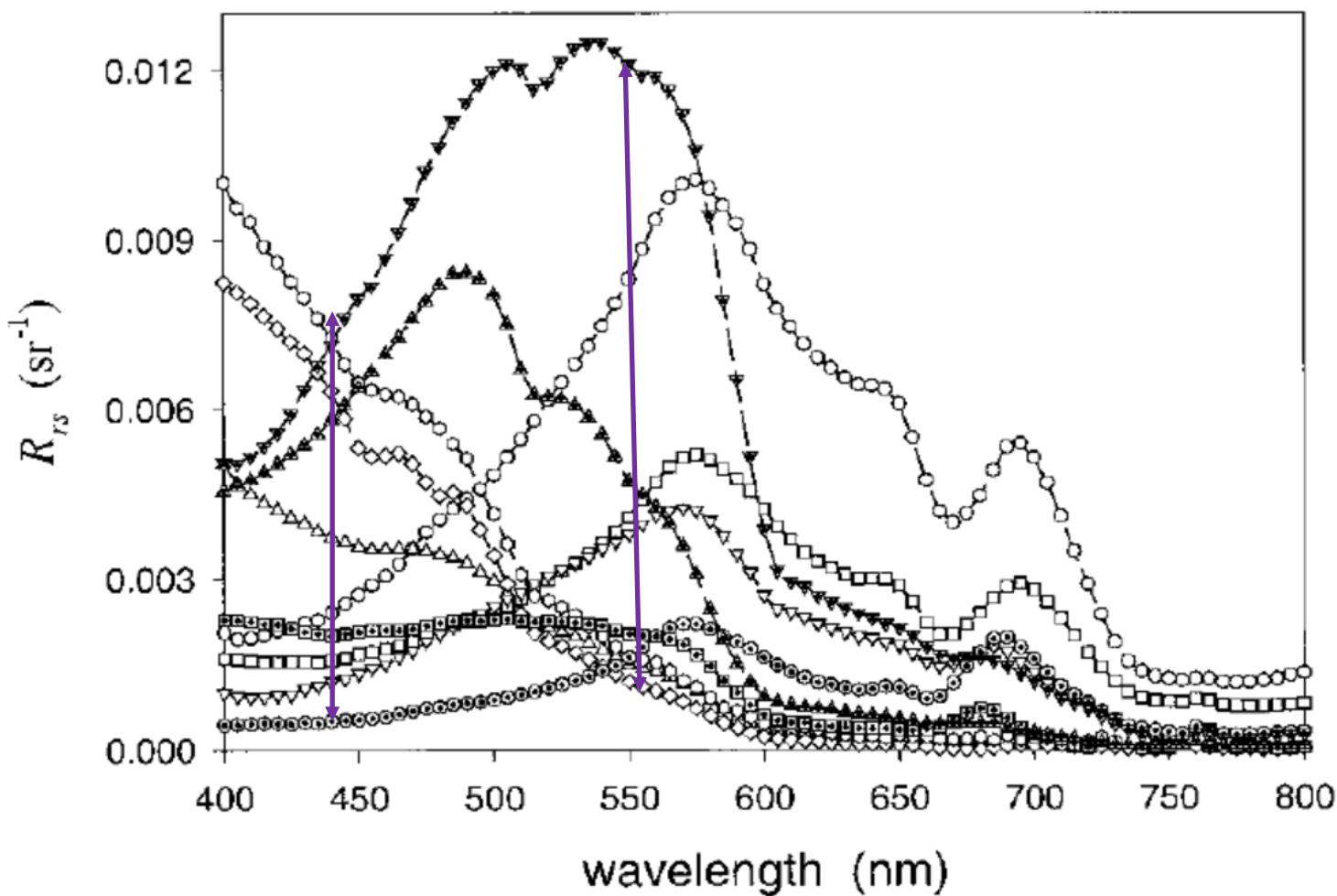
Bio-optical models: Yes

{ **Bottom Up Strategy (BUS)**
Top Down Strategy (TDS)

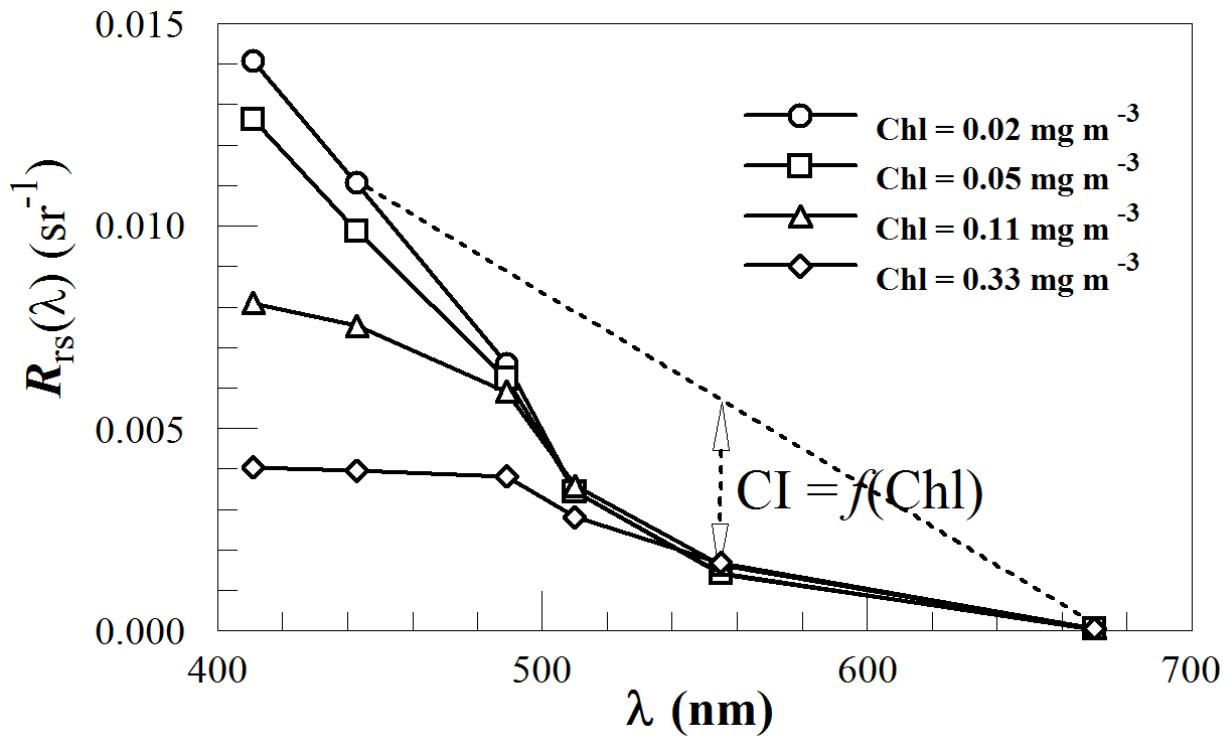
Chl centered band-ratio algorithms

Algorithm	Type	Result Equation(s)	Band Ratio (R), Coefficients (a)
Global processing (GPs)	power	$C_{13} = 10^{(a0+a1*R1)}$ $C_{23} = 10^{(a2+a3*R2)}$ $[C + P] = C_{13}; \text{ if } C_{13} \text{ and } C_{23} > 1.5 \mu\text{g L}^{-1} \text{ then } [C + P] = C_{23}$	$R1 = \log(Lwn443/Lwn550)$ $R2 = \log(Lwn520/Lwn550)$ $a = [0.053, 1.705, 0.522, 2.440]$
Clark three-band (C3b)	power	$[C + P] = 10^{(a0+a1*R)}$	$R = \log((Lwn443 + Lwn520)/Lwn550)$ $a = [0.745, -2.252]$
Aiken-C	hyperbolic + power	$C_{21} = \exp(a0 + a1*\ln(R))$ $C_{23} = (R + a2)/(a3 + a4*R)$ $C = C_{21}; \text{ if } C < 2.0 \mu\text{g L}^{-1} \text{ then } C = C_{23}$	$R = Lwn490/Lwn555$ $a = [0.464, -1.989, -5.29, 0.719, -4.23]$
Aiken-P	hyperbolic + power	$C_{21} = \exp(a0 + a1*\ln(R))$ $C_{24} = (R + a2)/(a3 + a4*R)$ $[C + P] = C_{22}; \text{ if } [C + P] < 2.0 \mu\text{g L}^{-1} \text{ then } [C + P] = C_{24}$	$R = Lwn490/Lwn555$ $a = [0.696, -2.085, -5.29, 0.592, -3.48]$
OCTS-C	power	$C = 10^{(a0+a1*R)}$	$R = \log((Lwn520 + Lwn565)/Lwn490)$ $a = [0.55006, 3.497]$
OCTS-P	multiple regression	$[C + P] = 10^{(a0+a1*R1+a2*R2)}$	$R1 = \log(Lwn443/Lwn520)$ $R2 = \log(Lwn490/Lwn520)$ $a = [0.19535, -2.079, -3.497]$
POLDER	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs443/Rrs565)$ $a = [0.438, -2.114, 0.916, -0.851]$
CalCOFI two-band linear	power	$C = 10^{(a0+a1*R)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.444, -2.431]$
CalCOFI two-band cubic	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs490/Rrs555)$ $a = [0.450, -2.860, 0.996, -0.3674]$
CalCOFI three-band	multiple regression	$C = \exp(a0 + a1*R1 + a2*R2)$	$R1 = \ln(Rrs490/Rrs555)$ $R2 = \ln(Rrs510/Rrs555)$ $a = [1.025, -1.622, 1.238]$
CalCOFI four-band	multiple regression	$C = \exp(a0 + a1*R1 + a2*R2)$	$R1 = \ln(Rrs443/Rrs555)$ $R2 = \ln(Rrs412/Rrs510)$ $a = [0.753, -2.583, 1.389]$
Morel-1	power	$C = 10^{(a0+a1*R)}$	$R = \log(Rrs443/Rrs555)$ $a = [0.2492, -1.768]$
Morel-2	power	$C = \exp(a0 + a1*R)$	$R = \ln(Rrs490/Rrs555)$ $a = [1.077835, -2.542605]$
Morel-3	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs443/Rrs555)$ $a = [0.20766, -1.82878, 0.75885, -0.73979]$
Morel-4	cubic	$C = 10^{(a0+a1*R+a2*R^2+a3*R^3)}$	$R = \log(Rrs490/Rrs555)$ $a = [1.03117, -2.40134, 0.3219897, -0.291066]$

(O'Reilly et al 1998⁵)



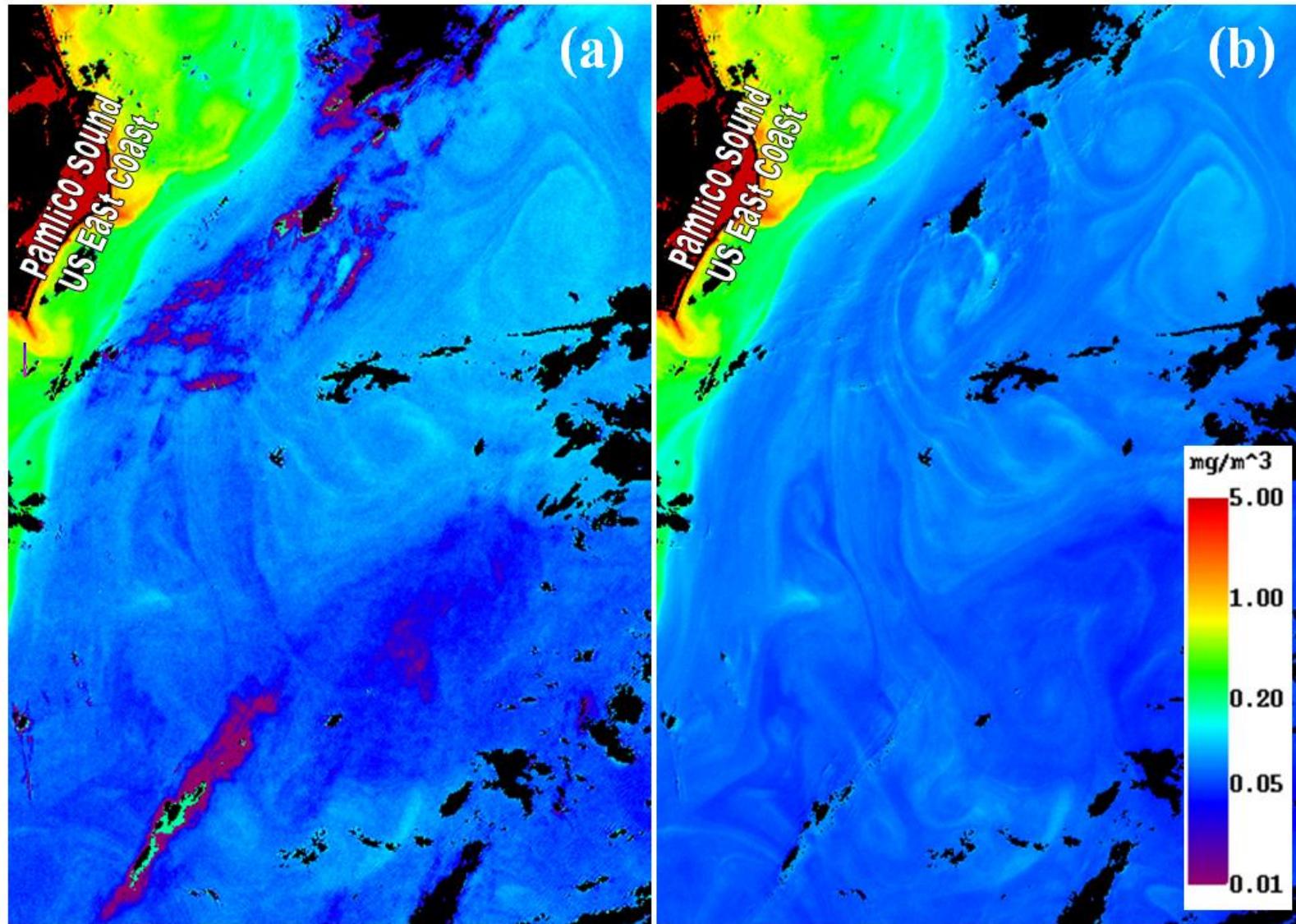
Chl based on band difference



$$CI = R_{rs}(555) - \left\{ R_{rs}(443) + \frac{555-443}{670-443} \times [R_{rs}(670) - R_{rs}(443)] \right\}$$

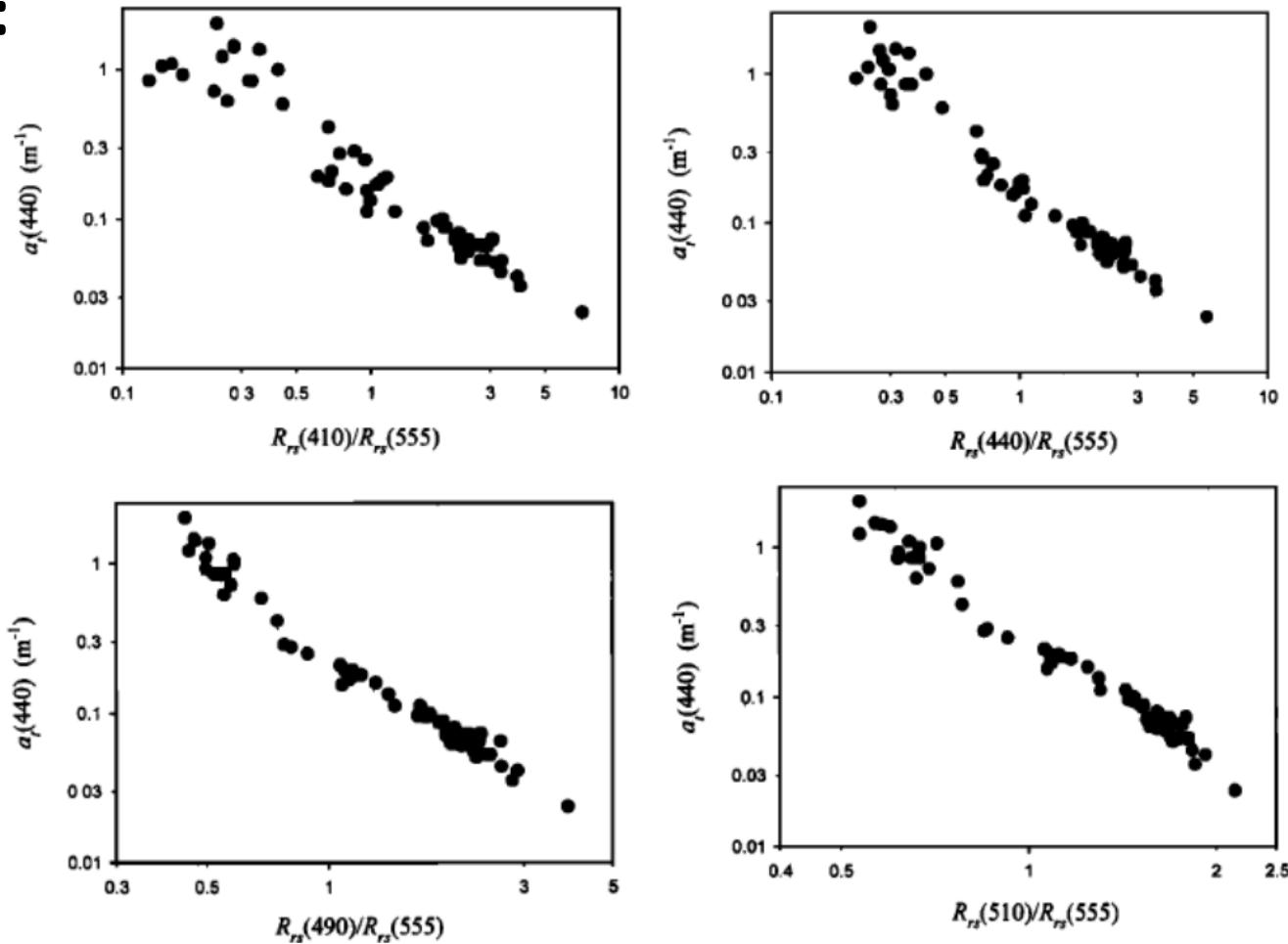
$$Chl = 10^{-0.49+191.66CI}; \quad CI \leq -0.0005 \text{ sr}^{-1}$$

(Hu et al 2012)



(Hu et al 2012)

Empirical:



$$a_t(440) = 10^{-0.674 - 0.531\rho_{25} - 0.745\rho_{25}^2 - 1.469\rho_{35} + 2.375\rho_{35}^2}, \quad (14)$$

$$a_\phi(440) = 10^{-0.919 + 1.037\rho_{25} - 0.407\rho_{25}^2 - 3.531\rho_{35} + 1.579\rho_{35}^2}, \quad (20)$$

(Lee et al 1998)

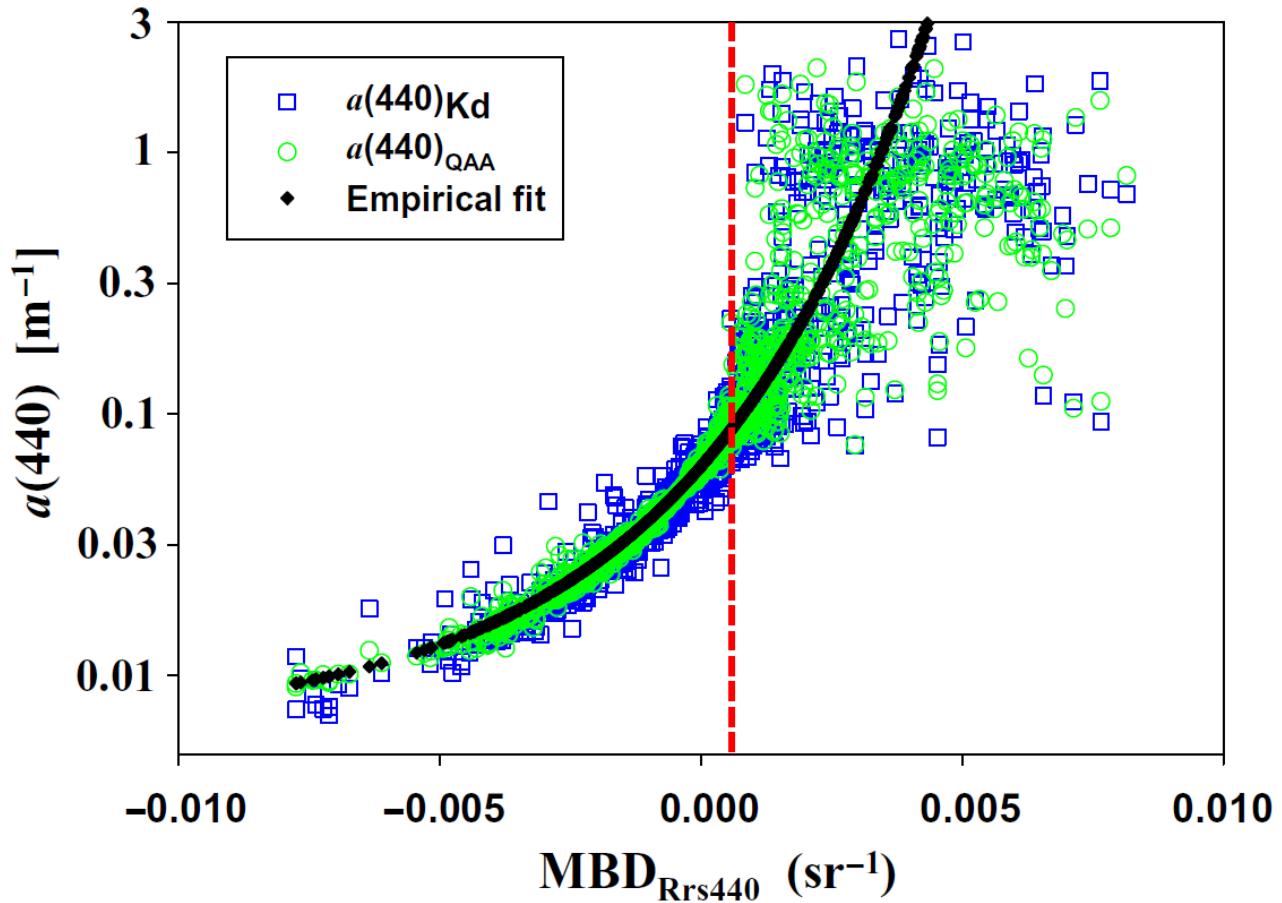


Fig.3. Relationship between $a(440)$ and $\text{MBD}_{\text{Rrs440}}$. The red vertical line indicates the location of $\text{MBD}_{\text{Rrs440}} = 0.0005 \text{ sr}^{-1}$.

$$\text{MBD}_{\text{Rrs440}} = R_{rs}(555) - \left[R_{rs}(443) + \frac{555 - 443}{670 - 443} (R_{rs}(670) - R_{rs}(443)) \right] \quad (\text{Lee et al., 2023})$$

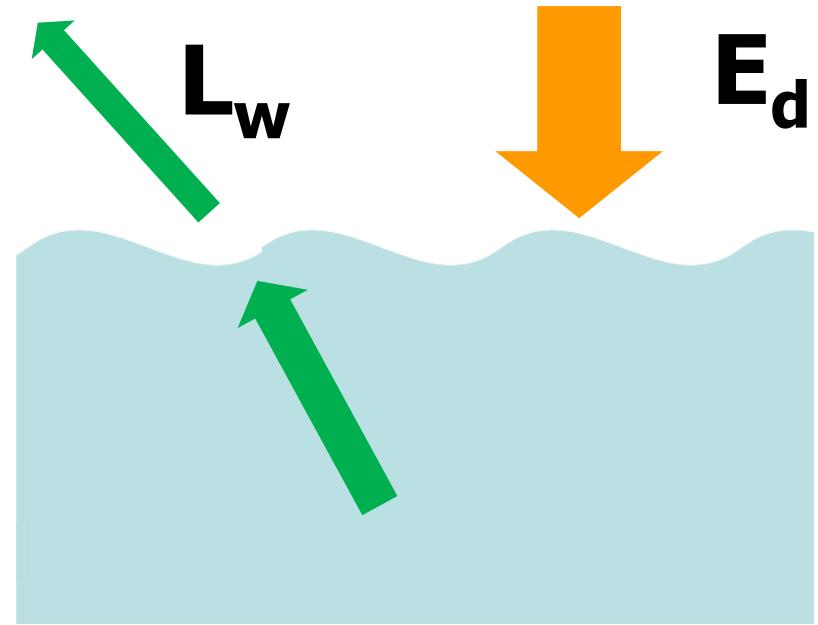
$$R_{rs}^{Sat}(\lambda) = R_{rs}(\lambda) + \delta(\lambda) = R_{rs}(\lambda) + y\lambda + x$$

$$MBD(R_{rs}^{Sat}) = MBD_{Rrs}$$

Physics-based algorithms (mechanistic)

Remote-sensing reflectance (sr^{-1}):

$$R_{rs}(\lambda) = \frac{L_w(\lambda, 0^+)}{E_d(\lambda, 0^+)}$$



How is R_{rs} related to water's optical (biogeochemical) properties?

