Steps and calculations of the Quasi-Analytical Algorithm (QAA_v6)

Steps	Calculations	
1	$r_{rs}(\lambda) = R_{rs}(\lambda)/(0.52 + 1.7\, R_{rs}(\lambda))$	
2	$u(\lambda) = \dfrac{-g_0 + \sqrt{(g_0)^2 + 4g_1 * r_{rs}(\lambda)}}{2g_1}$, where g_0=0.089 and g_1=0.1245	
	If $R_{rs}(670) < 0.0015\ sr^{-1}$ (55x nm is λ_0; this 55x is: 547 nm for MODIS; 555 for SeaWiFS or VIIRS; 560 for MERIS or OLCI)	**Else (670 nm is λ_0)**
3	$\chi = \log\left(\dfrac{r_{rs}(443) + r_{rs}(490)}{r_{rs}(55x) + 5\dfrac{r_{rs}(670)}{r_{rs}(490)} r_{rs}(670)}\right)$ $a(\lambda_0) = a(55x) = a_w(\lambda_0) + 10^{h0 + h1\chi + h2\chi^2}$ h_0 =-1.146; h_1 =-1.366; h_2 =-0.469	$a(\lambda_0) = a(670)$ $= a_w(670) + 0.39\left(\dfrac{r_{rs}(670)}{r_{rs}(443) + r_{rs}(490)}\right)^{1.14}$
4	$b_{bp}(\lambda_0) = b_{bp}(55x) = \dfrac{u(\lambda_0) \times a(\lambda_0)}{1 - u(\lambda_0)} - b_{bw}(\lambda_0)$	$b_{bp}(\lambda_0) = b_{bp}(670) = \dfrac{u(\lambda_0) \times a(\lambda_0)}{1 - u(\lambda_0)} - b_{bw}(\lambda_0)$
5	$\eta = 2.0\left(1 - 1.2\ \exp\left(-0.9\dfrac{r_{rs}(443)}{r_{rs}(55x)}\right)\right)$	
6	$b_{bp}(\lambda) = b_{bp}(\lambda_0)\left(\dfrac{\lambda_0}{\lambda}\right)^{\eta}$	
7	$a(\lambda) = (1 - u(\lambda))(b_{bw}(\lambda) + b_{bp}(\lambda))/u(\lambda)$	
8a & 8b	$\zeta = 0.74 + \dfrac{0.2}{0.8 + r_{rs}(443)/r_{rs}(55x)}$ $\xi = e^{S(442.5-415.5)}, S = 0.015 + \dfrac{0.002}{0.6 + r_{rs}(443)/r_{rs}(55x)}$	
9a & 9b	$a_{dg}(443) = \dfrac{a(412) - \zeta a(443)}{\xi - \zeta} - \dfrac{a_w(412) - \zeta a_w(443)}{\xi - \zeta}$ $a_{dg}(\lambda) = a_g(443) e^{-S(\lambda - 443)}$, $a_{ph}(\lambda) = a(\lambda) - a_{dg}(\lambda) - a_w(\lambda)$	

Descriptions

The Quasi-Analytical Algorithm (QAA) was originally developed by *Lee et al.* [2002] to derive the absorption and backscattering coefficients by analytically inverting the spectral remote-sensing reflectance ($R_{rs}(\lambda)$). QAA starts with the calculation of the total absorption coefficient (a) at a reference wavelength (λ_0), and then propagate the calculation to shorter wavelengths. Component absorption coefficients (contributions by detritus/gelbstoff and phytoplankton pigments) are further algebraically decomposed from the total absorption spectrum. To summarize, briefly, QAA is consist of the following elements:

1) The ratio of backscattering coefficient (b_b) to the sum of backscattering and absorption coefficients ($b_b/(a+b_b)$) at a wavelength (λ) is calculated algebraically based on the models of *Gordon et al*. [1988] and *Lee et al*. [1999],

$$\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)} = \frac{-0.0895+\sqrt{0.008+0.499\,r_{rs}(\lambda)}}{0.249}. \qquad (1)$$

