# Inclusion of variables in semi-analytical model to retrieve marine inherent optical properties from deep waters

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**Abstract**

In optically deep waters, remote sensing reflectance (Rrs) is expressed as the ratio of the backscattering coefficient (bb) and the sum of absorption and backscattering coefficients (a+bb) with a multiplicative model parameter "g". Parameter "g" itself is expressed as function of g0, g1 and u (= bb/ (a+bb)). For oceanic case 1 waters and coastal waters, different constant values for g0 and g1 are proposed owing to varying scattering conditions and particle phase function. In this study, we used g0 and g1 as variables (instead of constants) in the semi-analytical model to retrieve marine Bulk Inherent Optical Properties (IOPs – a and bb) from Rrs. To assess the performance of proposed increase in variables, Rrs values at six SeaWiFS wavelengths 410, 443, 490, 510, 550 and 670 nm are taken from NASA bio-Optical Marine Algorithm Dataset, with Particle Swarm Optimization (PSO) as the optimization technique for inversion of Rrs. Results show that the Multiplicative Bias values obtained with g0 and g1 considered as variables for Bulk IOPs (a – 0.79, bb – 1.27) are better than standard semi-analytical model (a – 0.77, bb – 1.32). We observed similar results using another statistic: Mean Absolute Error. We propose to include g_0 and g_1 as variables for retrieval of IOPs from rrs using semi-analytical models.

Keywords: Semi-analytical model, deep waters, Inherent Optical Properties, PSO

## 1. INTRODUCTION

Ocean color is measured by subsurface remote sensing reflectance ($r_{rs}$) [1][2] , defined as a ratio of upwelling radiance $[L_u(0-)]$ to downwelling irradiance $[E_d(0-)]$ at zero depth:

$$r_{rs} = \frac{L_u(0-)}{E_d(0-)} \tag{1}$$

The relation between $r_{rs}$ and in – water constituents can be used to estimate water properties from remotely sensed data of $r_{rs}$. Various numerical simulation tools such as Monte Carlo method [3], [4] or the Hydrolight model [5] are used to develop relations between $r_{rs}$ and Inherent Optical Properties (IOPs) of water. But, numerical simulations alone cannot completely describe the ocean color and water properties relations. Owing to some of the limitations of the existing remote sensing reflectance models, semi analytical models with molecular and particle scattering functions are developed [2]. In this study, we propose an improved semi-analytical model to overcome some of the limitations and compare with standard Semi-analytical model. The order of the paper is as follows: Section – II will briefly describe the general semi-analytical model used for generation of model spectra and the proposed modifications. Section – III will give information about the standard dataset used for the study. Section – IV will mention about the optimization routine used for finding optimal values of IOPs in $r_{rs}$ inversion. Section – V will discuss the results and discussion from the study.

## 2. FORWARD SEMI-ANALYTICAL MODEL

In this section, we briefly mention about the generally used semi-analytical model used for generation of model spectra. Remote sensing reflectance above the surface ($R_{rs}$, $sr^{-1}$), is defined as ratio of water – leaving radiance to downwelling irradiance just above the surface for optically deep waters and is measured by sensors. To convert $R_{rs}$ to subsurface remote sensing reflectance ($r_{rs}(\lambda), sr^{-1}$) for a nadir – viewing angle, the following relation given by [6] is used

$$r_{rs}(\lambda) = \frac{R_{rs}(\lambda)}{0.52+1.7\, R_{rs}(\lambda)} \tag{2}$$

$r_{rs}$ is modelled as a function of absorption and backscattering coefficients as in [3].

$$r_{rs}(\lambda) = g_0 u(\lambda) + g_1[u(\lambda)]^2 \tag{3}$$

With

$$u = \frac{b_b}{a+b_b} \tag{4}$$

For nadir – viewed $r_{rs}$ and oceanic case 1 waters, [3] proposed the values of $g_0 \approx 0.0949$ and $g_1 \approx 0.0794$. Here, a is the total absorption coefficient expressed as sum of absorption coefficients for pure water, phytoplankton pigments and gelbstoff. $b_b$ is the total backscattering coefficient expressed as sum of scattering coefficients for pure seawater and particles. $\lambda$ is the wavelength. The modelling of coefficients a and $b_b$ is mentioned below briefly

$$a(\lambda) = a_w(\lambda) + a_\phi(\lambda) + a_g(\lambda) \tag{5}$$

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda) \tag{6}$$

For a given temperature and salinity, $a_w(\lambda)$ and $b_{bw}(\lambda)$ are laboratory measured absorption and backscattering coefficients of pure sea water taken as constants in the semi-analytical model. The $a_w(\lambda)$ are taken from [7] and $b_{bw}(\lambda)$ values from [8]. $a_\phi(\lambda)$ is phytoplankton absorption is based on model given by [9]

$$a_\phi(\lambda) = \left(a_0(\lambda) + a_1(\lambda)\, ln\left(a_\phi(443)\right)\right)\, a_\phi(443) \tag{7}$$

The values of $a_0(\lambda)$ and $a_1(\lambda)$ are mentioned in [9]. $a_g(\lambda)$ is absorption coefficient of gelbstoff and detritus expressed as in [10]–[13].

$$a_g(\lambda) = a_g(443)\, exp[-S\,(\lambda - 443)] \tag{8}$$

S is a empirically determined spectral slope reported in the range of 0.011 – 0.021 $nm^{-1}$. A value of 0.0206 $nm^{-1}$ is used as a representative average as in [14]. $a_g$ represents sum of gelbstoff and detritus absorption spectra.