Radiative Transfer Equation (inelastic scattering omitted):

$$\frac{d L(\Omega)}{d l} = -c L(\Omega) + \int L(\Omega') \beta(\Omega', \Omega) d\omega$$

$$r_{rs}(\lambda, \Omega) = \frac{L_u(0^-, \Omega)}{E_d(0^-)}$$

Exact solution (no inelastic scattering):

$$r_{rs}(\lambda, \Omega) \equiv \frac{D_d(\lambda, \theta_S)}{c(\lambda) + k_L(\lambda, \Omega) - f_L(\lambda, \Omega)b_f(\lambda)} \frac{\int_0^{2\pi} \int_0^{\pi/2} \beta(\Omega', \Omega) L(\lambda, \Omega') \sin(\theta') d\theta' d\phi'}{E_{od}(0^-, \lambda, \theta_S)} \quad (\text{Zaneveld 1995})$$

$$r_{rs} \cong \frac{1}{\bar{\mu}_d} \frac{\beta(\psi)}{b_b} / \left[\frac{a}{b_b} \left(1 - \cos(\theta_v) \Psi_{K_{Lu}} \bar{\mu}_{\infty}^{-1} \right) + f_L \left(1 - \tilde{b}_b^{-1} \right) + \tilde{b}_b^{-1} \right], \quad (12)$$

(Twardowski and Tonizzo, 2018)

Approximations:

Albert and Mobley (2003) :

$$r_{rs}(\lambda, \Omega) = q(\Omega, w) \sum_{i=1}^4 p_i \left(\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \right)^i$$

Park and Ruddick (2005)

$$r_{rs}(\lambda, \Omega) = \sum_{i=1}^4 g_i(\Omega, v_b) \left(\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \right)^i$$

Van Der Woerd and Pasterkamp (2008)

$$\ln[r_{rs}(\lambda, \Omega)] = \sum_{i=1}^4 \sum_{j=1}^4 P_{ij}(\Omega) [\ln(a(\lambda))]^i [\ln(b(\lambda))]^j$$

Morel et al (1993, 1996, 2002):

$$r_{rs}(\lambda, \Omega) = g(\lambda, Chl, \Omega) \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

Gordon et al (1988):

$$r_{rs}(\lambda, \pi) = \sum_{i=1}^2 g_i \left(\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \right)^i;$$

$$g_1 = 0.0949, g_2 = 0.0794$$

Lee et al (2004)

$$r_{rs}(\lambda, \Omega) = g_w(\Omega) \frac{b_{bw}(\lambda)}{a(\lambda) + b_b(\lambda)} + g_p(\lambda, \Omega) \frac{b_{bp}(\lambda)}{a(\lambda) + b_b(\lambda)}$$

$r_{rs} \rightarrow R_{rs}$?

$$R_{rs} = \frac{L_w}{E_d(0^+)}$$

$$E_d(0^-) = t_E E_d(0^+) + \gamma E_u(0^-)$$

$$L_w = \frac{t_L}{n_w^2} L_u(0^-)$$

(for nadir viewing)

$$R_{rs} = \frac{t_E t_L}{n_w^2} \frac{r_{rs}}{1 - \gamma R} = \frac{0.52 r_{rs}}{1 - 1.7 r_{rs}}$$

Solve Rrs for IOPs or in-water constituents?

Two basic strategies:

1. Bottom-up strategy (BUS):

Assume we know the spectral shapes of the optically active components

2. Top-down strategy (TDS):

Only need the spectral shape information when it is necessary

What are we facing in RS algorithms?

$$R_{rs}(\lambda) = F(a(\lambda), b_b(\lambda))$$



$$R_{rs}(\lambda) = F(a_w(\lambda), a_{ph}(\lambda), a_{dg}(\lambda), b_{bw}(\lambda), b_{bp}(\lambda))$$



$$\begin{cases} R_{rs}(\lambda_1) = F(a_w(\lambda_1), a_{ph}(\lambda_1), a_{dg}(\lambda_1), b_{bw}(\lambda_1), b_{bp}(\lambda_1)) \\ R_{rs}(\lambda_2) = F(a_w(\lambda_2), a_{ph}(\lambda_2), a_{dg}(\lambda_2), b_{bw}(\lambda_2), b_{bp}(\lambda_2)) \\ \vdots \\ R_{rs}(\lambda_n) = F(a_w(\lambda_n), a_{ph}(\lambda_n), a_{dg}(\lambda_n), b_{bw}(\lambda_n), b_{bp}(\lambda_n)) \end{cases}$$

of unknowns > # of equations.

An ill formulated math problem!

Have to increase # of equations or decrease # of unknowns.

1. Bottom-up strategy (BUS):

Build-up an R_{rs} spectrum block-by-block:

$$a(\lambda) = a_w(\lambda) + \sum a_{xi}(\lambda) \quad b_b(\lambda) = b_{bw}(\lambda) + \sum b_{bxi}(\lambda)$$

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_d(\lambda) + a_g(\lambda)$$

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{dg}(\lambda)$$

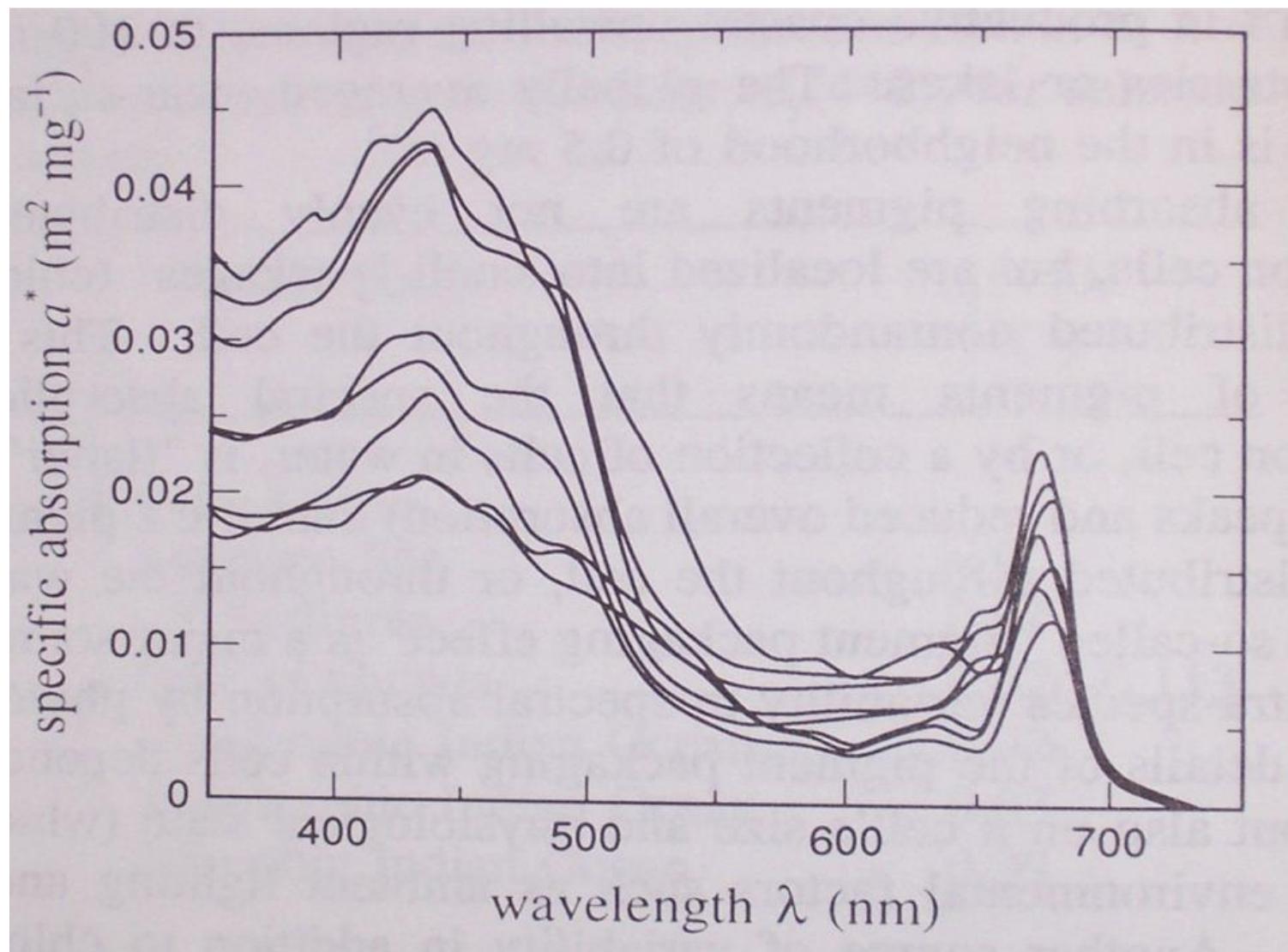
$$a(\lambda) = a_w(\lambda) + M_1 \langle a_{ph}(\lambda) \rangle + M_2 \langle a_{dg}(\lambda) \rangle$$

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda)$$

$$b_b(\lambda) = b_{bw}(\lambda) + M_3 \langle b_{bp}(\lambda) \rangle$$



Bio-optical models (forward model)



Modeling a_{ph} spectrum

Example of **one** parameter hyperspectral $a_{ph}(\lambda)$ model:

Bricaud et al (1995):

$$a_{ph}(\lambda) = A_{ph}(\lambda) Chl^{1-B_{ph}(\lambda)}$$

Lee (1994); Lee et al (1998):

$$a_{ph}(\lambda) = (a_0(\lambda) + a_1(\lambda) \ln(P)) P$$

$$P = a_{ph}(440)$$

Table 2. Parameters for the Empirical $a_{ph}(\lambda)$ Simulation by Eq. (12)^a

Table 2. Spectral Values of the Constants Obtained When Fitting the Variations of $a_{ph}^*(\lambda)$ Versus the (chl a + div a) Concentration (Chl) to Power Laws of the Form $a_{ph}^*(\lambda) = A(\lambda) (\text{Chl})^{-B(\lambda)}$ and Determination Coefficients on the Log-Transformed Data r^2

λ , nm	A	B	r^2	λ , nm	A	B	Wavelength	$a_0(\lambda)$	$a_1(\lambda)$
400	0.0263	0.282	0.702	402	0.0271	0.281	390	0.5813	0.0235
404	0.0280	0.282	0.706	406	0.0290	0.281	400	0.6843	0.0205
408	0.0301	0.282	0.710	410	0.0313	0.283	410	0.7782	0.0129
412	0.0323	0.286	0.718	414	0.0333	0.291	420	0.8637	0.006
416	0.0342	0.293	0.725	418	0.0349	0.296	430	0.9603	0.002
420	0.0356	0.299	0.733	422	0.0359	0.306	440	1.0	0
424	0.0362	0.313	0.746	426	0.0369	0.316	450	0.9634	0.006
428	0.0376	0.317	0.749	430	0.0386	0.314	460	0.9311	0.0109
432	0.0391	0.318	0.750	434	0.0395	0.324	470	0.8697	0.0157
436	0.0399	0.328	0.757	438	0.0401	0.332	480	0.789	0.0152
440	0.0403	0.332	0.762	442	0.0398	0.339	490	0.7558	0.0256
444	0.0390	0.348	0.774	446	0.0383	0.355	500	0.7333	0.0559
448	0.0375	0.360	0.783	450	0.0371	0.359	510	0.6911	0.0865
452	0.0365	0.362	0.783	454	0.0358	0.366	520	0.6327	0.0981
456	0.0354	0.367	0.789	458	0.0351	0.368	530	0.5681	0.0969
460	0.0350	0.365	0.789	462	0.0347	0.366	540	0.5046	0.09
464	0.0343	0.368	0.792	466	0.0339	0.369	550	0.4262	0.0781
468	0.0335	0.369	0.793	470	0.0332	0.368	560	0.3433	0.0659
472	0.0325	0.371	0.792	474	0.0318	0.375	570	0.295	0.06
476	0.0312	0.378	0.793	478	0.0306	0.379	580	0.2784	0.0581
480	0.0301	0.377	0.791	482	0.0296	0.377	590	0.2585	0.0574
484	0.0290	0.376	0.788	486	0.0285	0.373	600	0.2385	0.0563
488	0.0279	0.369	0.783	490	0.0274	0.361	610	0.2185	0.0552
492	0.0267	0.356	0.774	494	0.0258	0.349	620	0.1985	0.0541
496	0.0249	0.341	0.763	498	0.0240	0.332	630	0.1785	0.0530
500	0.0230	0.321	0.747	502	0.0220	0.311	640	0.1585	0.0519
504	0.0209	0.300	0.722	506	0.0199	0.288	650	0.1385	0.0508
508	0.0189	0.275	0.686	510	0.0180	0.260	660	0.1185	0.0497
512	0.0171	0.249	0.641	514	0.0163	0.237	670	0.0985	0.0486
516	0.0156	0.224	0.578	518	0.0149	0.211	680	0.0785	0.0475
520	0.0143	0.196	0.498	522	0.0137	0.184	690	0.0585	0.0464
524	0.0131	0.173	0.417	526	0.0126	0.162	700	0.0385	0.0453
528	0.0121	0.151	0.332	530	0.0117	0.139	710	0.0185	0.0442
532	0.0113	0.129	0.248	534	0.0108	0.119	720	0.0085	0.0431
536	0.0104	0.109	0.176	538	0.0100	0.100	730	0.0085	0.0420
540	0.0097	0.090	0.116	542	0.0093	0.081	740	0.0085	0.0409

Example of a two-variable model: (Ciotti et al 2002)

$$a_\phi(\lambda) = a_\phi(505) \left[[S_f \cdot \bar{a}_{<pico>}(\lambda)] + [(1 - S_f) \cdot \bar{a}_{<micro>}(\lambda)] \right]$$

Table 3. Basis vectors representing the normalized absorption for the smallest ($\bar{a}_{(pico)}(\lambda)$, *Prochlorococcus*) and biggest ($\bar{a}_{(micro)}(\lambda)$, average microplankton) cell sizes in our data set. Wavelength (λ) in nm. Basis vectors for $a_{ph}^*(\lambda)$ can be constructed by setting $\bar{a}_{(pico)}(676)$ to 0.023 m² mg⁻¹, $\bar{a}_{(micro)}(674)$ to 0.0086 m² mg⁻¹, and scaling for the other wavelengths accordingly.

λ	Pico	Micro												
400	1.682	1.574												
402	1.734	1.584	462	2.526	1.623	522	0.544	1.013	582	0.111	0.459	642	0.191	0.528
404	1.800	1.600	464	2.455	1.616	524	0.522	0.992	584	0.072	0.452	644	0.174	0.526
406	1.890	1.617	466	2.402	1.606	526	0.486	0.977	586	0.073	0.452	646	0.197	0.528
408	1.978	1.633	468	2.331	1.592	528	0.448	0.959	588	0.073	0.449	648	0.176	0.538
410	2.057	1.654	470	2.281	1.568	530	0.391	0.944	590	0.099	0.443	650	0.168	0.549
412	2.162	1.669	472	2.205	1.542	532	0.375	0.927	592	0.070	0.433	652	0.160	0.574
414	2.269	1.674	474	2.136	1.509	534	0.336	0.909	594	0.095	0.424	654	0.217	0.605
416	2.327	1.684	476	2.063	1.481	536	0.305	0.888	596	0.085	0.416	656	0.244	0.655
418	2.398	1.697	478	2.049	1.459	538	0.292	0.868	598	0.090	0.406	658	0.286	0.720
420	2.457	1.708	480	1.998	1.437	540	0.288	0.847	600	0.086	0.401	660	0.381	0.798
422	2.533	1.710	482	1.930	1.415	542	0.261	0.826	602	0.068	0.400	662	0.437	0.889
424	2.614	1.716	484	1.918	1.399	544	0.245	0.806	604	0.078	0.403	664	0.520	0.979
426	2.663	1.737	486	1.897	1.387	546	0.214	0.785	606	0.069	0.408	666	0.660	1.068
428	2.749	1.763	488	1.867	1.377	548	0.194	0.764	608	0.090	0.416	668	0.716	1.147
430	2.804	1.793	490	1.812	1.367	550	0.187	0.737	610	0.096	0.429	670	0.824	1.207
432	2.840	1.812	492	1.776	1.349	552	0.138	0.711	612	0.094	0.443	672	0.846	1.243
434	2.915	1.827	494	1.701	1.338	554	0.137	0.682	614	0.084	0.458	674	0.816	1.249
436	2.947	1.830	496	1.648	1.319	556	0.111	0.653	616	0.105	0.473	676	0.891	1.227
438	2.978	1.834	498	1.522	1.301	558	0.094	0.626	618	0.128	0.487	678	0.869	1.174
440	3.014	1.824	500	1.439	1.271	560	0.095	0.604	620	0.119	0.495	680	0.812	1.096
442	3.032	1.800	502	1.373	1.242	562	0.070	0.580	622	0.126	0.499	682	0.741	1.004
444	3.011	1.771	504	1.270	1.222	564	0.053	0.555	624	0.138	0.504	684	0.605	0.893

Multiple-parameters model:

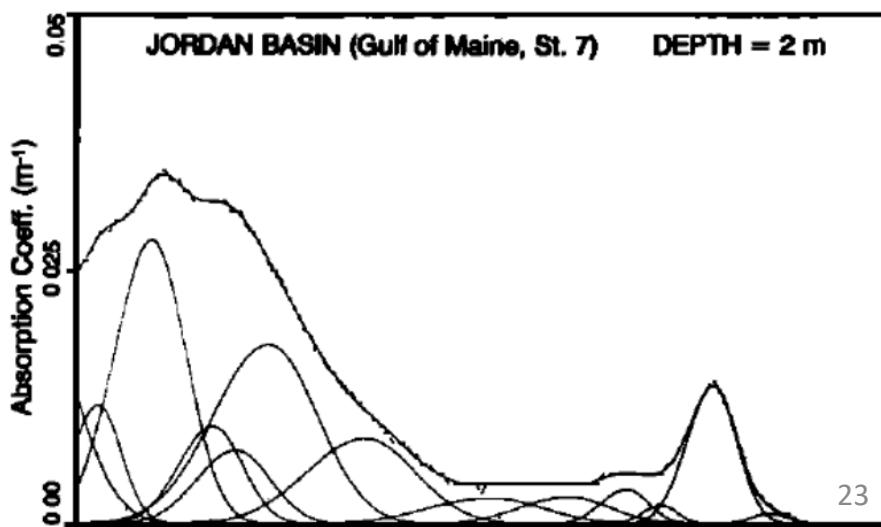
$$a_{ph}(\lambda) = \sum_{j=1}^l C_j a_j^*(\lambda_{mj}) \exp \left[\frac{(\lambda - \lambda_{mj})^2}{2\sigma_j^2} \right] \quad (7)$$

TABLE 2. Input Values and Mean Characteristics of Gaussian Bands Reflecting Absorption by Chlorophylls and Carotenoids