Here $r_{rs}(\lambda)$ is the nadir-viewing spectral remote-sensing reflectance just below the surface and is calculated from nadir-viewing $R_{rs}(\lambda)$ through,

$$r_{rs}(\lambda) = R_{rs}(\lambda)/(0.52 + 1.7\,R_{rs}(\lambda)). \qquad (2)$$

2) The spectral $b_b(\lambda)$ is modeled with the widely used expression [*Gordon and Morel*, 1983; *Smith and Baker*, 1981],

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda_0)\left(\frac{\lambda_0}{\lambda}\right)^{\eta}, \qquad (3)$$

where b_{bw} and b_{bp} are the backscattering coefficients of pure seawater and suspended particles, respectively. Values of $b_{bw}(\lambda)$ are provided in *Morel* [1974].

3) When $a(\lambda_0)$, the ratio of $b_b/(a+b_b)$ at λ_0, and $b_{bw}(\lambda_0)$ are known, $b_{bp}(\lambda_0)$ in Eq. 3 can be easily derived with the combination of Eqs. 1 and 3. The values of $b_b(\lambda)$ at the shorter wavelengths are then calculated after the power parameter (η) is estimated [*Lee et al.*, 2002].

4) Applying $b_b(\lambda)$ to the ratio of $b_b/(a+b_b)$ at λ (Eq. 1), the total absorption coefficient at λ, $a(\lambda)$, is then calculated algebraically.

5) After $a(\lambda)$ is known, $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$ is calculated through

$$a_{dg}(443) = \frac{a(412) - \zeta a(443)}{\xi - \zeta} - \frac{a_w(412) - \zeta a_w(443)}{\xi - \zeta}$$

$$a_{dg}(\lambda) = a_g(443) e^{-S(\lambda - 443)}, \; a_{ph}(\lambda) = a(\lambda) - a_{dg}(\lambda) - a_w(\lambda) \qquad (4)$$

Here $\zeta = a_{ph}(411)/a_{ph}(443)$ and $\xi = a_{dg}(411)/a_{dg}(443)$.

The updates of the QAA (related to the calculation of $a(\lambda_0)$, η, ζ, and ξ)

In QAA_v4 [*Lee et al.*, 2007] an estimated $R_{rs}(640)$ was proposed for the calculation of $a(\lambda_0)$ for both oceanic and coastal waters. As many satellite sensors do not have a band around 640 nm, the measured $R_{rs}(670)$ (or a wavelength in the near vicinity) is now incorporated. This is in particular useful because that all operational satellite sensors (SeaWiFS, MODIS, and MERIS) have a band around this wavelength, although some minor contamination from chlorophyll fluorescence is possible in the measured $R_{rs}(670)$.

Therefore, in this updated version of QAA, $a(\lambda_0)$ is now estimated as follow (for $R_{rs}(670) < 0.0015\ sr^{-1}$),

$$\chi = \log\left(\frac{r_{rs}(443) + r_{rs}(490)}{r_{rs}(55x) + 5\frac{r_{rs}(670)}{r_{rs}(490)} r_{rs}(670)}\right), \qquad (5)$$

$$a(\lambda_0) = a_w(\lambda_0) + 10^{-1.146 - 1.366\chi - 0.469\chi^2}, \qquad (6)$$

with λ_0 as 550, 555, or 560 nm that corresponding to SeaWiFS, MODIS, and MERIS sensors.

Constants in Eq. 6 were the average of the coefficients obtained by least-square fitting $a(\lambda_0)$ of the synthetic data set adopted by the IOCCG [2006] for SeaWiFS, MODIS, and MERIS bands. In short, one set of parameters is proposed for the three sensors (good enough for comparison of derived IOPs with in situ measurements), except the change of $a_w(\lambda_0)$ values for each sensor. Separate sets of constants for each sensor, however, are necessary if long-term and consistent IOP results from the three sensors are the goal.