$b_{bp}(\lambda)$ is backscattering due to particulate material which is modelled as a hyperbolic function of wavelength as in [6]. The hyperbolic slope is determined empirically based on ratio of $r_{rs}(443)$ and $r_{rs}(555)$.

$$b_{bp}(\lambda) = b_{bp}(555) * \left[\frac{555}{\lambda}\right]^{Y} \quad (9)$$

$$Y = 2.2\left[1 - 1.2\, exp\left(-0.9\frac{r_{rs}(443)}{r_{rs}(555)}\right)\right] \quad (10)$$

With above spectral models using empirical constants, $r_{rs}$ can be described as a function below and is mentioned hereafter as SAA3v (Semi Analytical Model with 3 variables) with wavelength consideration.

$$r_{rs} = fun\left(a_{\phi}, a_{dg}, b_{bp}, \lambda\right) \quad (11)$$

**Parameter "g" and its variations:**

In Eq. 3 and 4, the values of $g_0 \approx 0.0949$ and $g_1 \approx 0.0794$ were originally obtained by least squares regression of Monte Carlo simulated data for Oceanic Case 1 waters by [3]. Later, for higher scattering coastal waters, [13] proposed values of $g_0 \approx 0.084$ and $g_1 \approx 0.17$. In development of QAA (Quasi – analytical algorithm), averaged values of $g_0 = 0.0895$ and $g_1 = 0.1247$ are used by [6] with an aim to develop a model suitable for both coastal and open – ocean waters. However, the values of $g_0$ and $g_1$ may vary with particle phase function and not known remotely [6].

As mentioned in [2], the Eq.n. 3 has some limitations which are 1. The values provided by [3] for $g_0$ and $g_1$ are for nadir viewing sensors and are not applicable to sensors measuring water color away from nadir to avoid sun glint. 2. Eq.n 3 will give the same g value for different a and $b_b$ values as long as they result in same $b_b/(a + b_b)$ value. A semi-analytical $r_{rs}$ model is developed by [2] to overcome some of the above limitations, by partitioning parameter "g" to include effects of molecular and particle scattering to $r_{rs}$ as below

$$g = g_w\frac{b_{bw}}{b_b} + g_p\frac{b_{bp}}{b_b} \quad (12)$$

$$g_p = G_0\left[1 - G_1\, exp\left(-G_2\frac{b_{bp}}{a+b_b}\right)\right] \quad (13)$$

Here $g_w$ and $g_p$ are two independent model parameters for molecular and particle scattering. $b_{bw}$ and $b_{bp}$ are molecular and particle contribution as in [15]. The values $G_0, G_1$ and $G_2$ for various viewing angles and a particle phase function are calculated in [2].

In this study, we propose to treat $g_0$ and $g_1$ as variables in Eq.ns 3 and 4 with their variation in between oceanic case 1 and coastal waters i.e. $g_0$ will vary from 0.084 – 0.0949 and $g_1$ from 0.0794 – 0.17. The standard semi-analytical model described in Section - II with $g_0$ and $g_1$ as variables is hereby mentioned as SAA5v (Semi analytical model with 5 variables). For every $r_{rs}$, different $g_0$ and $g_1$ will be generated even if the ratio of $b_b/(a + b_b)$ is same, thus overcoming some of the limitations mentioned before. To understand the performance of the proposed inclusion of variables, we compare the proposed SAA5v with SAA3v with values given for nadir viewing sensor.

## 3. STANDARD DATASETS

To validate the proposed SAA5v, we used the NASA Bio – Optical Marine Algorithm Data set (NOMAD [16]), available from SeaBASS website (http://seabass.gsfc.nasa.gov) which consists of field measurements made around the globe. NOMAD dataset provides $R_{rs}$ at bands of 411,443,489,510,555 and 670 nm with corresponding optical properties. We adjusted the absorption and backscattering coefficients of pure seawater (available at 550nm) while using NOMAD dataset. NOMAD data with $r_{rs}$ at first 6 SeaWiFS wavelengths and corresponding $a_{\phi}, a_{dg}, bb_p$ are extracted. Hereafter, called as NOMAD6w. Table 1 gives number of spectra available for individual and bulk IOPs.