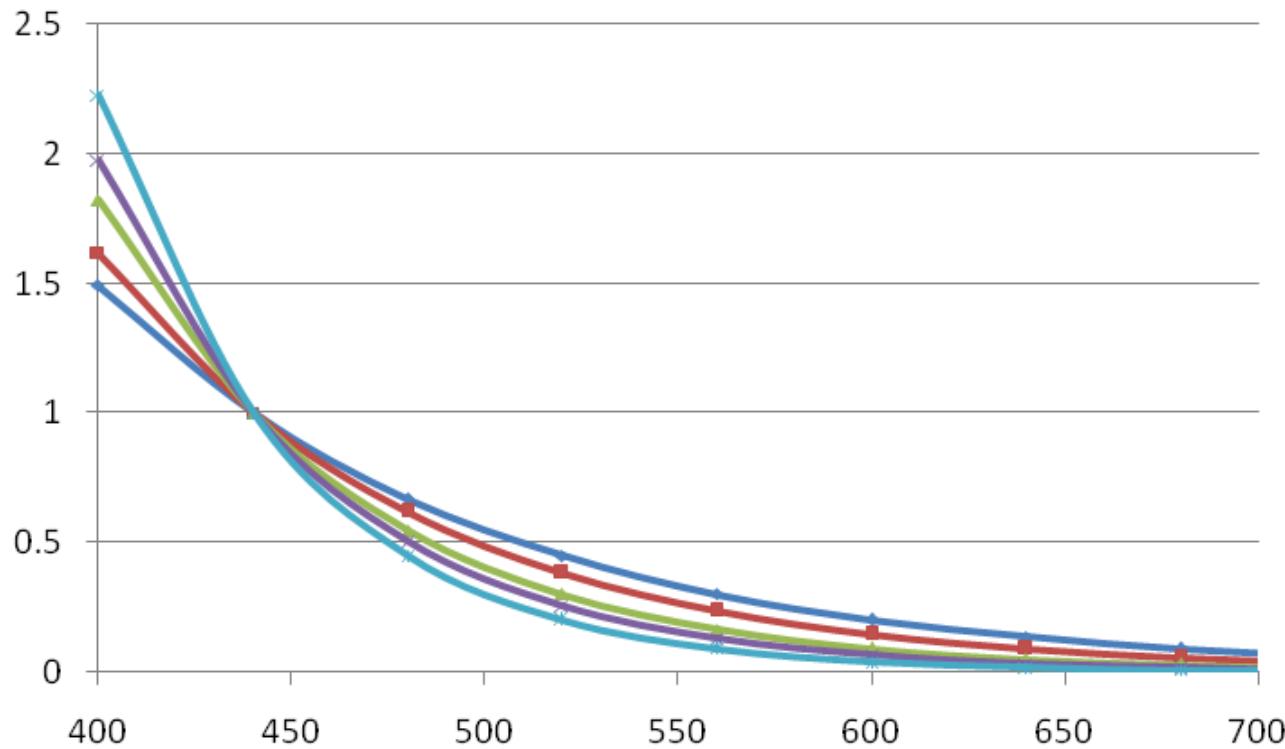
Characteristic	Gaussian Band Number and Associated Pigment Species												
	1 chl a	2 chl a	3 chl a	4 chl c	5 chl b	6 carot.	7 carot.	8 chl c	9 chl a	10 chl c	11 chl b	12 chl a	13 chl a
Input parameters													
Half width, nm	53.8	21.3	32.1	27.2	45.0	45.4	45.9	46.3	35.0	28.9	24.4	21.6	33.5
Center, nm	384	413	435	461	464	490	532	583	623	644	655	676	700
Output parameters													
Half width, nm	43.2	22.7	34.5	29.3	36.0	46.8	49.6	46.8	38.0	24.9	25.4	24.7	29.0
Center, nm	381.5	410.8	433.5	459.2	466.6	487.8	532.0	585.6	620.6	640.7	652.9	675.6	699.8
Specific absorption coefficient, m^2 (mg pigment) $^{-1}$	0.042	0.019	0.047	0.110	0.115	0.035	0.019	0.044	0.005	0.044	0.029	0.021	0.002

Specific absorption coefficients of each pigment are ratios of Gaussian band absorptions (in reciprocal meters) to high-performance liquid chromatography concentrations (in milligrams per cubic meter) of that pigment. Chl, chlorophyll; Carot., carotenoid.

(Hoepffner and Sathyendranath, 1993)



Absorption components: a_{dg} spectrum shapes



$$\langle a_{dg}(\lambda) \rangle = e^{-S(\lambda - 440)}$$

S: 0.01 – 0.02 nm⁻¹

(Bricaud et al 1981)

$$\left\langle b_{bp}(\lambda)\right\rangle = \left(\frac{440}{\lambda}\right)^{\eta}$$

$$R_{rs}(\lambda) = G \frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}$$



$$R_{rs}(\lambda) = G \frac{b_{bw}(\lambda) + M_3 \langle b_{bp}(\lambda) \rangle}{a_w(\lambda) + M_1 \langle a_{ph}(\lambda) \rangle + M_2 \langle a_{dg}(\lambda) \rangle + b_{bw}(\lambda) + M_3 \langle b_{bp}(\lambda) \rangle}$$

3-variable model to describe an Rrs spectrum

(Sathyendranath et al 1989)

M₁₋₃ are wavelength-independent variables.

Then they could be derived by comparing the modeled Rrs spectrum with the measured Rrs spectrum.

Spectral ranges used for solutions (e.g. examples of BUS):

The **blue-green** domain: e.g., Hoge and Lyon (1996), Carder et al (1999)

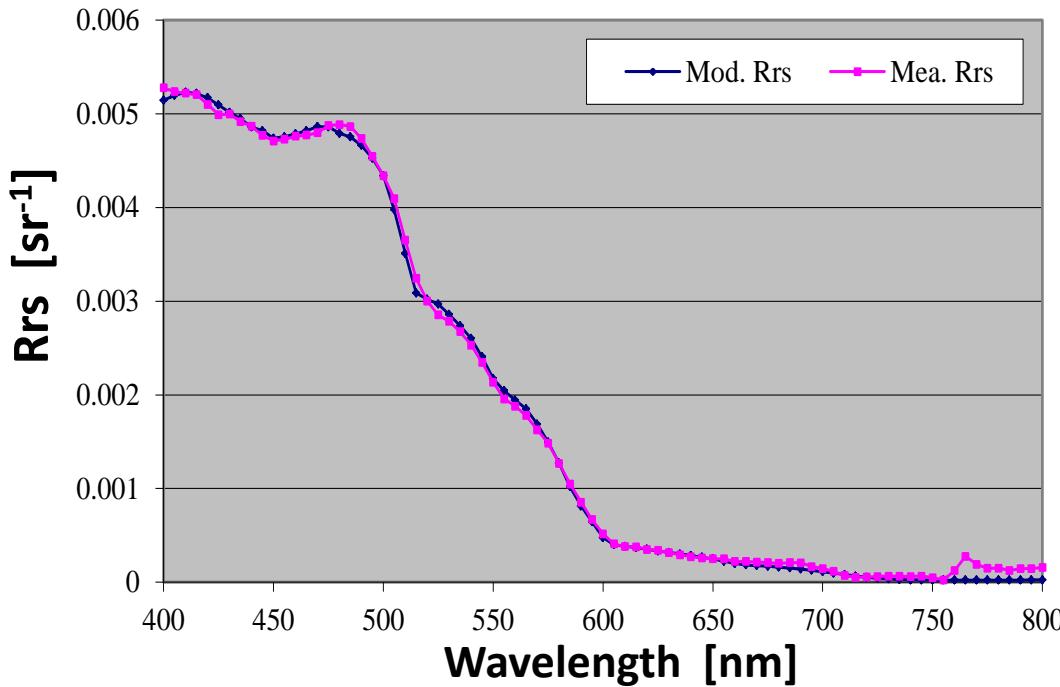
The **red-infrared** domain: e.g., Binding et al (2012)

The **entire spectrum (spectral optimization)**: e.g., Bukata et al (1995), Lee et al (1994,1996,1999), Maritorena et al (2002), Boss and Roesler (2006), Brando et al (2012), Werdell et al (2013)

Look-Up-Tables (LUT): e.g., Carder et al (1991); Mobley et al (2005)

Spectral Optimization

Matching between measured and modeled R_{rs}



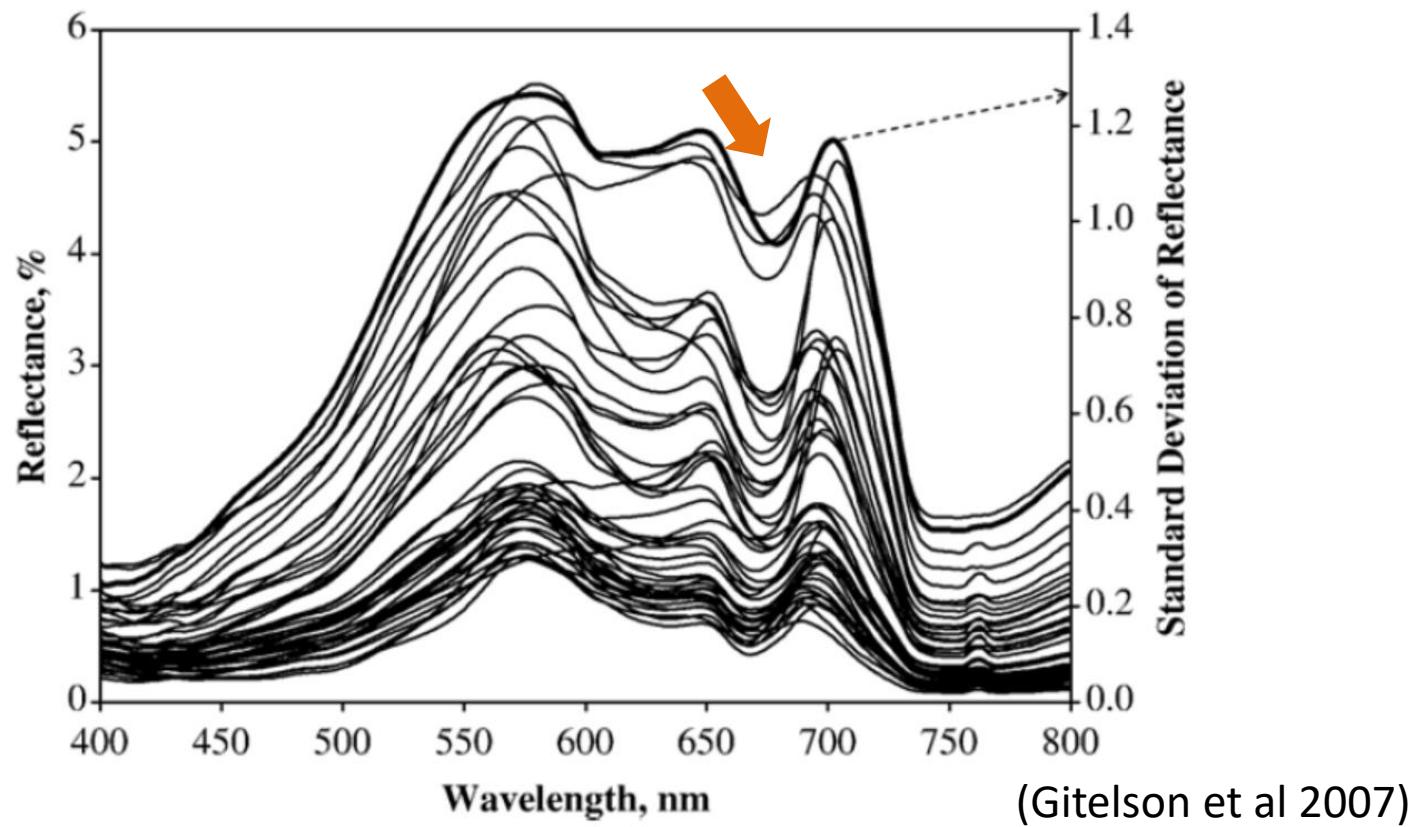
Quantitative measure of the closure (**error function**):

$$\delta_{R_{rs}} = \frac{\sqrt{\sum_{\lambda_1}^{\lambda_2} (\tilde{R}_{rs}(\lambda) - R_{rs}(\lambda))^2}}{\sum_{\lambda_1}^{\lambda_2} R_{rs}(\lambda)} = \sqrt{n} \frac{\sqrt{\sum_{\lambda_1}^{\lambda_2} (\tilde{R}_{rs}(\lambda) - R_{rs}(\lambda))^2}}{\sum_{\lambda_1}^{\lambda_2} R_{rs}(\lambda)}$$

Logic (assumption) behind SOA:

A unique set of bio-optical properties for each Rrs spectrum.

Algorithms using information in the red-infrared bands



Two bands

$$Chl = f \left(\frac{Rrs(75x)}{Rrs(67x)} \right)$$

Three bands

$$Chl = f \left(\frac{Rrs(75x)}{Rrs(67x)} - \frac{Rrs(75x)}{Rrs(70x)} \right)$$

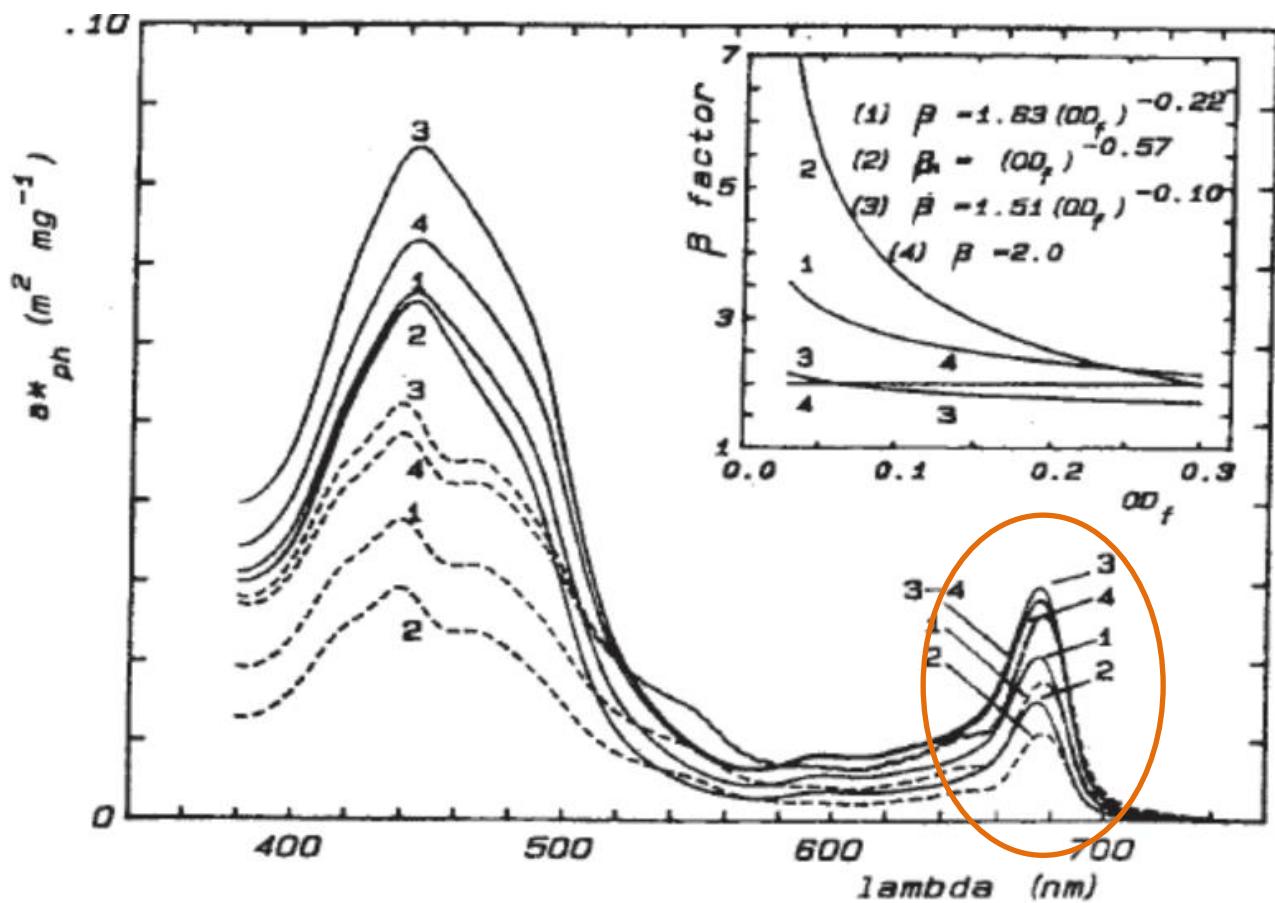
$$R_{rs}(\lambda) = G \frac{b_{bw}(\lambda) + M_3 \langle b_{bp}(\lambda) \rangle}{a_w(\lambda) + M_1 \langle a_{ph}(\lambda) \rangle + M_2 \langle a_{dg}(\lambda) \rangle + b_{bw}(\lambda) + M_3 \langle b_{bp}(\lambda) \rangle}$$

$$R_{rs}(\lambda) \approx G \frac{M_3 \langle b_{bp}(\lambda) \rangle}{a_w(\lambda) + M_1 \langle a_{ph}(\lambda) \rangle}$$

$$\frac{R_{rs}(\lambda_{red1})}{R_{rs}(\lambda_{red2})} = \frac{\langle b_{bp}(\lambda_{red1}) \rangle}{\langle b_{bp}(\lambda_{red2}) \rangle} \frac{a_w(\lambda_{red2}) + M_1 \langle a_{ph}(\lambda_{red2}) \rangle}{a_w(\lambda_{red1}) + M_1 \langle a_{ph}(\lambda_{red1}) \rangle}$$

Proper contrast of Rrs at λ_1 and λ_2 then leads to M_1 .

a_{ph}



2. Top-down strategy (TDS):

$$R_{rs} = G \frac{b_b}{a + b_b}$$

$$R_{rs} \rightarrow b_b \& a \rightarrow a_x$$



Clarity (Secchi depth, light depth, SPM, etc.)

Remote sensing measures the *total* effect:

Water clarity (or turbidity) is also a measure of total effect.

Examples of TDS:

Loisel & Stramski (2000), QAA (Lee et al, 2002); Smyth et al (2006);
Doran et al (2007).

The Quasi-Analytical Algorithm (QAA)

Forward modeling:

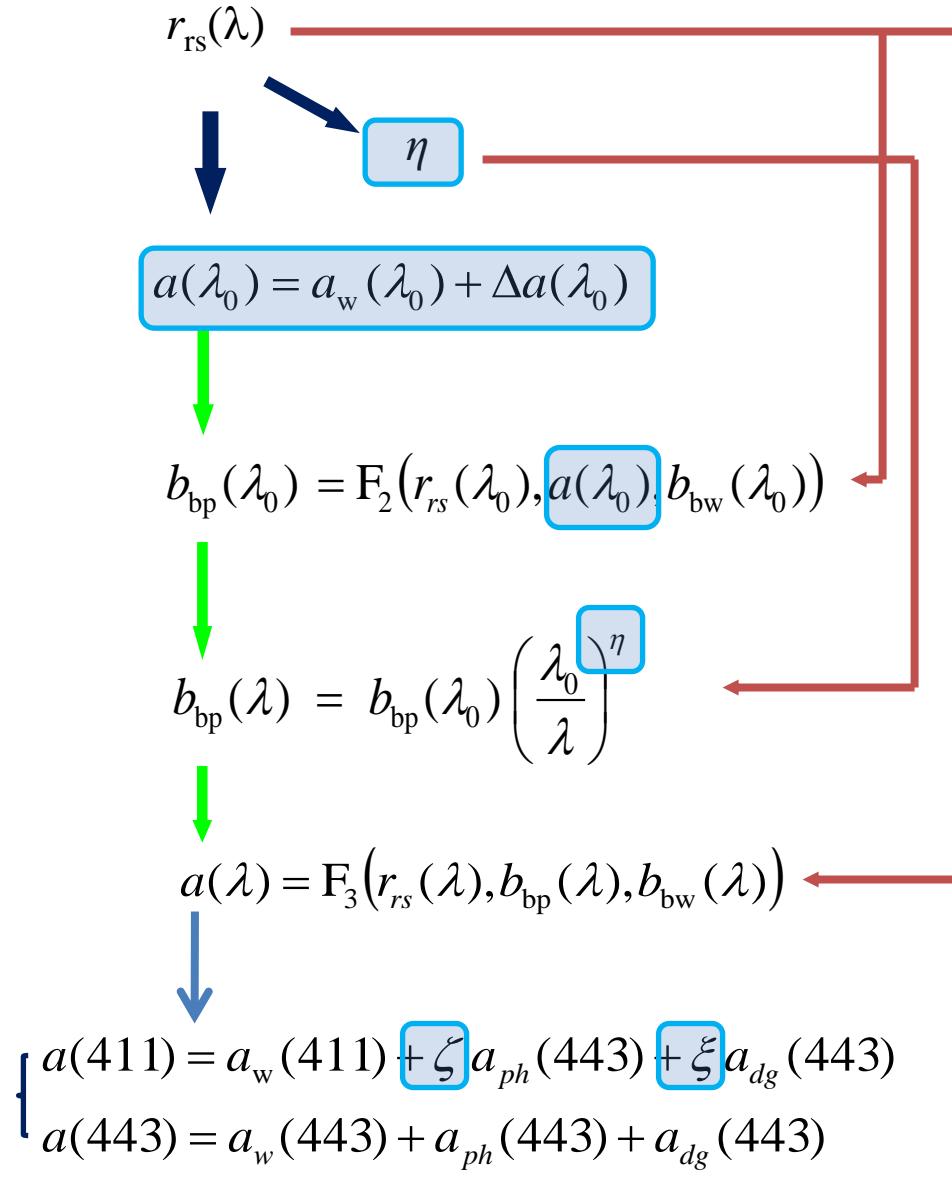
$$(a, b_b, \text{etc}) \longrightarrow R_{rs}$$

$$R_{rs} \approx 0.05 \frac{b_b}{a + b_b}$$

QAA:

$$(a, b_b) \longleftarrow R_{rs}$$

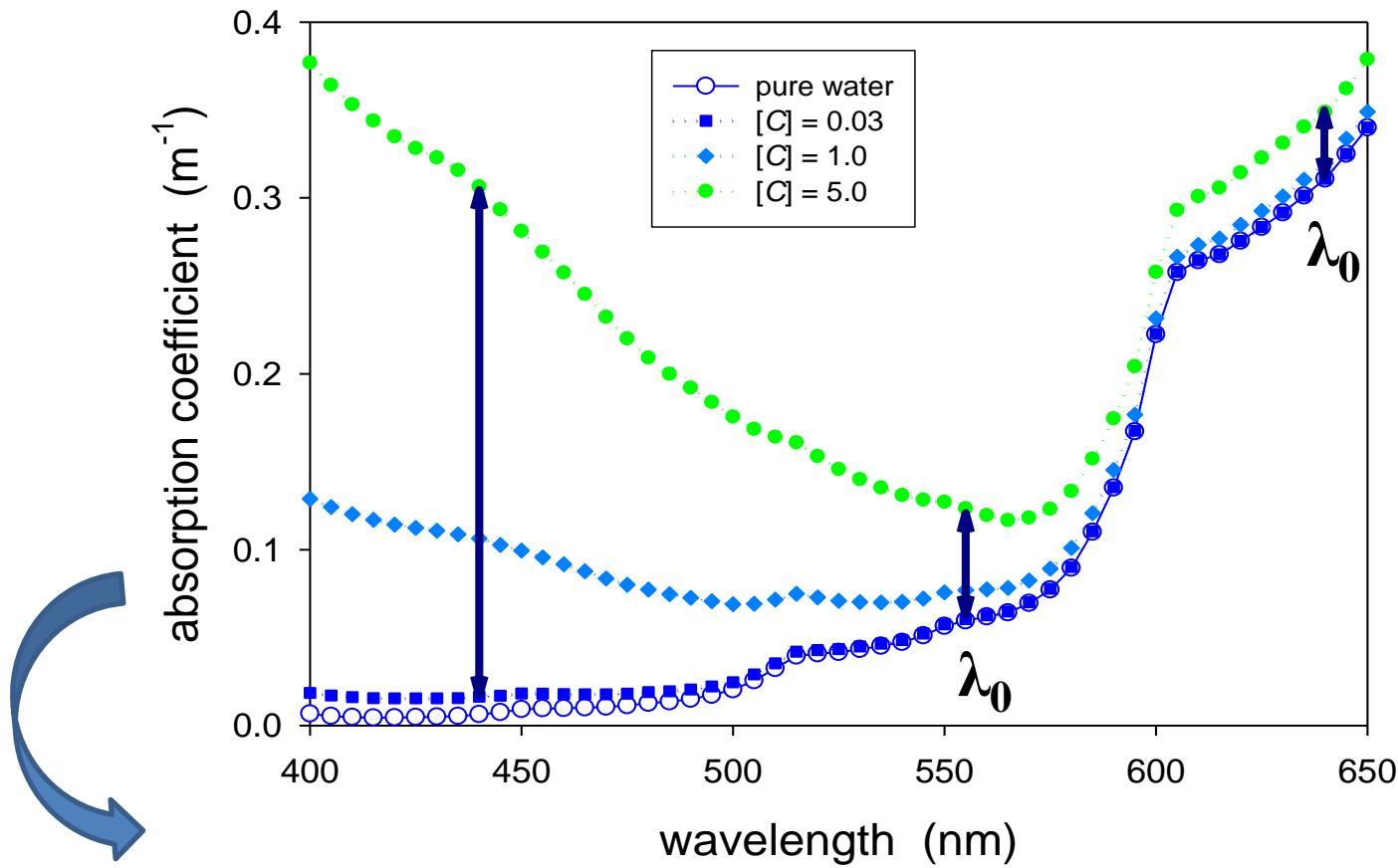
The data flow of QAA:



$$\zeta = \frac{a_{ph}(411)}{a_{ph}(443)}$$

$$\xi = \frac{a_{dg}(411)}{a_{dg}(443)}$$

Logic behind QAA (and its updated versions):



For a reference wavelength, λ_0 , variation of $a(\lambda_0)$ is limited.

Known $a(\lambda_0)$, enables calculation of $b_b(\lambda_0)$ from $R_{rs}(\lambda_0)$; propagate $b_b(\lambda_0)$ to $b_b(\lambda)$, then enables calculation of $a(\lambda)$ from $R_{rs}(\lambda)$.

No need of spectral model of $a_x(\lambda)$ in this process.

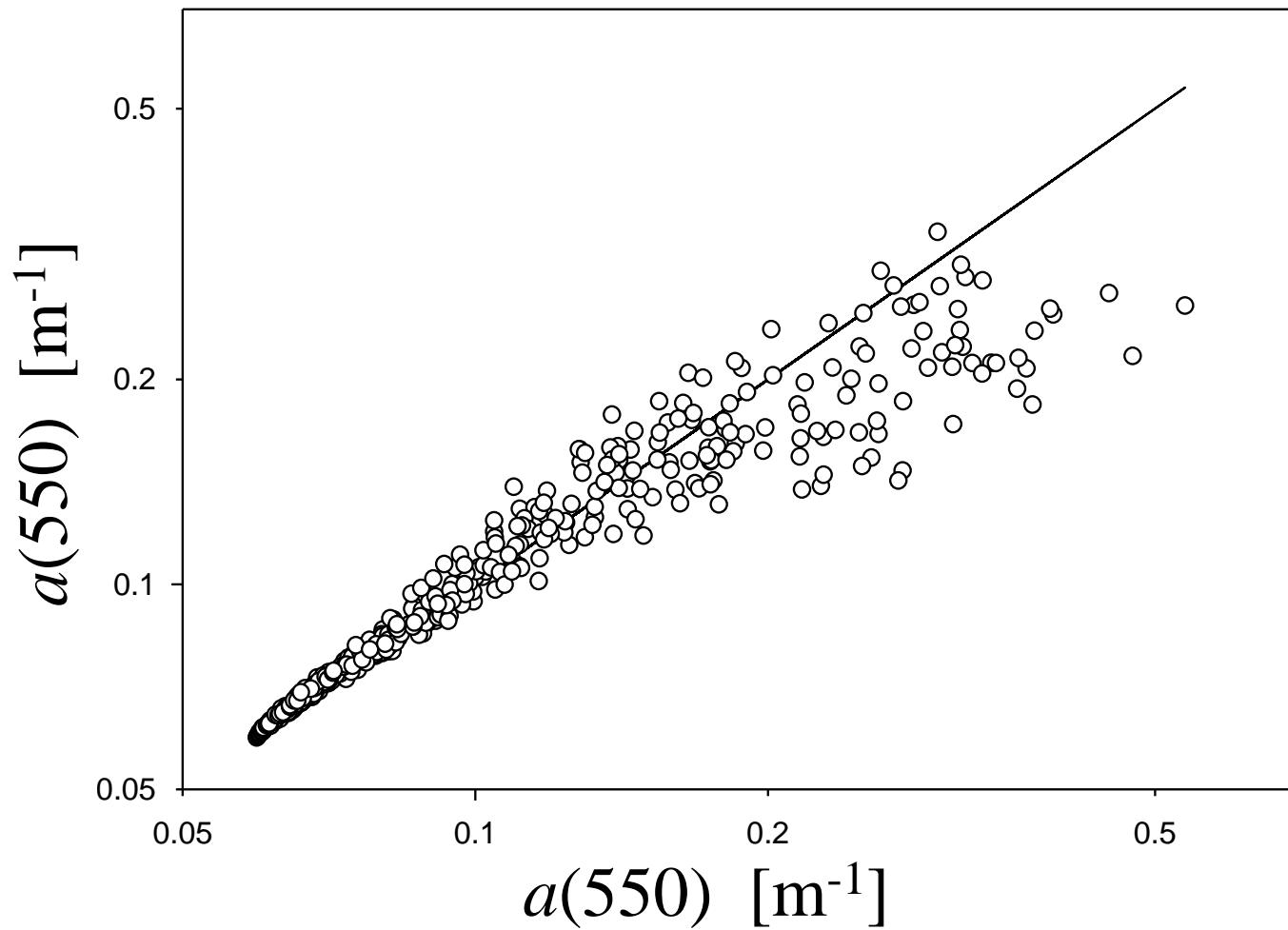
When 550 nm as the reference wavelength (λ_0)

$$a(550) = a_w(550) + 10^{-1.146 - 1.366\chi - 0.469\chi^2}$$

$$\chi = \log \left(\frac{r_{rs}(443) + r_{rs}(490)}{r_{rs}(\lambda_0) + 5 \frac{r_{rs}(667)}{r_{rs}(490)} r_{rs}(667)} \right)$$

$$a_w(550) = 0.0565$$

Empirical!



Invert Rrs:

$$R_{rs} \xrightarrow{\hspace{1cm}} r_{rs} \xrightarrow{\hspace{1cm}} \{a \& b_b\}$$

$$r_{rs}(\lambda) = R_{rs}(\lambda)/(0.52 + 1.7 R_{rs}(\lambda))$$

$$r_{rs} = g_0 \left(\frac{b_b}{a + b_b} \right) + g_1 \left(\frac{b_b}{a + b_b} \right)^2$$

$g_0=0.089, g_1=0.125$

$$u(\lambda) = \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} = \frac{-g_0 + \sqrt{(g_0)^2 + 4 g_1 * r_{rs}(\lambda)}}{2g_1}$$

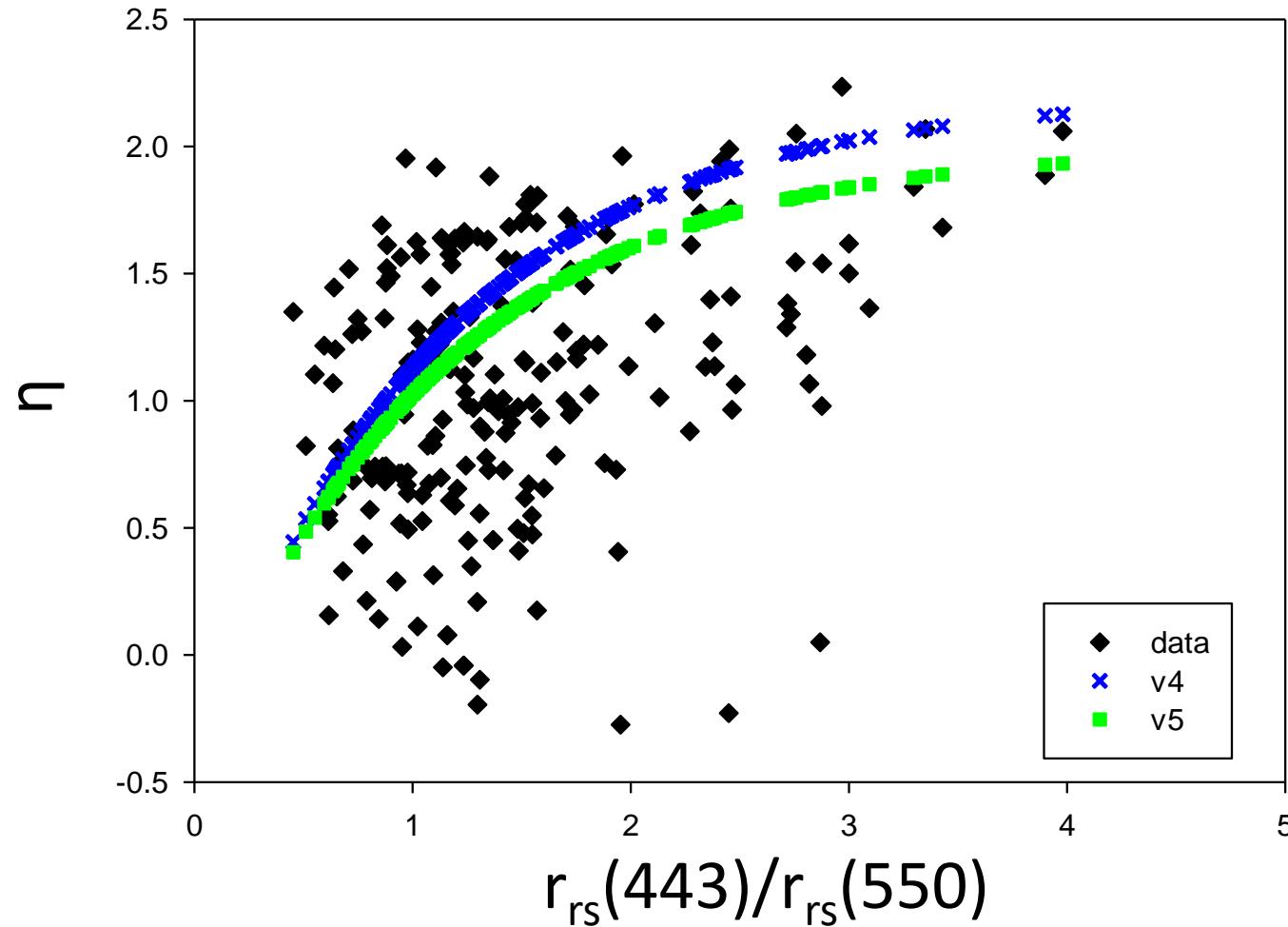
$$a(550) = a_w(550) + 10^{-1.146 - 1.366\chi - 0.469\chi^2}$$

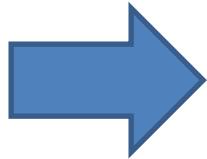
→ $b_{bp}(550) = \frac{u(550) a(550)}{1 - u(550)} - b_{bw}(550)$

$$b_{bp}(\lambda) = b_{bp}(550) \left(\frac{550}{\lambda} \right)^{\eta}$$

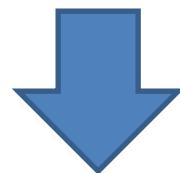
Empirical:

$$\eta = 2.0 \left(1 - 1.2 \exp \left(-0.9 \frac{r_{rs}(443)}{r_{rs}(550)} \right) \right)$$





$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda)$$



$$a(\lambda) = \frac{(1 - u(\lambda)) b_b(\lambda)}{u(\lambda)}$$

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{dg}(\lambda)$$



$$\begin{cases} a(410) = a_w(410) + a_{ph}(410) + a_{dg}(410), \\ a(440) = a_w(440) + a_{ph}(440) + a_{dg}(440). \end{cases}$$

$$\zeta = \frac{a_{ph}(410)}{a_{ph}(440)} \quad \quad \xi = \frac{a_{dg}(410)}{a_{dg}(440)}$$



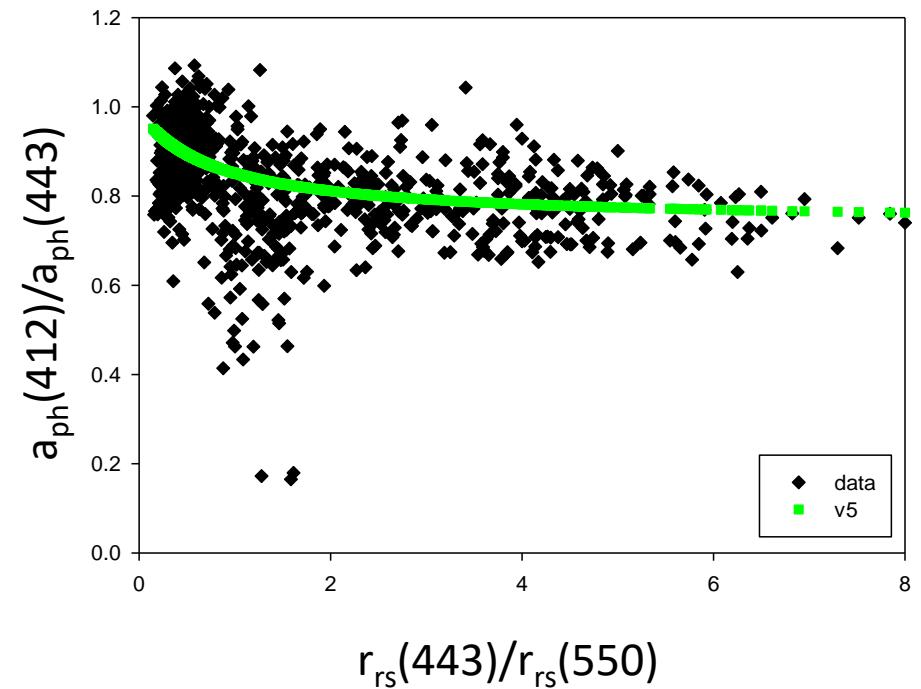
$$\begin{cases} a(410) = a_w(410) + \zeta a_{ph}(440) + \xi a_{dg}(440), \\ a(440) = a_w(440) + a_{ph}(440) + a_{dg}(440). \end{cases}$$



$$\begin{cases} a(410) = a_w(410) + \zeta a_{ph}(440) + \xi a_{dg}(440), \\ a(440) = a_w(440) + a_{ph}(440) + a_{dg}(440). \end{cases}$$

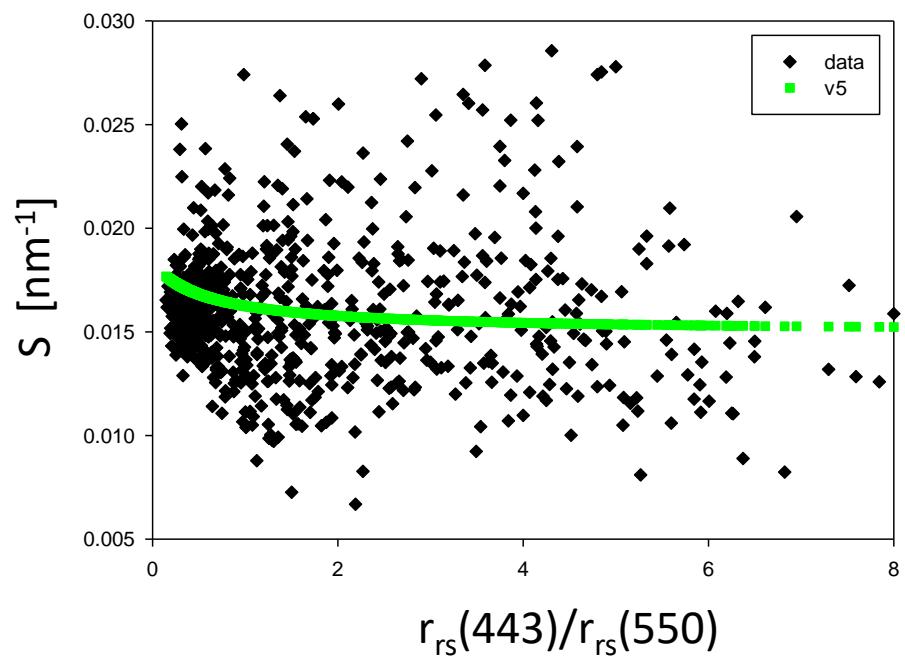


$$\begin{cases} a_g(440) = \frac{(a(410) - \zeta a(440)) - (a_w(410) - \zeta a_w(440))}{\xi - \zeta}, \\ a_{ph}(440) = a(440) - a_w(440) - a_{dg}(440). \end{cases}$$



$$\zeta = 0.74 + \frac{0.2}{0.8 + r_{rs}(443)/r_{rs}(550)}$$

Empirical!