When processing data from satellite imageries, $R_{rs}(670)$ could be erroneous due to imperfect atmospheric correction. Consequently, constraints for the $R_{rs}(670)$ value are necessary in order to avoid the impact of erroneous $R_{rs}(670)$ on IOPs at the shorter wavelengths. Based on *in situ* measurements and Hydrolight simulated data, Figure 1a shows the range of $R_{rs}(670)$ for the different $R_{rs}(555)$, along with the upper and lower bands: For each $R_{rs}(555)$, $R_{rs}(670)$ is proposed to be kept within

Upper limit:

$$R_{rs}(670) = 20.0\left(R_{rs}(555)\right)^{1.5} \tag{7}$$

Lower limit

$$R_{rs}(670) = 0.9\left(R_{rs}(555)\right)^{1.7} \tag{8}$$

If there is no $R_{rs}(670)$ measurement or $R_{rs}(670)$ value is out of the limits, an estimated $R_{rs}(670)$ is recommended, i.e.

$$R_{rs}(670) = 1.27\left(R_{rs}(555)\right)^{1.47} + 0.00018\left(R_{rs}(490)/R_{rs}(555)\right)^{-3.19} \tag{9}$$

Which is the best regression (Figure 1b) between $R_{rs}(670)$ and $R_{rs}(555)$ as well as $R_{rs}(490)/R_{rs}(555)$.

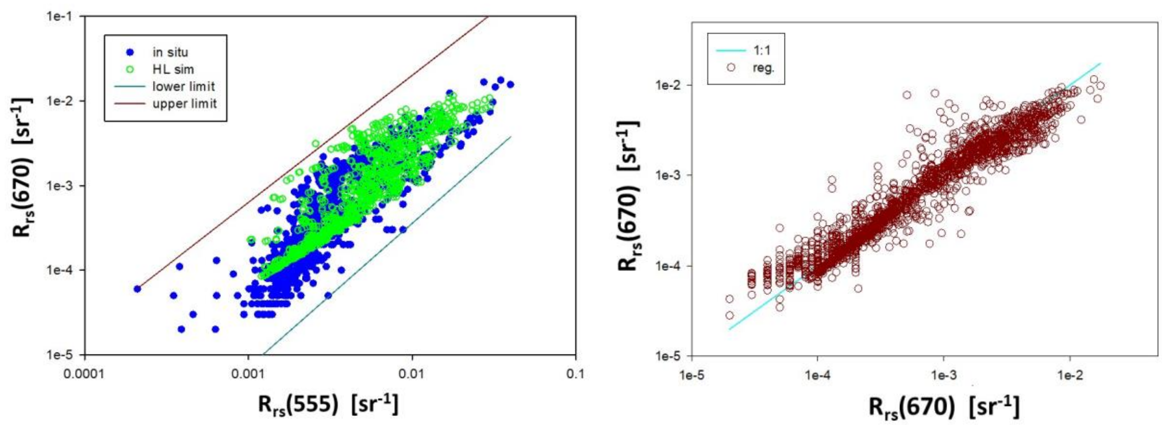

Figure 1a (left), upper and lower limits of $R_{rs}(670)$. 1b (right): empirical $R_{rs}(670)$ from $R_{rs}(555)$ and $R_{rs}(490)/R_{rs}(555)$.

Value of η, required for extrapolation of b_{bp} at λ_0 to shorter wavelengths, is now slightly adjusted to the following based on NOMAD dataset (see Fig.2)

$$\eta = 2.0\left(1 - 1.2\ \exp\left(-0.9\frac{r_{rs}(443)}{r_{rs}(555)}\right)\right). \tag{10}$$

The 555 nm used in Eqs. 7-10 can be changed to 550 nm (for MODIS) or 560 nm (for MERIS) without causing significant impacts on final IOP results.