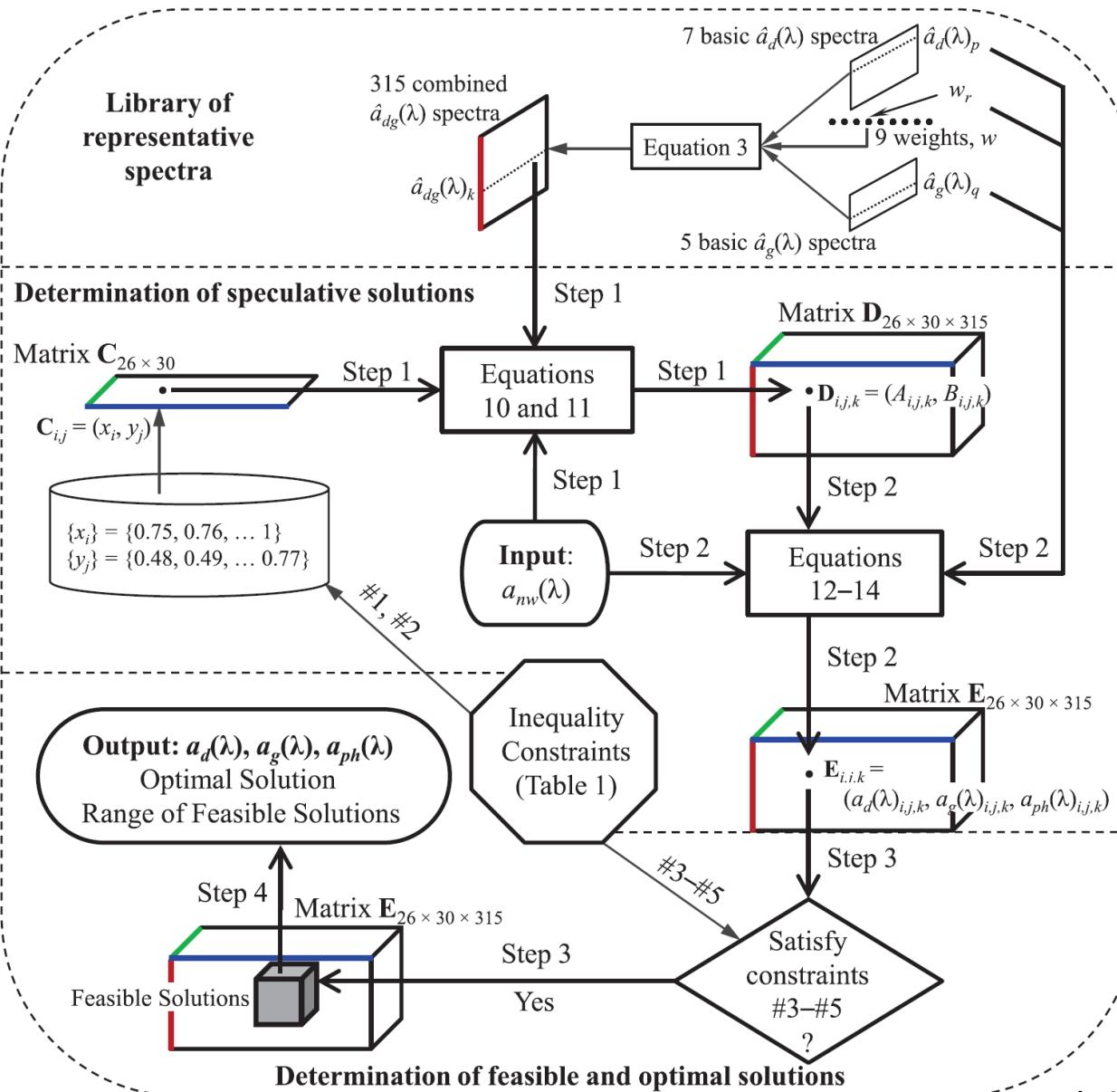
$$\xi = e^{S(443-411)},$$

$$S = 0.015 + \frac{0.002}{0.6 + r_{rs}(443)/r_{rs}(550)}$$

Ensemble solutions:

Wang et al. 2005; Zheng et al. 2015

$$a(\lambda) = a_w(\lambda) + M_1 \langle a_{ph}(\lambda) \rangle + M_2 \langle a_{dg}(\lambda) \rangle$$



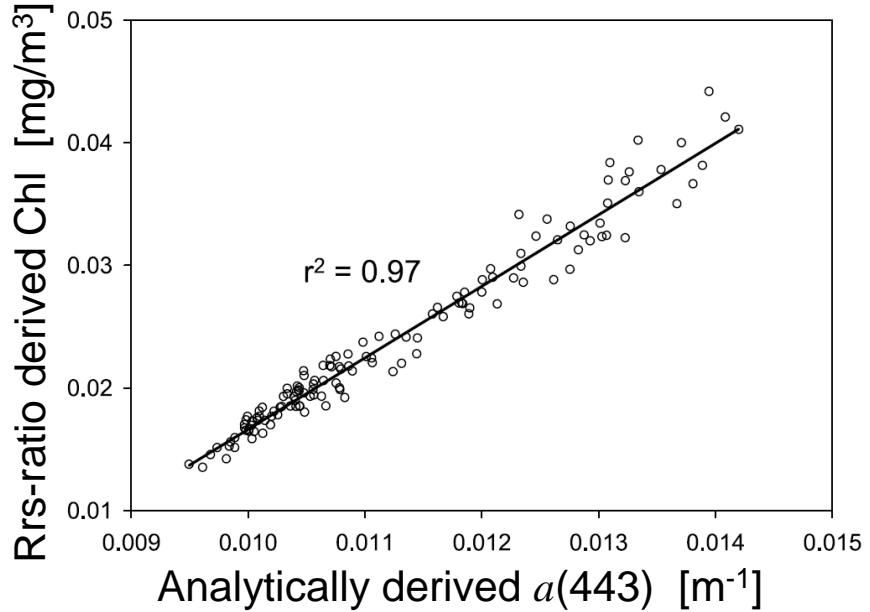
(Zheng et al. 2015)

What is band-ratio derived [Chl]?

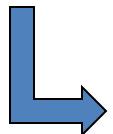
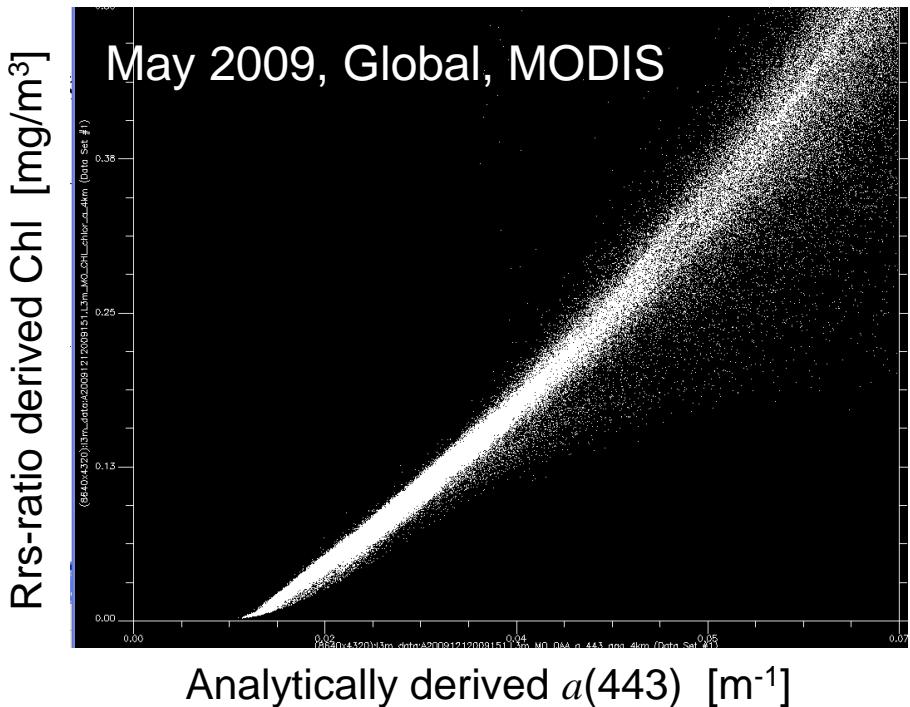
$$[Chl] = f_1 \left(R_{rs}(\lambda_i) / R_{rs}(\lambda_j) \right)$$

$$R_{rs}(\lambda_i) / R_{rs}(\lambda_j) = f_2 \left(\frac{b_{bw}(\lambda_i) + b_{bp}(\lambda_i)}{b_{bw}(\lambda_j) + b_{bp}(\lambda_j)} \frac{a_w(\lambda_j) + a_{ph}(\lambda_j) + a_{dg}(\lambda_j)}{a_w(\lambda_i) + a_{ph}(\lambda_i) + a_{dg}(\lambda_i)} \right)$$

[Chl] is actually an IOP product



At the center of South Pacific Gyre



Ratio-derived “Chl” is re-scaled total absorption coefficient.

Correction of Raman-Scattering contribution:

$$R_{rs}^T(\lambda) = R_{rs-E}(\lambda) + R_{rs-Ram}(\lambda)$$

$$\begin{aligned} R_{rs-Ram}(\lambda) &= \frac{t^2}{n^2} \frac{\tilde{\beta}^r(\theta_s \rightarrow \pi) b_r(\lambda_{\text{em}}) E_d(0^+, \lambda_{\text{ex}})}{(K_d(\lambda_{\text{ex}}) + \kappa_L(\lambda_{\text{em}})) E_d(0^+, \lambda_{\text{em}})} \\ &\times \left[1 + \frac{b_b(\lambda_{\text{ex}})}{\mu_u(K_d(\lambda_{\text{ex}}) + \kappa(\lambda_{\text{ex}}))} + \frac{b_b(\lambda_{\text{em}})}{2\mu_u\kappa(\lambda_{\text{em}})} \right]. \end{aligned} \quad (7)$$

(Mobley 2012, Westberry et al 2013)

Solve for $R_{rs-\text{Ram}}$ and IOPs through iteration

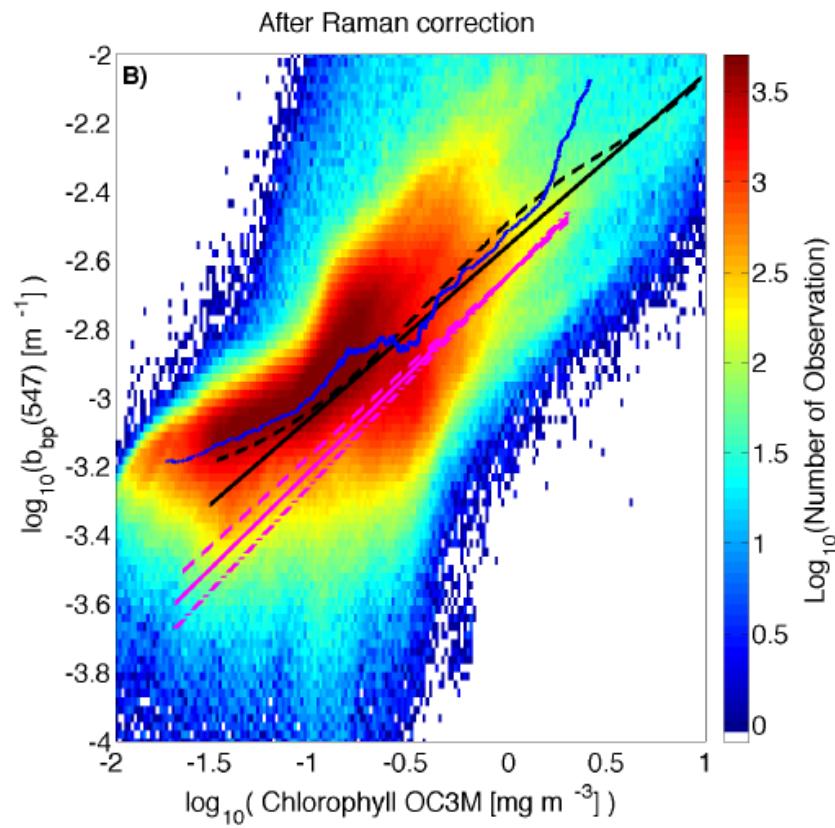
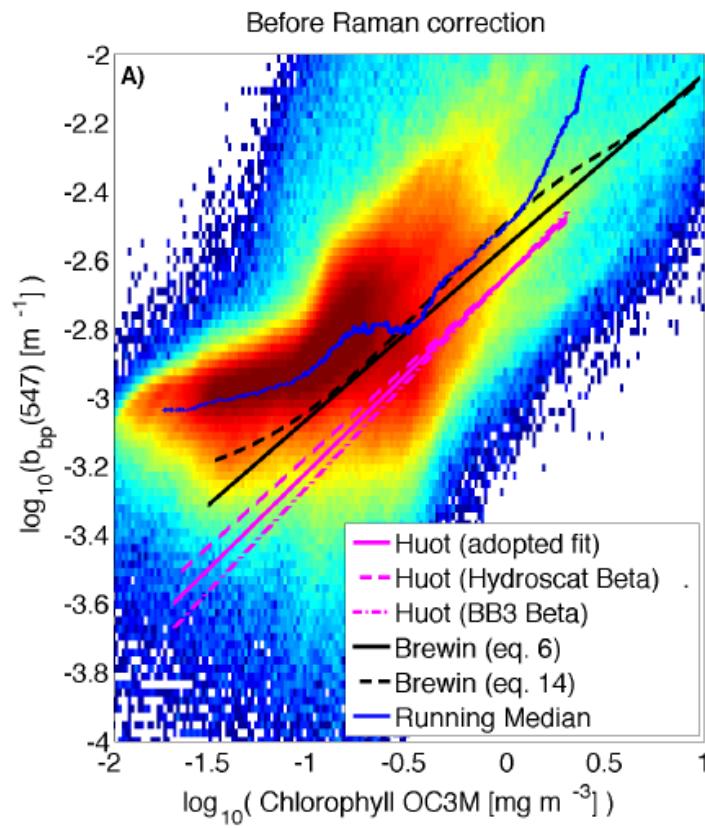
Empirical scheme:

$$R_{rs-E}(\lambda) = \frac{R_{rs}^T(\lambda)}{1 + RF(\lambda)}$$

$$RF(\lambda) = \alpha(\lambda) \left(\frac{R_{rs}^T(440)}{R_{rs}^T(550)} \right) + \beta_1(\lambda) (R_{rs}^T(550))^{\beta_2(\lambda)}.$$

(Lee et al 2013)

RF: Raman factor



(Lee and Huot, 2014)⁴⁸

Impact of Sensor Specifics on RS products

Sensor Specifics:

Spectral:

Number of bands

Position of bands

Width of bands

Signal-to-noise: **SNR**

Pixel size:

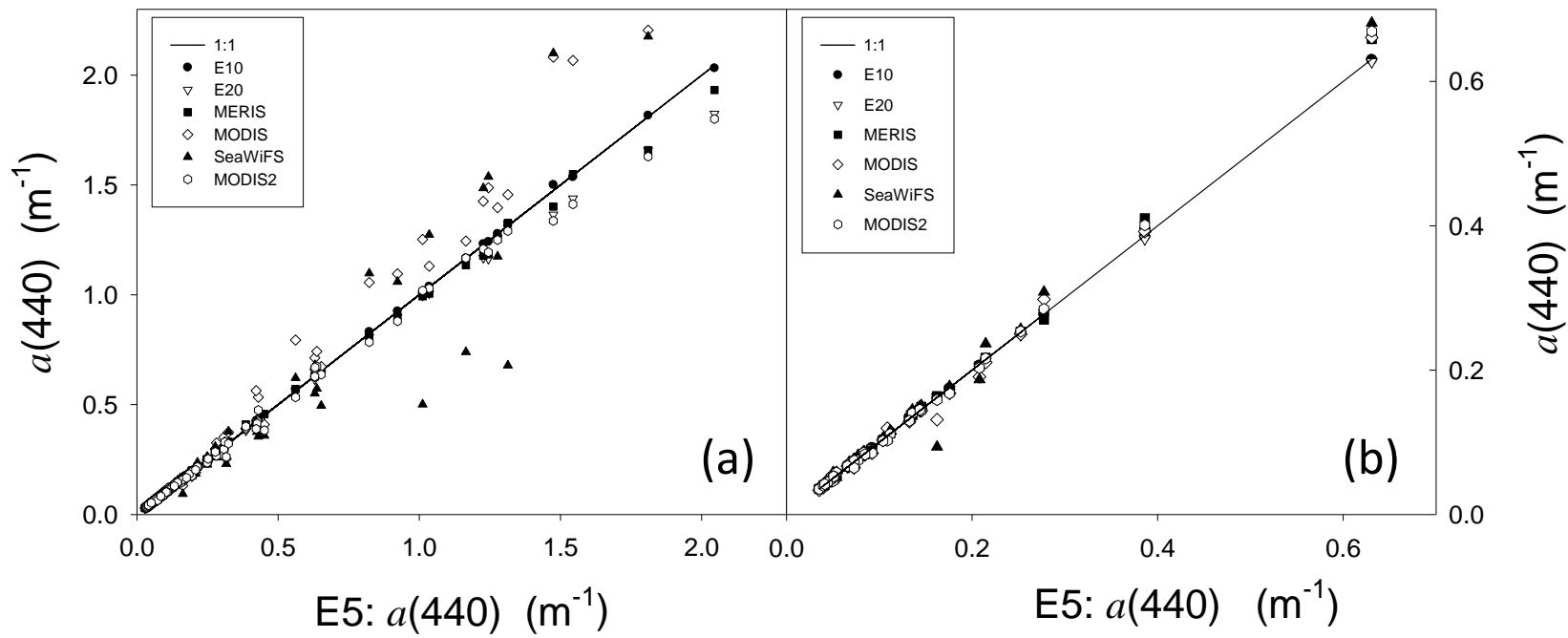
Spatial resolution

Revisit:

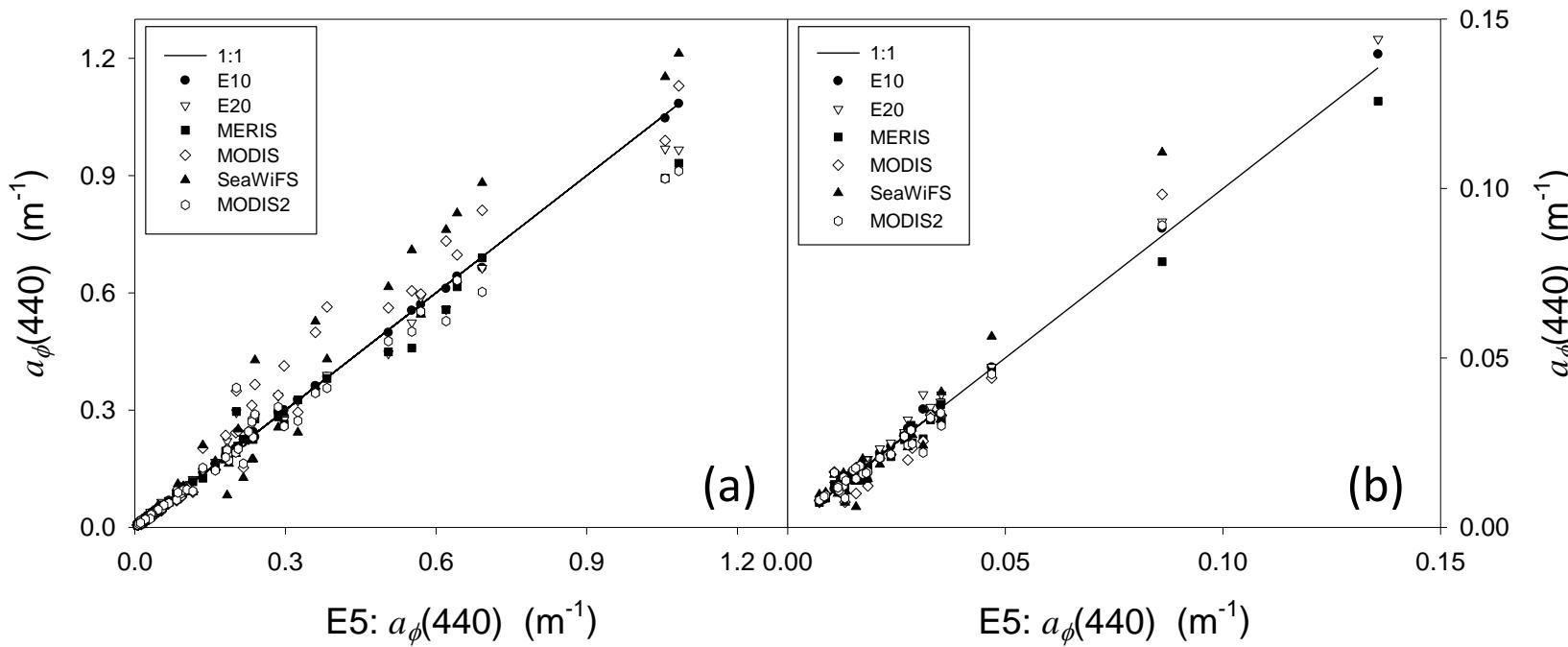
Temporal resolution

How these designs affect remote sensing products?

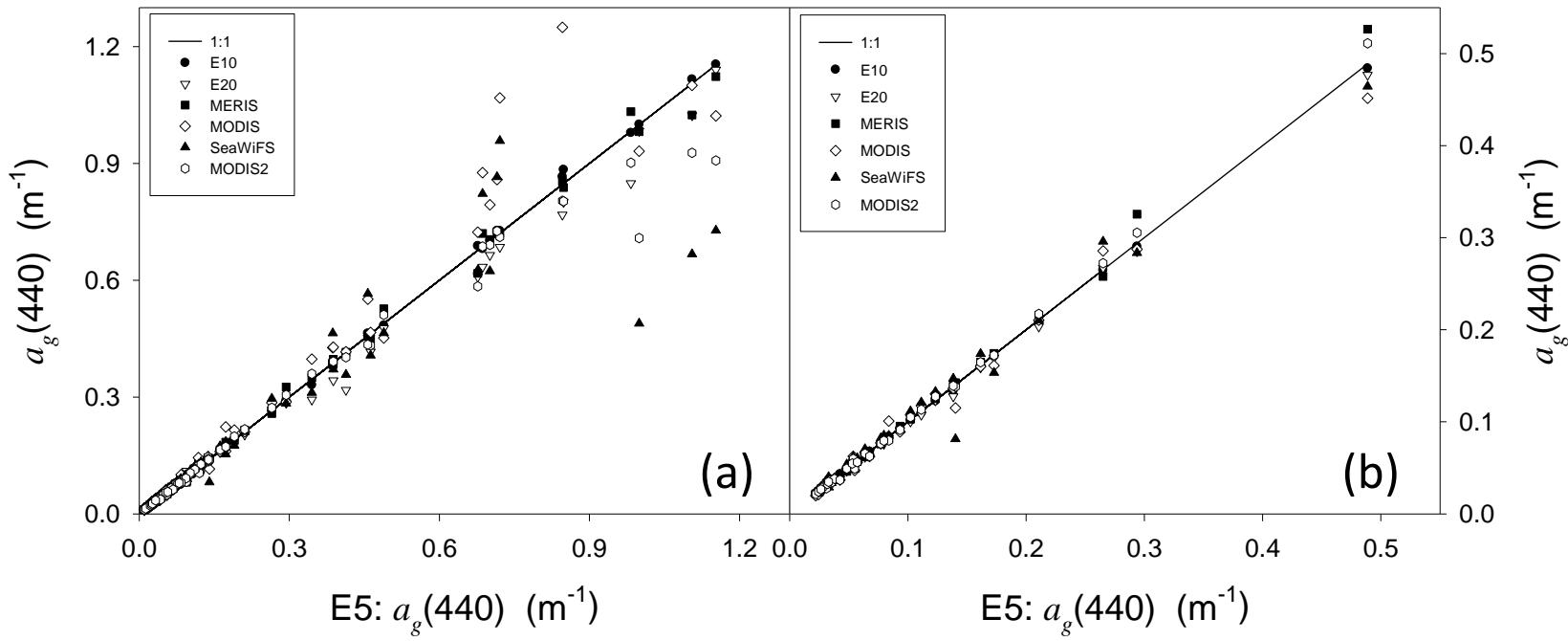
a) Inversion vs number of spectral bands:

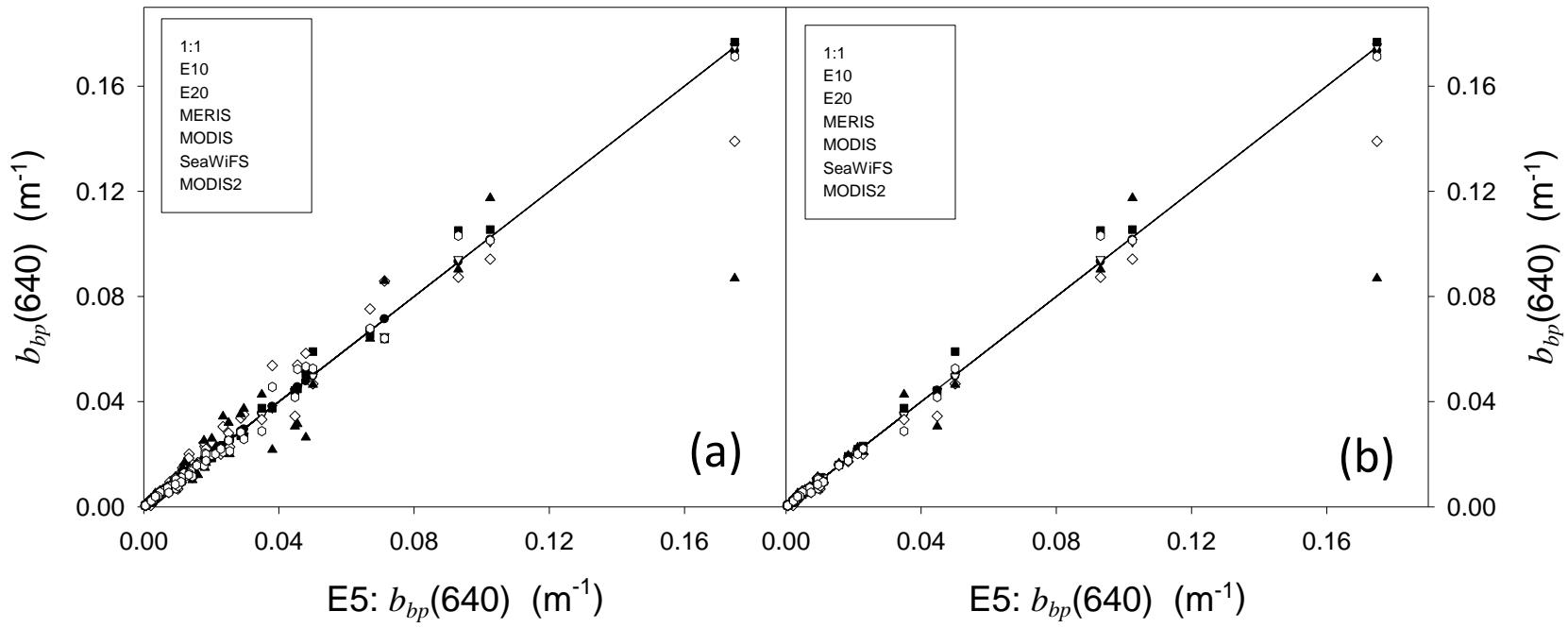


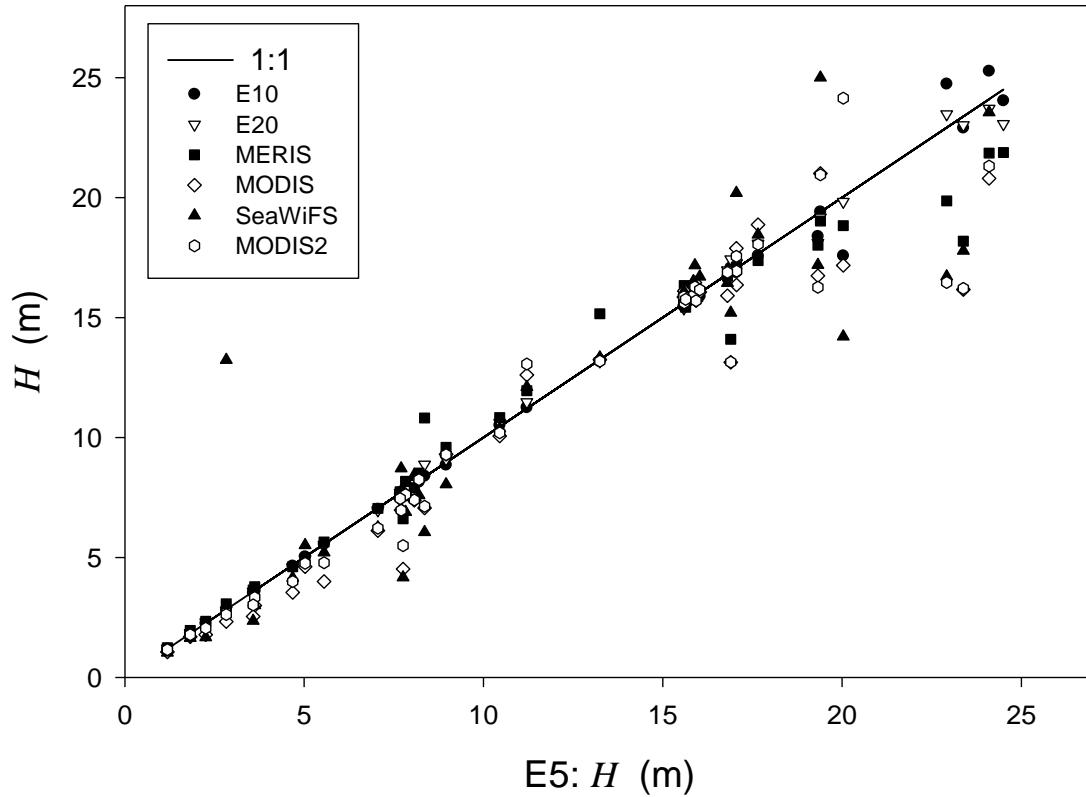
(Lee and Carder 2002)



(Lee and Carder 2002)

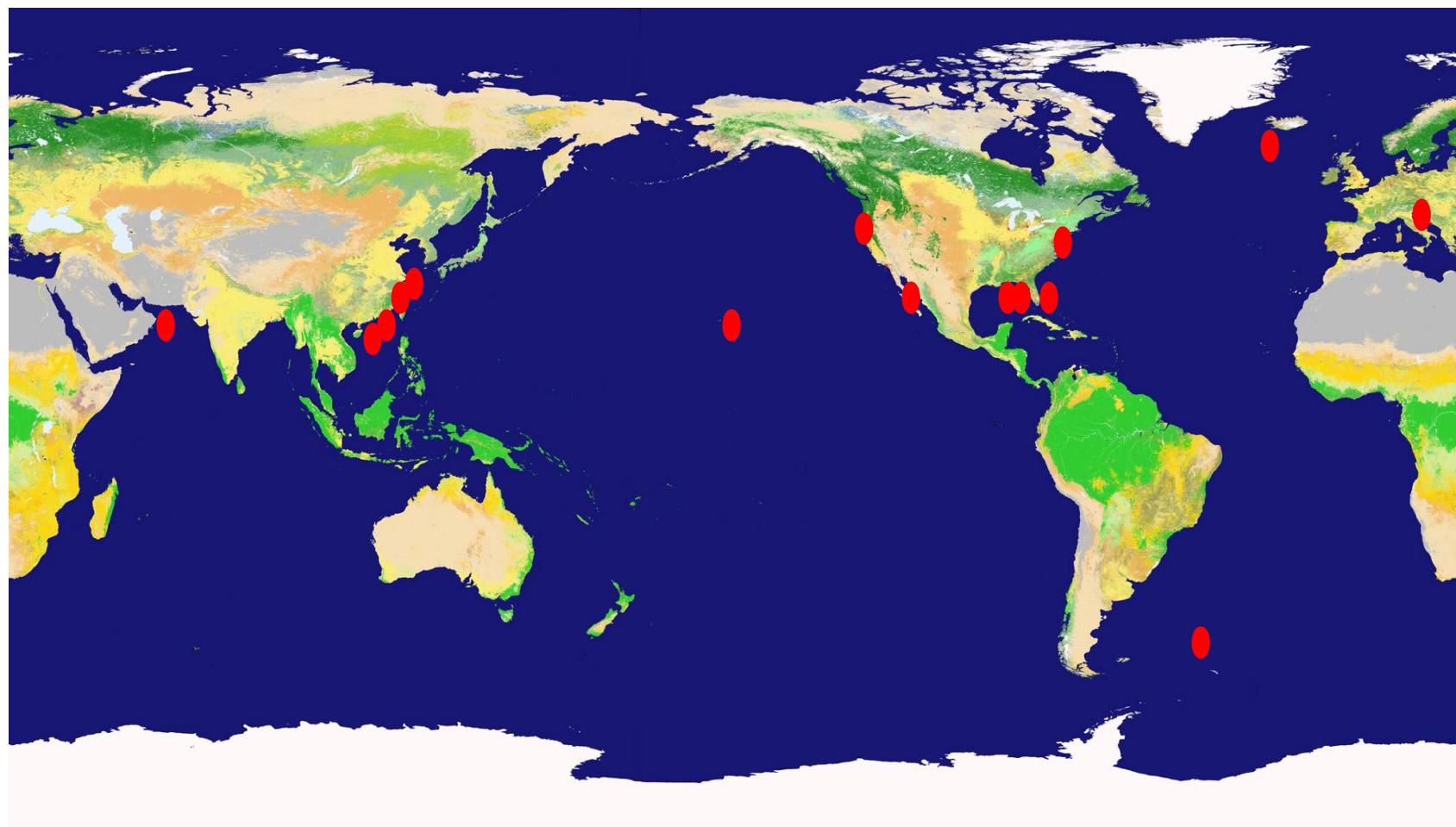




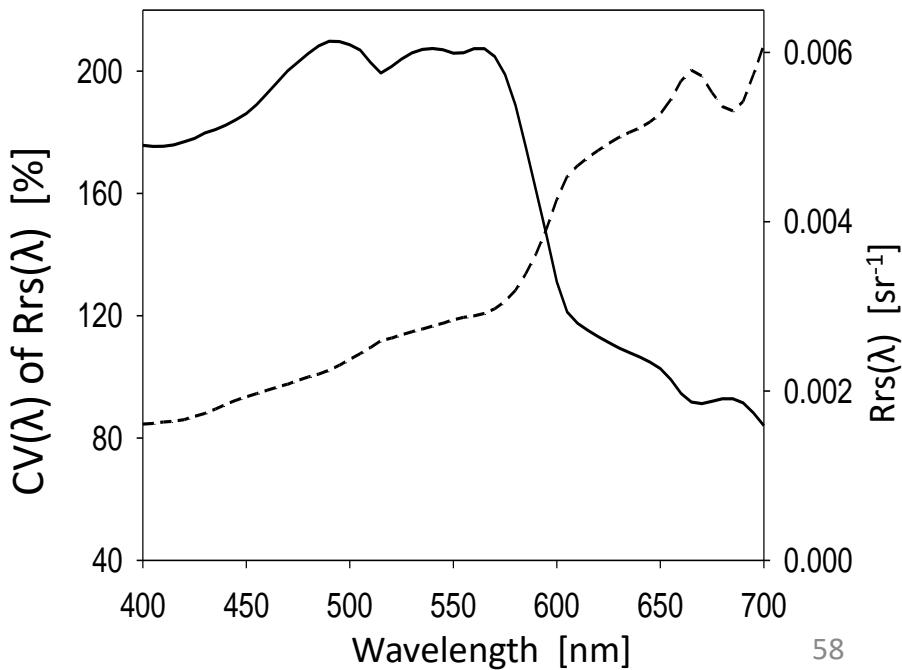
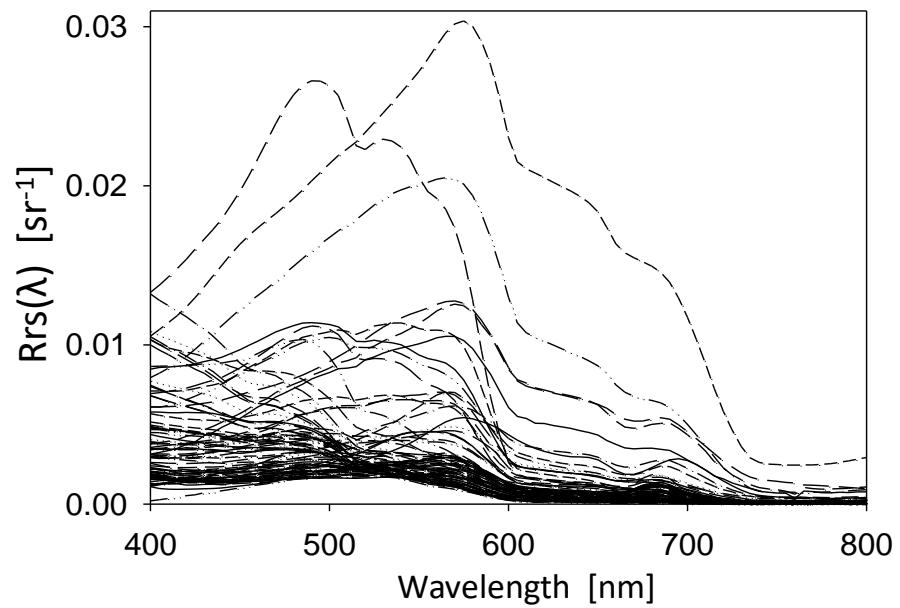


Retrievals with Rrs of ~15 bands are equivalent to that from hyperspectral Rrs.

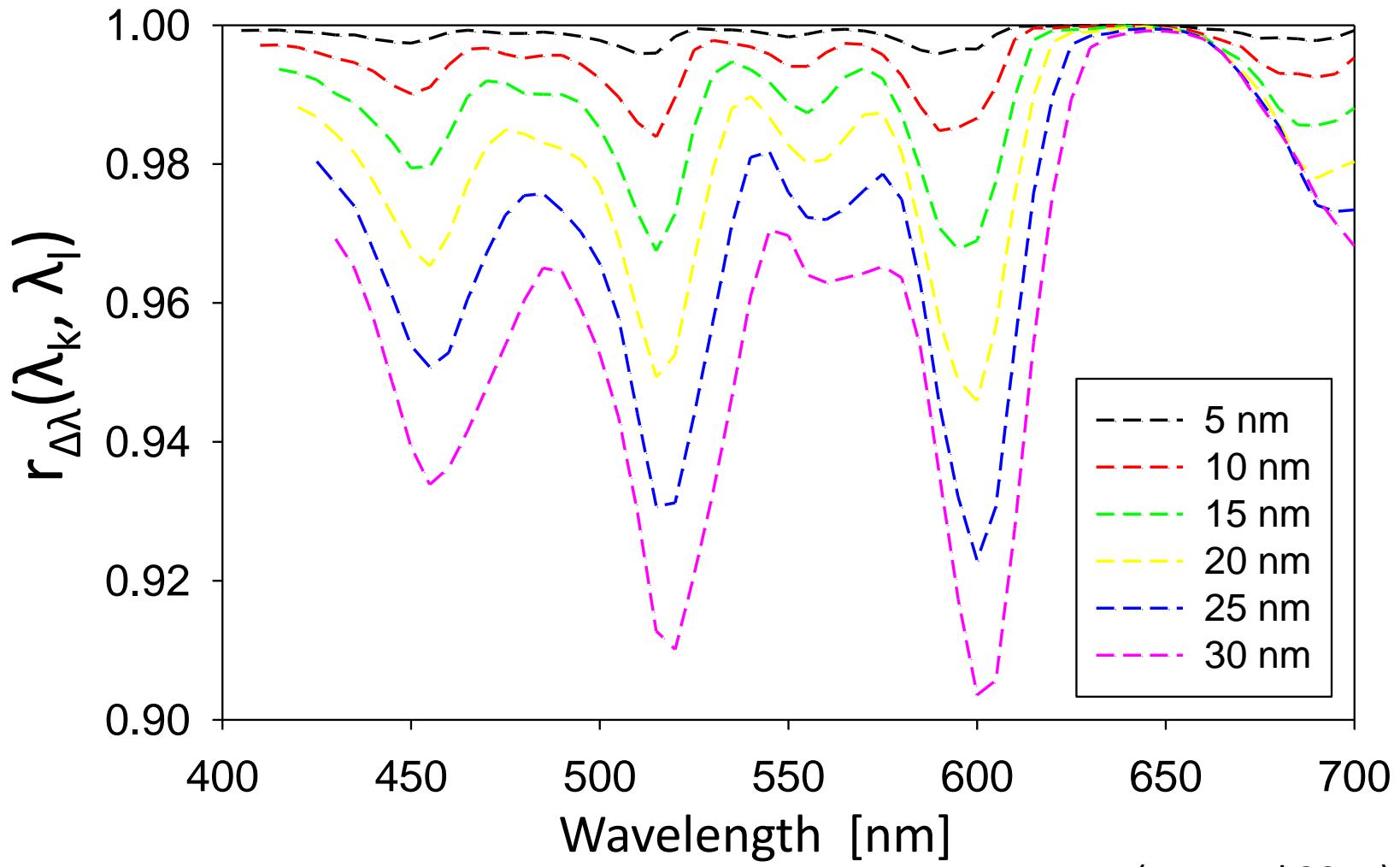
Why?



Characteristics of Rrs dataset (~1000 spectra)



Correlation coefficient of Rrs between neighbor bands:

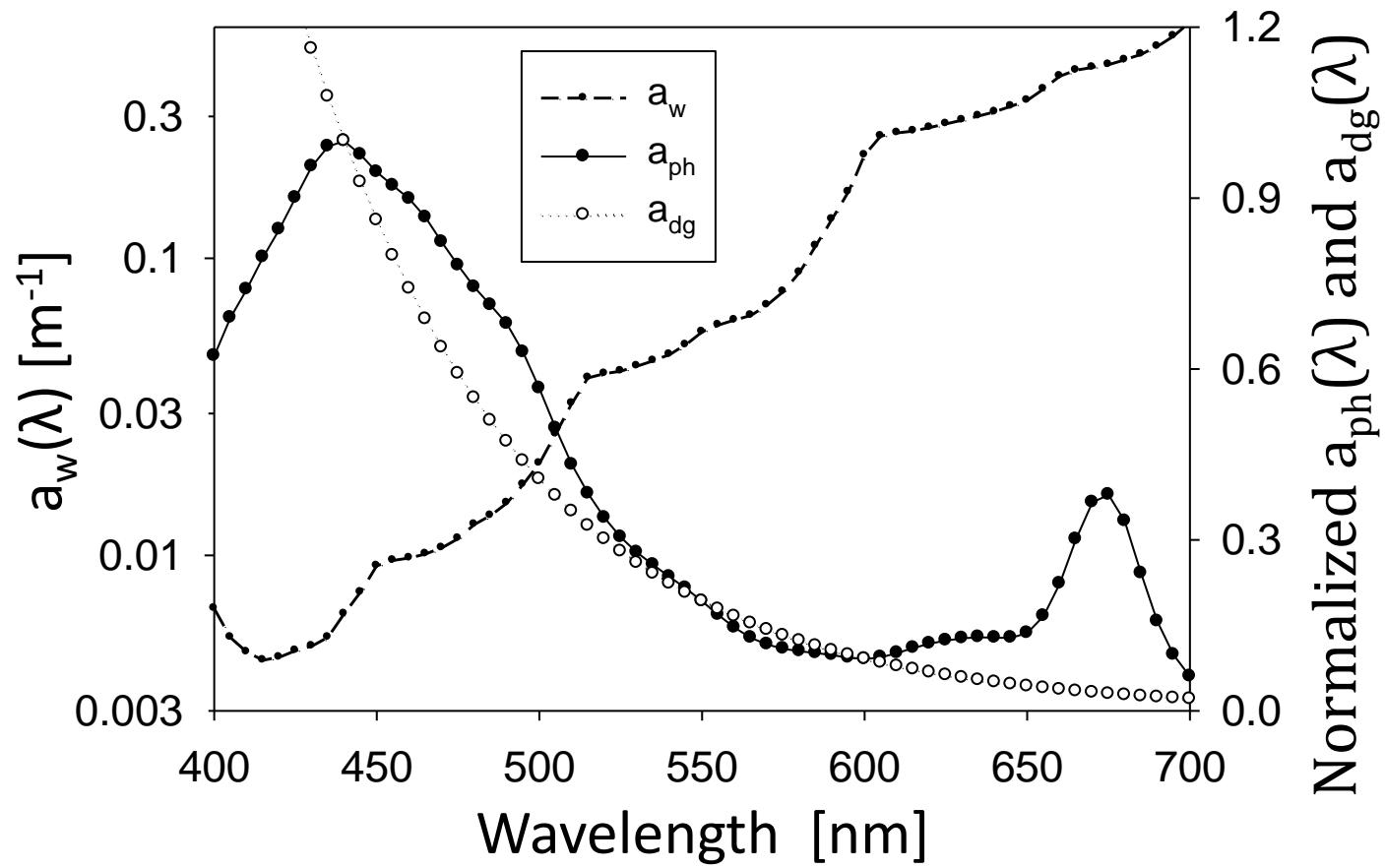


(Lee et al 2014)

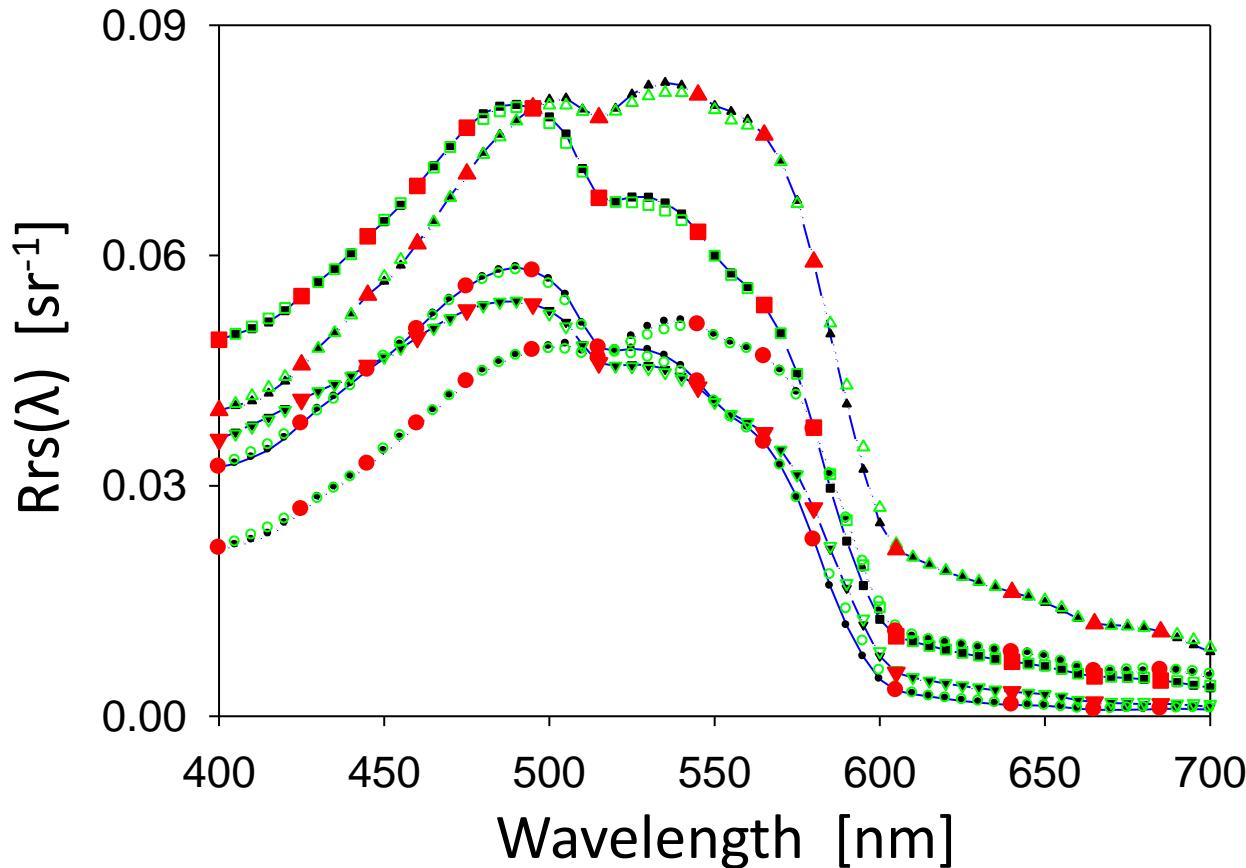


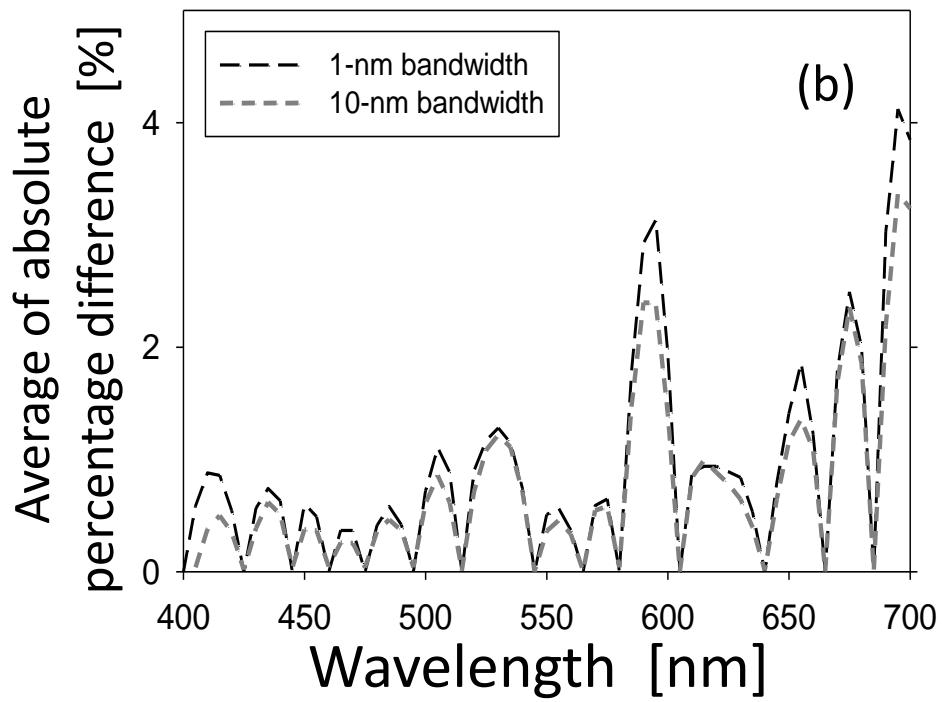
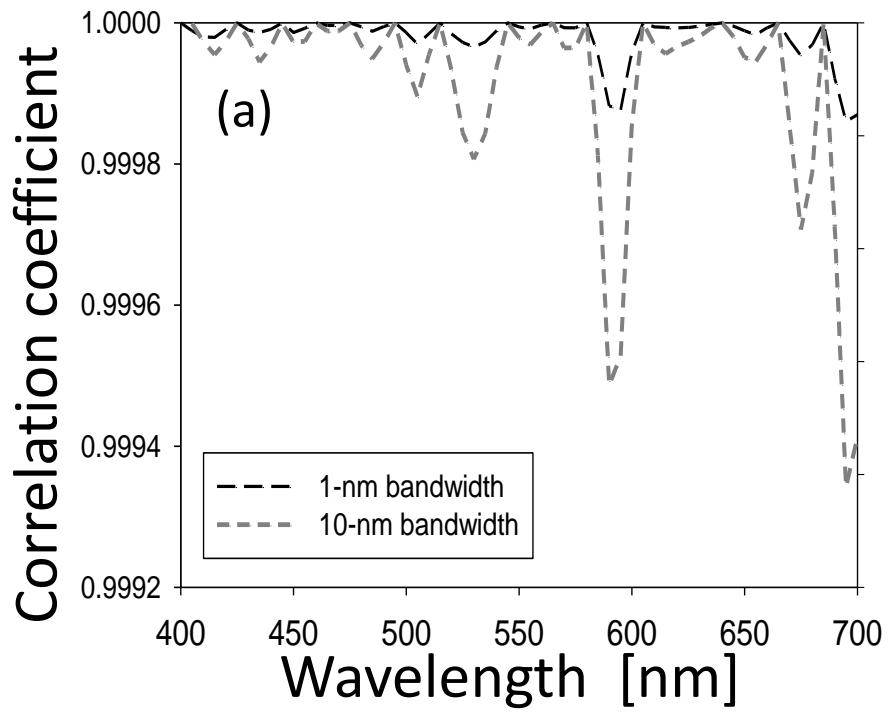
Spectral Rrs are highly correlated, especially for short gaps in wavelengths

$$R_{rs}(\lambda) = G \frac{b_{bw}(\lambda) + b_{bp}(\lambda)}{a_w(\lambda) + a_x(\lambda) + b_{bw}(\lambda) + b_{bp}(\lambda)}$$



Re-construct hyperspectral Rrs from multi-band Rrs



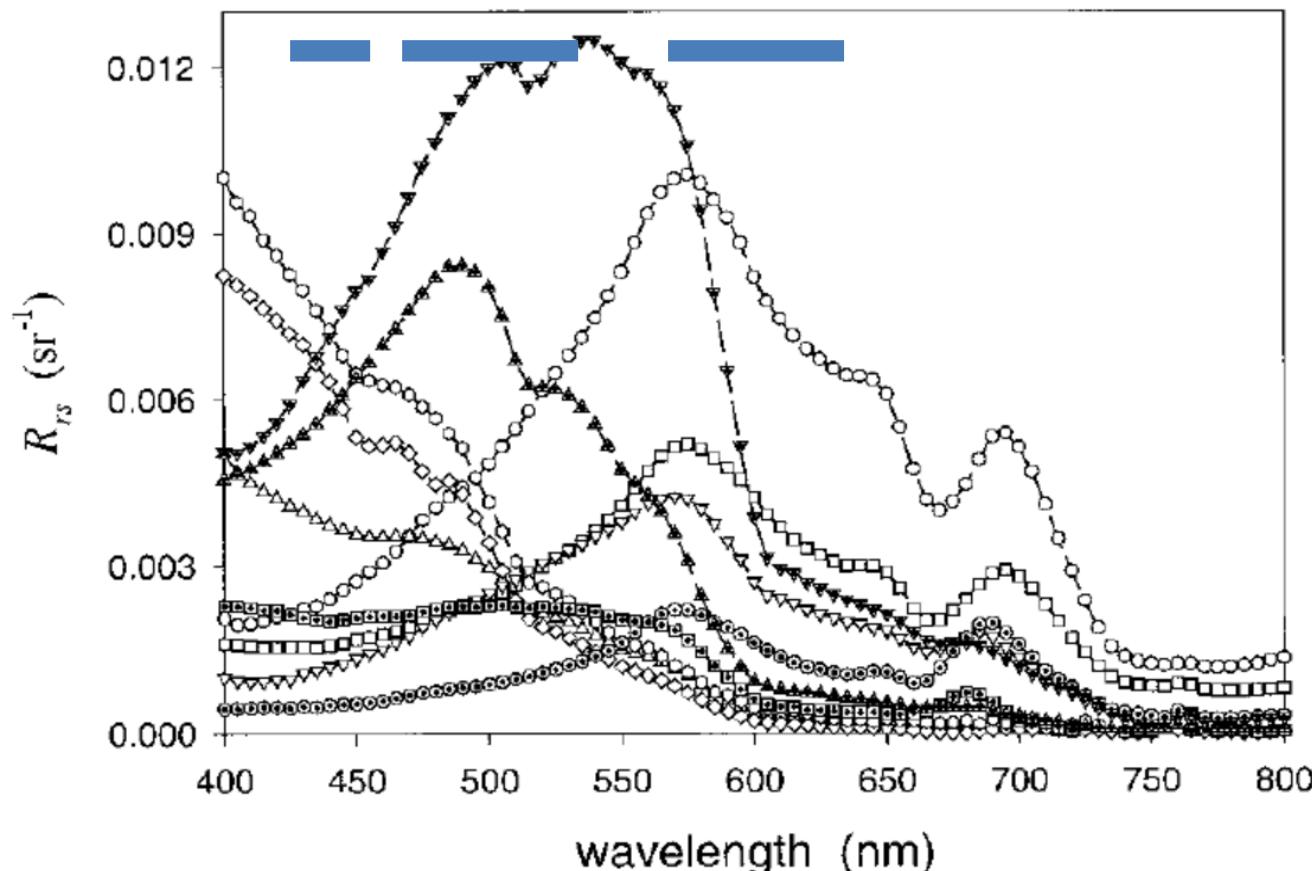


(Lee et al 2014)

→ hyperspectral Rrs can be well re-constructed from Rrs of ~15 bands

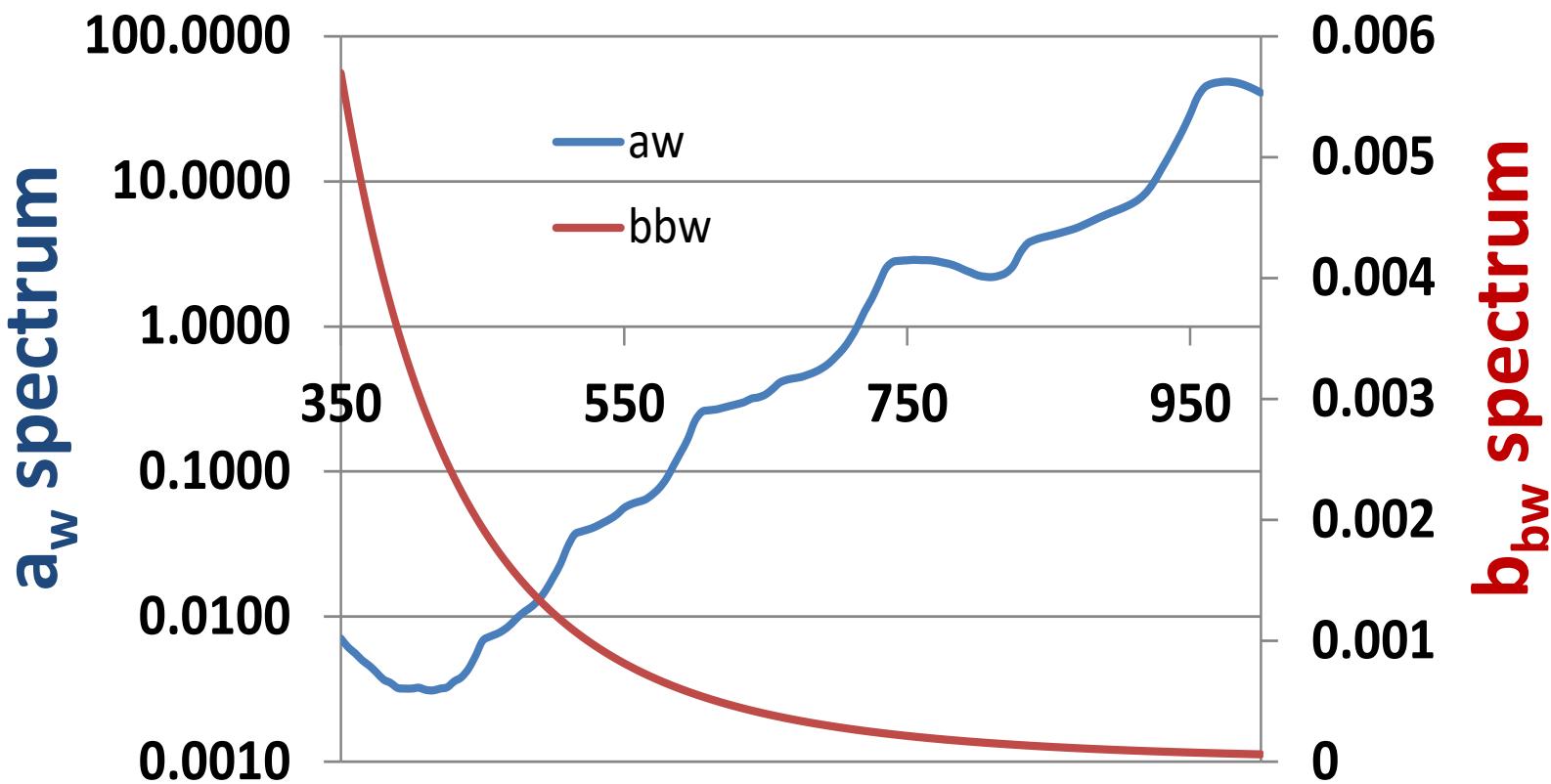
b). Effect of bandwidth

IOPs of wide-spectral bands



Landsat 8

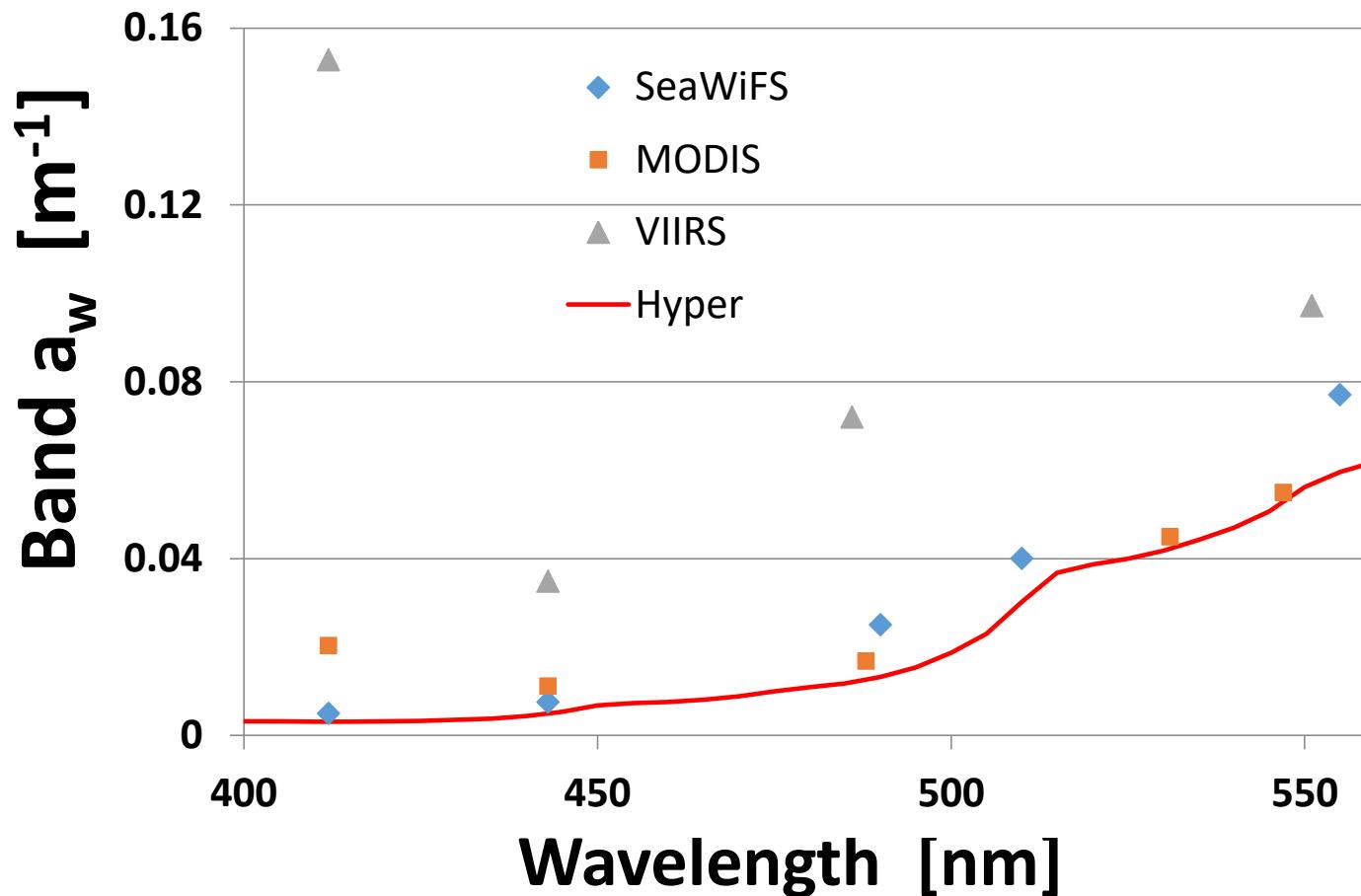
$$R_{rs}(\lambda) = G \frac{b_{bw}(\lambda) + b_{bp}(\lambda)}{a_w(\lambda) + a_x(\lambda) + b_{bw}(\lambda) + b_{bp}(\lambda)}$$



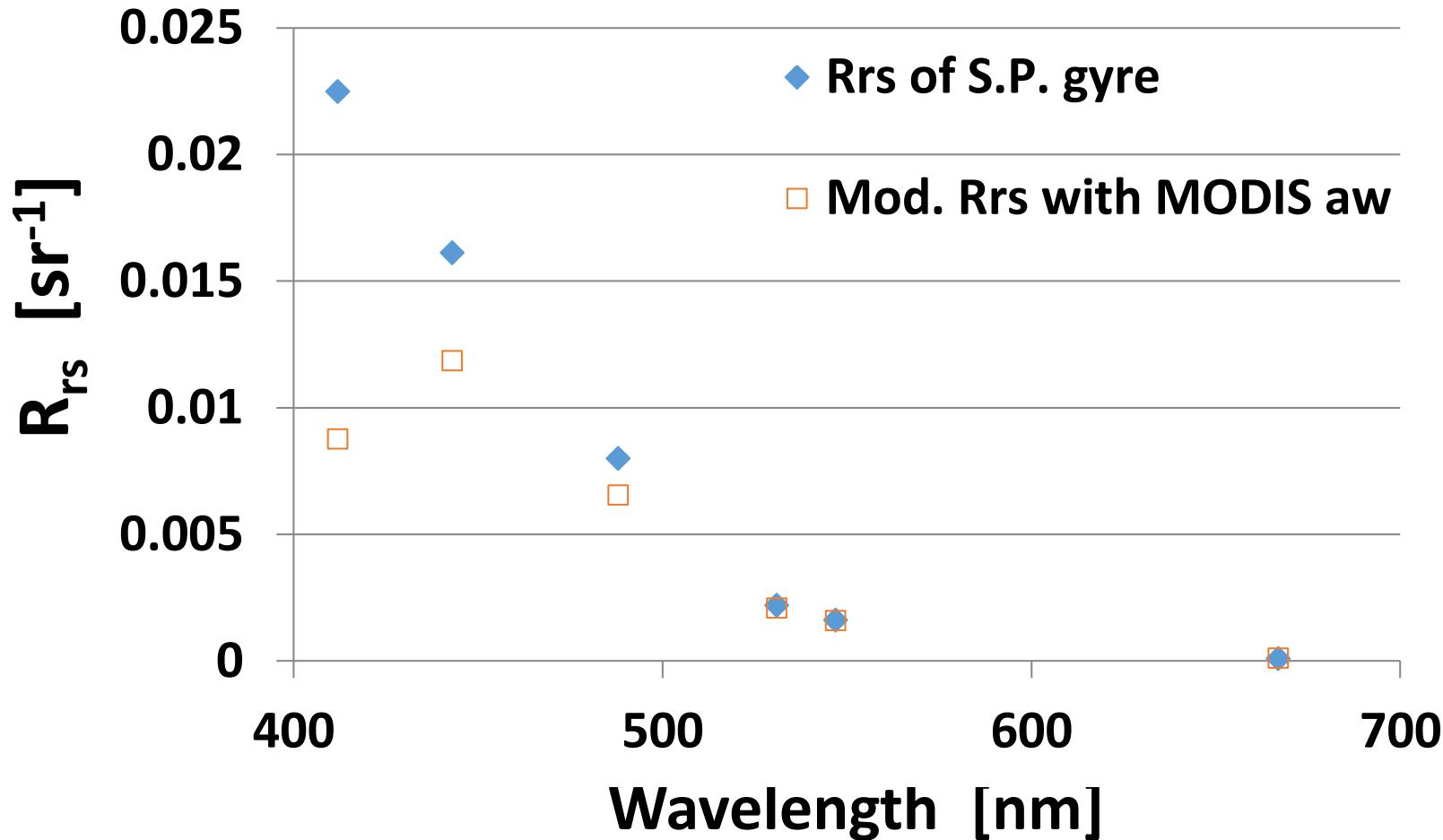
Band-averaged pure-water constants for remote sensing?