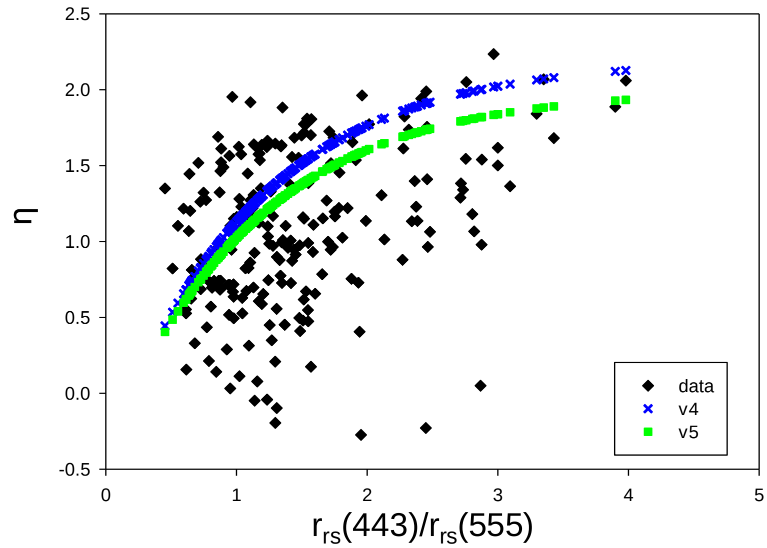

Figure 2. Relationship between η (Y-axis) and $r_{rs}(443)/r_{rs}(555)$ (X-axis). Symbol square for data, blue line for Eq.10, blue line for estimates by QAA-v4.

Values of ζ (= $a_{ph}411/a_{ph}443$), and ξ (= $a_{dg}411/a_{dg}443$) are required for the analytical decomposition of the total absorption spectrum, and their estimations are adjusted to the following, respectively (Fig.3)

$$\zeta = 0.74 + \frac{0.2}{0.8 + r_{rs}(443)/r_{rs}(55x)} \tag{11}$$

$$\xi = e^{S(443-411)}, \quad S = 0.015 + \frac{0.002}{0.6 + r_{rs}(443)/r_{rs}(555)} \tag{12}$$

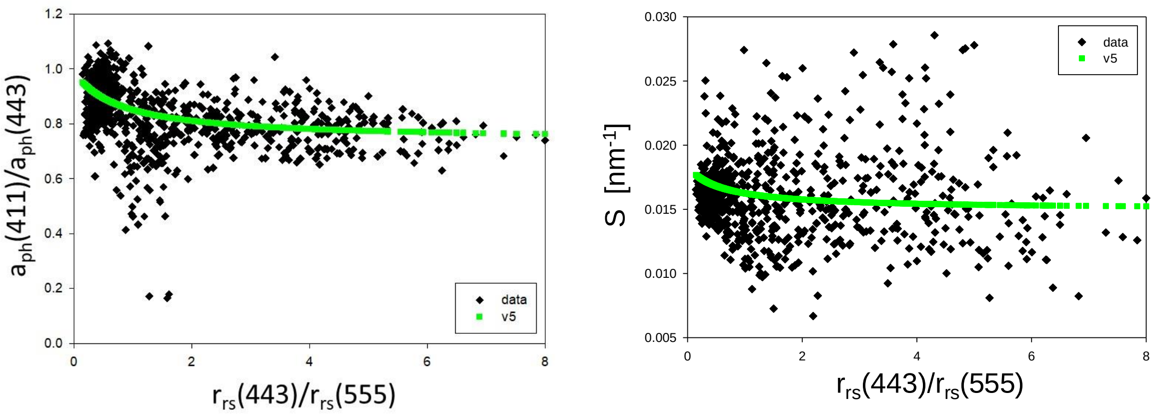

Figure 3. Relationships between $a_{ph}(411)/a_{ph}(443)$ (left), S (right), and $r_{rs}(443)/r_{rs}(555)$ (X-axis), respectively. Data points with $a_{ph}(411)/a_{ph}(443) > 1.1$ are excluded.

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