“standard” approach:

$$a_w(i) = \text{integral} \left\{ \frac{a_w(\lambda) * RSR_i(\lambda) * d\lambda}{\text{integral}\{RSR_i(\lambda) * d\lambda\}} \right\}$$



→ Consequence is no closure of Rrs



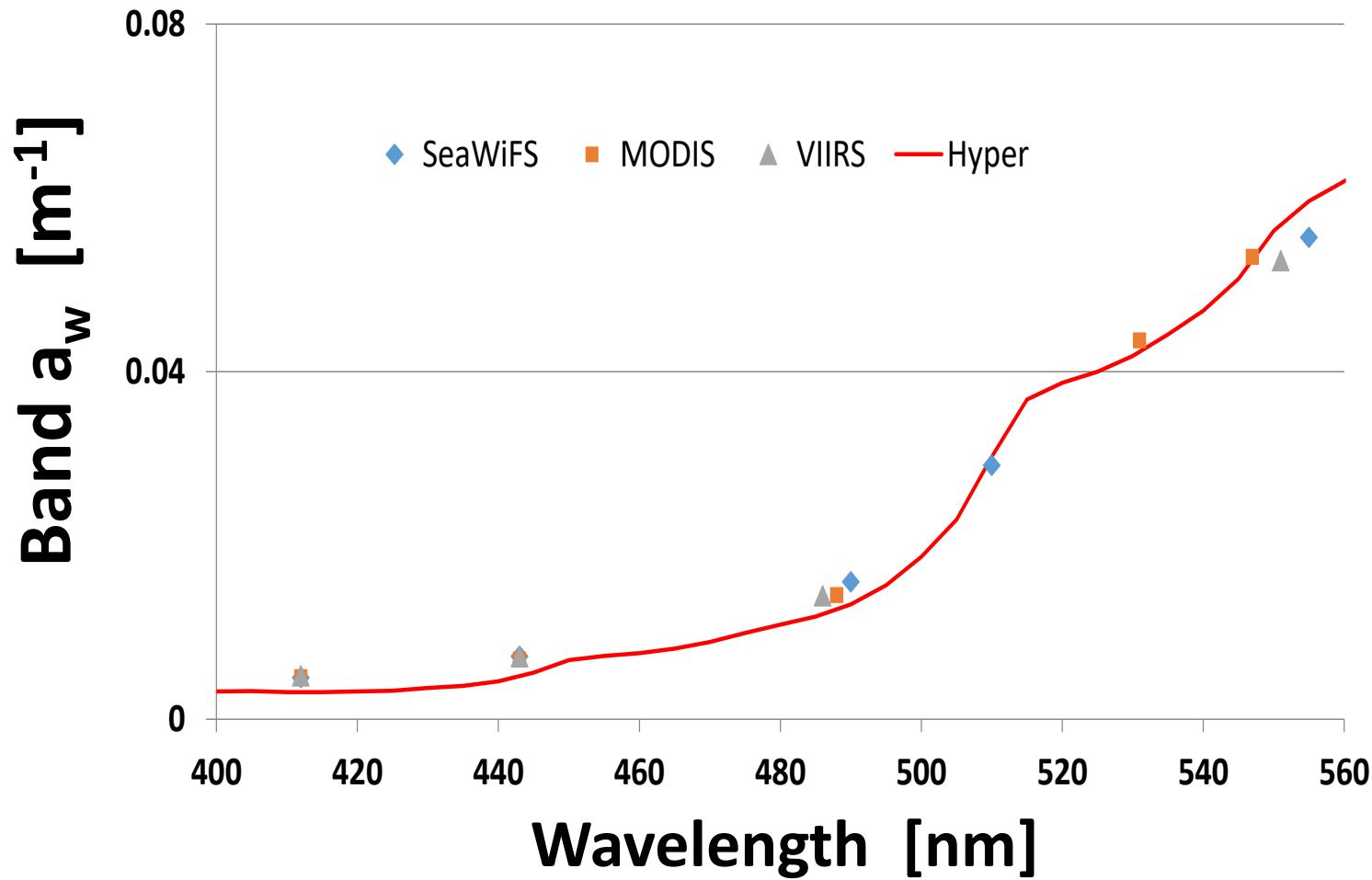
$$R_{rs}(\lambda) = G \frac{b_{bw}(\lambda) + b_{bp}(\lambda)}{a_w(\lambda) + a_x(\lambda) + b_{bw}(\lambda) + b_{bp}(\lambda)}$$

$$x_w(B_i) = \frac{\int RSR_i(\lambda) \left(1/a_w(\lambda)\right) d\lambda}{\int RSR_i(\lambda) d\lambda}$$

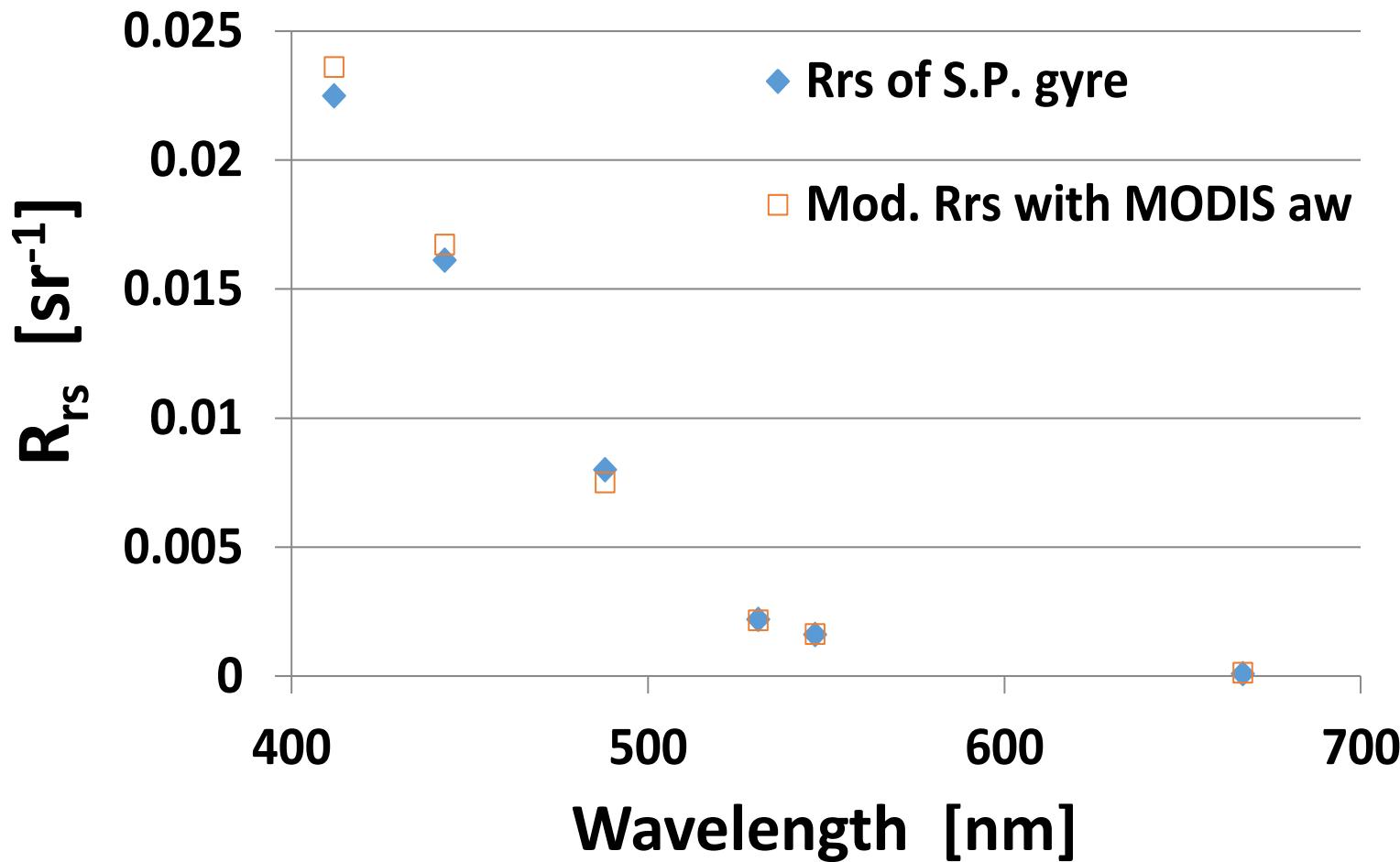
$$a_w(B_i) = \frac{1}{x_w(B_i)}$$

(Lee et al 2016)

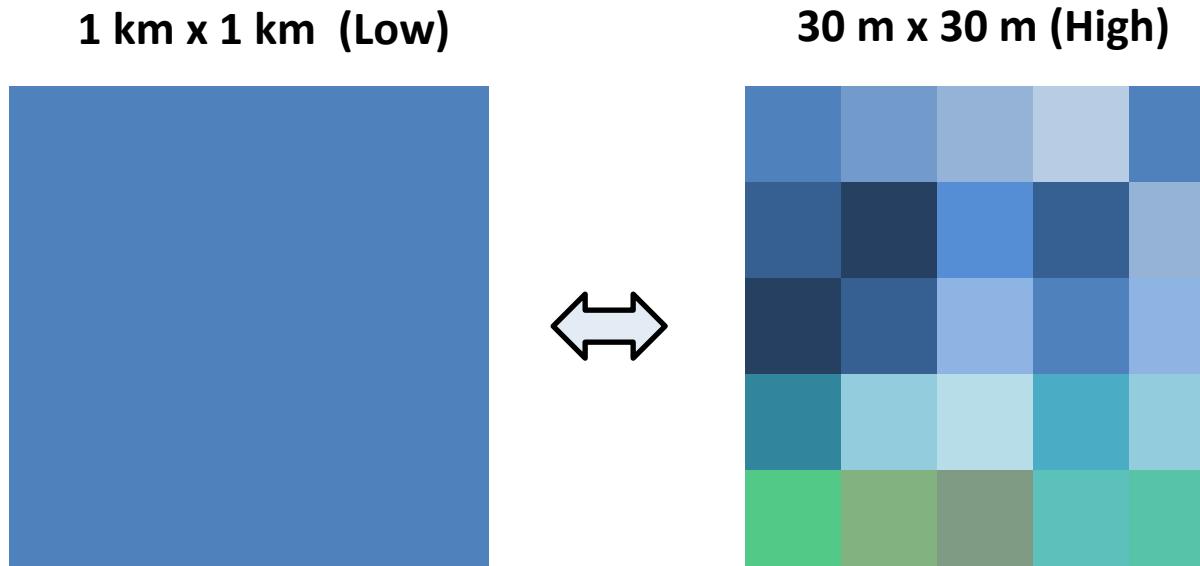
→ band-averaged a_w for Rrs



→ Closure of Rrs



c). Effect of spatial resolution (pixel size)



How to compare results from the two observations if the target is not uniform?

$$\text{Property}_{\text{lo}} = \text{average of Property}_{\text{hi}} \quad ??$$

$$\text{Chl}_{\text{lo}} = \text{average of Chl}_{\text{hi}} \quad ??$$

$$H_{\text{lo}} = \text{average of } H_{\text{hi}} \quad ??$$

What kind of “average”?

$$R_{rs}(\lambda) = \frac{L_w(\lambda)}{E_d(\lambda)}$$

Arithmetic average

$$Lw_{lo} = \overline{Lw_{hi}(i)}$$



$$Rrs_{lo} = \overline{Rrs_{hi}(i)}$$

$$Rrs = G \frac{b_b}{a + b_b}$$



$$a_{lo} \neq \overline{a_{hi}}(i)$$



Chl_{lo} ≠ average of Chl_{hi}

$$g^{\text{'}} \frac{{b_b}^{Lo}}{{a}^{Lo}} \approx \overline{g^{\text{'}} \frac{{b_b}^{Hi}(i)}{{a}^{Hi}(i)}}$$

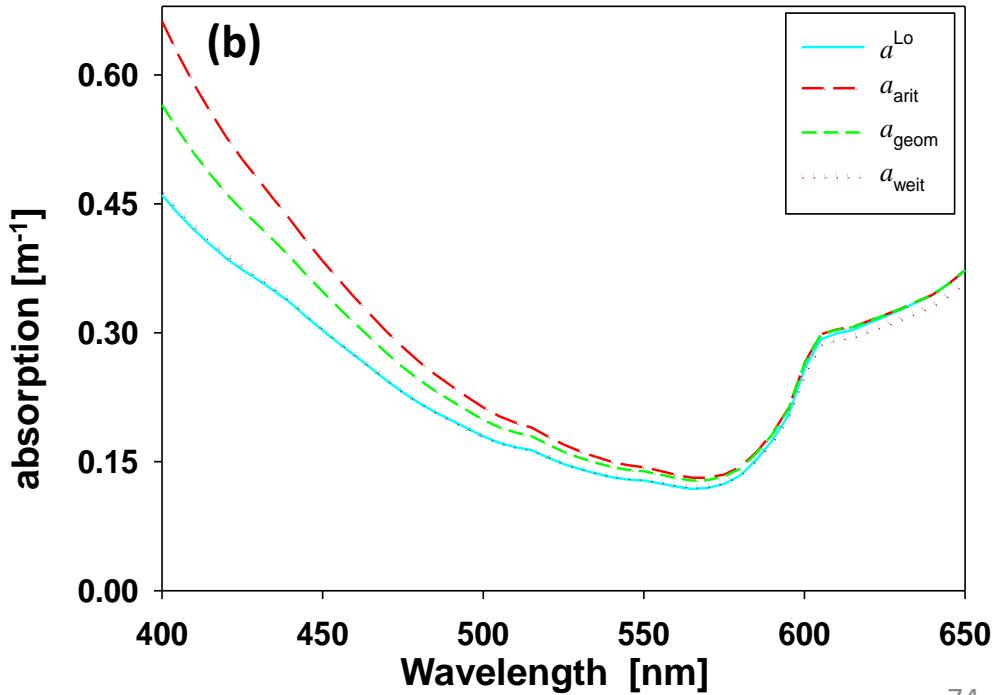
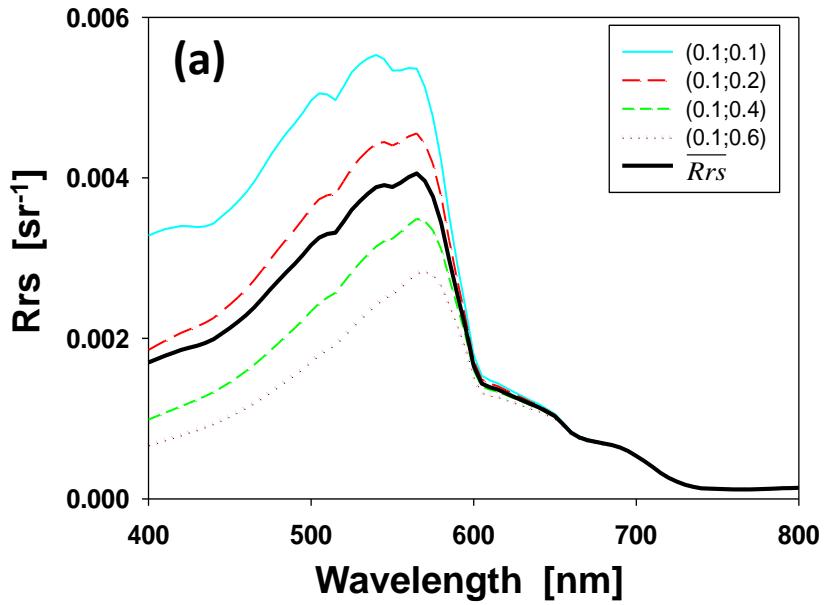
$$\frac{{b_b}^{Lo}}{{a}^{Lo}} \approx \frac{1}{n} \sum_{i=1}^n \frac{{b_b}^{Hi}(i)}{{a}^{Hi}(i)}$$

$${a}^{Lo} \approx \frac{n {b_b}^{Lo} \prod_{i=1}^n {a}^{Hi}(i)}{\sum_{i=1}^n \left({b_b}^{Hi}(i) \prod_{j=1, j \neq i}^{n-1} {a}^{Hi}(j) \right)}$$

Backscattering weighted average

$${b_b}^{Lo} \approx \overline{{b_b}^{Hi}(i)}$$

Lee et al (2012)
73



Shallow water:

$$H_{lo} = \text{average of } H_{hi} \quad ??$$

$$R_{rs} = G(r_{rs}^C + r_{rs}^B) = G \left[r_{rs}^{dp} \left(1 - e^{-D_C(a+b_b)H} \right) + \frac{\rho}{\pi} e^{-D_B(a+b_b)H} \right]$$

$$\rho^{Lo} e^{-D_B(a+b_b)H^{Lo}} \approx \overline{\rho^{Hi}(i) e^{-D_B(a+b_b)H^{Hi}(i)}}$$

$$H^{Lo} \approx \frac{-1}{D_B(a+b_b)} \ln \left\{ \frac{1}{\rho^{Lo}} \overline{\rho^{Hi}(i) e^{-D_B(a+b_b)H^{Hi}(i)}} \right\}$$

Lee et al (2012)

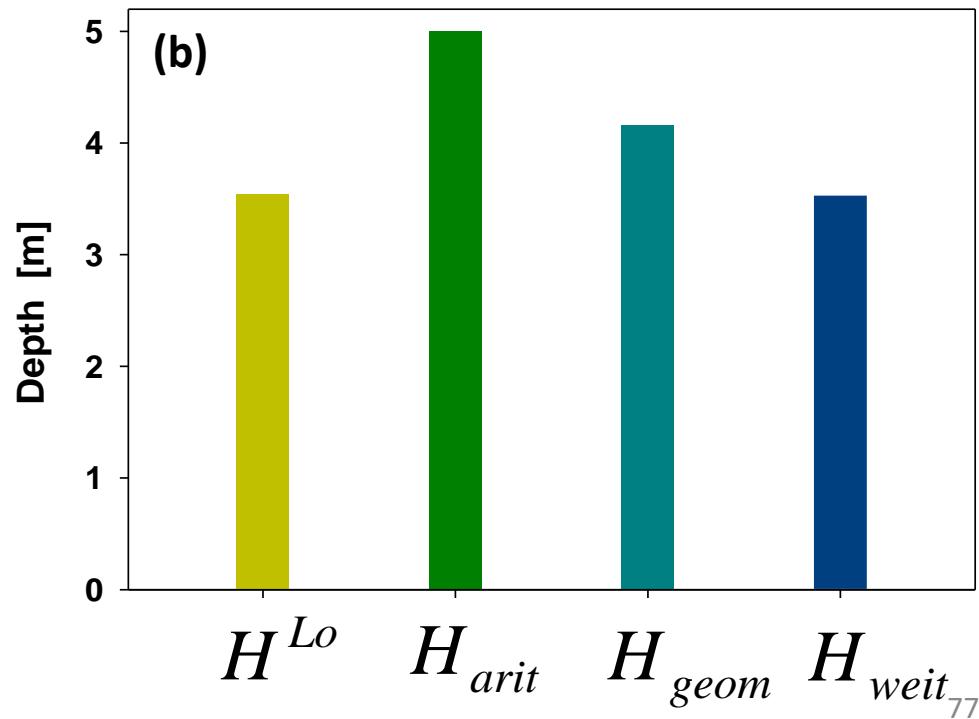
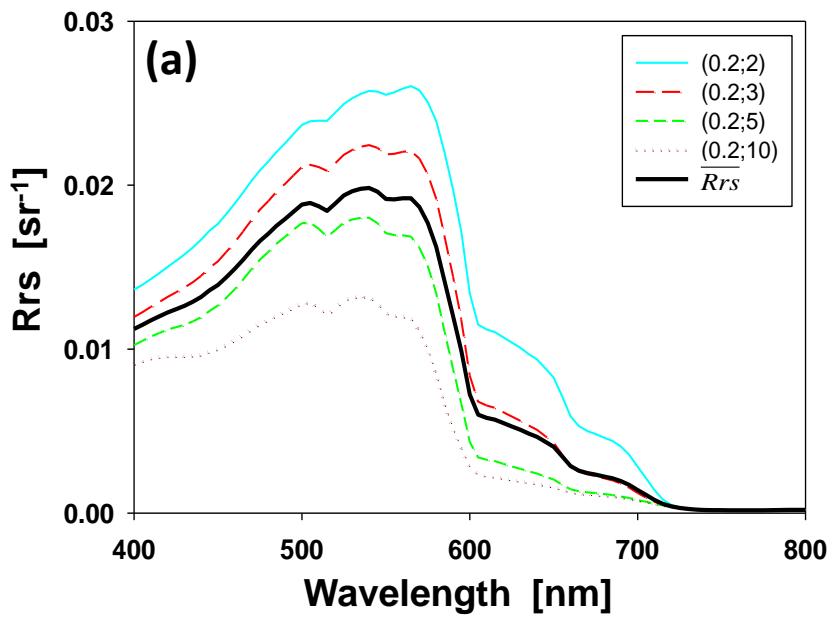
$$\frac{\rho^{Lo}}{H^{Lo}} \approx \frac{\overline{\rho^{Hi}(i)}}{H^{Hi}(i)}$$

$$H^{Lo} \approx \frac{n \rho^{Lo} \prod_{i=1}^n H^{Hi}(i)}{\sum_{i=1}^n \left(\rho^{Hi}(i) \prod_{j=1, j \neq i}^{n-1} H^{Hi}(j) \right)}$$

For same type of bottom:

$$H^{Lo} \approx \frac{n}{\sum_{i=1}^n \frac{1}{H^{Hi}(i)}}$$

Lee et al (2012)



Lee et al (2012)

Key Points:

1. Various inversion algorithms for IOPs have been developed; but more/better ones are also expected.
2. BUS derives every component first, then (simultaneously) derives the total optical property.

Assume the spectral shapes of the optically active components are well characterized.
BUS relies more on the accuracy of forward bio-optical models.

3. TDS derives total first, then decompose it to separate components.

TDS relies more on the accuracy of Rrs measurement

4. Spectral details of input Rrs have various impact on the analytical retrieval of IOPs.

5. For spatially varying water properties, it is necessary to be careful to compare properties of different pixel sizes. It may not be a simply arithmetic average.

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