## 4. OPTIMIZATION TECHNIQUE

To find the optimal values for $a_{\phi}, a_{dg}, b_{bp}, g_0$ and $g_1$ in SAA5v and SAA3v, we followed spectral optimization technique for inversion of $r_{rs}$ spectra generated using SAA5v and SAA3v. Various computational methods are used to obtain optimized values of variables in Semi-analytical models. Local optimization techniques like Levenberg – Marquardt [17], [18], Nelder – Mead [19] and global optimization techniques like Genetic algorithm (GA) [20], Particle Swarm Optimization (PSO) [21] and Simulated Annealing [22] are used as optimization routines. PSO outperformed GA in terms of both processing time and better retrievals in a study to retrieve IOPs from deep waters [21]. Hence, we used, Particle Swarm Optimization which as a global optimization technique is capable to overcome local minimums and achieve global optimization of an objective function. It is based on behaviour of swarming or flocking animals, such as birds or fish. More information about PSO can be found in ([23]–[25]). The values used as boundary constraints for different variables and for different datasets are mentioned in

Table 2.

For optimization, the following objective function, which minimizes the error between modelled and measured spectra is used as in ([21],[20])

$$\delta = \frac{\sqrt{\sum_{w=1}^{n}\left(r_{rs}(\lambda_w) - \widehat{r_{rs}}(\lambda_w)\right)^2}}{\sum_{w=1}^{n} r_{rs}(\lambda_w)} \tag{14}$$

where $r_{rs}$ represents observed spectra and $\widehat{r_{rs}}$ represents modelled spectra with n as number of wavelengths.

## 5. RESULTS AND DISCUSSIONS

Statistics based on mean squared errors, like $r^2$ (coefficient of determination), Root Mean Square Error (RMSE) and regression slopes are suitable for data with Gaussian distributions and not ideal for ocean color algorithm performance assessment owing to limited amount of data availability. Hence, we used two statistical measures, bias and mean absolute error (MAE) for algorithm performance assessment as suggested by [26] calculated as in Eq.ns 15 and 16. The advantages and disadvantages of different metrics are also discussed in [26].

$$Bias = 10 \wedge \left(\frac{\sum_{i=1}^{n} log_{10}(M_i) - log_{10}(O_i)}{n}\right) \tag{15}$$

$$MAE = 10 \wedge \left(\frac{\sum_{i=1}^{n} |log_{10}(M_i) - log_{10}(O_i)\,|}{n}\right) \tag{16}$$

Where $M_i$ and $O_i$ are modelled and observed values of parameter, n is number of total observations.

The two statistics considered are multiplicative metrics and are dimensionless and the values given are interpreted as: A multiplicative bias of 0.75 (as in $a_{\phi}(443)$ for SAA5v, NOMAD6w dataset) indicates that the model is 25% lesser on average than the observed variable. The bias values obtained closest to unity indicates least bias and bias less than one indicates negative and more than one indicates positive bias. Multiplicative MAE always exceeds unity, and a value of 1.5 indicates relative measurement error of 50%.

The bias and MAE values obtained for different IOPs using two SAA's are presented in **Error! Reference source not found.**. The bias values for $a_{\phi}$ and $a_{dg}$ are below one, implying negative bias for NOMAD 6w dataset. In case of $b_{bp}$, positive bias values are obtained. For $a_{tot}$, both SAA5v and SAA3V models gave negative bias values. As $bb_{tot}$ is sum of $b_{bp}$and $b_{bw}$, with $b_{bw}$ a constant value, the $bb_{tot}$ bias values followed the similar trend as in $bb_{p}$. From the **Error! Reference source not found.**, it is evident that SAA5v performed better than SAA3V for total absorption and backscattering coefficients. In case of metrics for individual component absorption and particulate backscattering coefficients, SAA5v performed better than SAA3v in case of $a_{\phi}$ and $bb_{p}$ but vice-versa in case of $a_{dg}$. This can be due to the choice of spectral models. The study further can be extended by using various spectral models available in Generalized Inherent Optical Property model (GIOPs) developed by [27]. Further, the study needs to be extended to use various optimization algorithms (global and local) to verify the results.

## 6. CONCLUSIONS

In the relation between $r_{rs}$, bulk absorption and backscattering coefficients, the parameter 'g' is often considered constant. The value of 'g' parameter vary with particle phase function and scattering properties of the water and is variable in nature. In this study, the parameter 'g' is taken as variable and is allowed to vary between the limits for deep and coastal water (high scattering). Our study shows that by including g0 and g1 as variables will improve the bias and MAE values for bulk IOPs retrieved from deep water $r_{rs}$. With suggested metrics like Multiplicative Bias and MAE, the study showed an improvement. Further studies can be conducted using other spectral models available for modelling $a_{\phi}, a_{dg}$and $b_{bp}$ to understand the performance of proposed SAA5v model. In the processing of satellite imagery to retrieve IOPs, the proposed SAA5v model can be tested.

## REFERENCES


[1] J. H. Jerome, R. P. Bukata, and J. R. Miller, "Remote sensing reflectance and its relationship to optical properties of natural waters," *Int. J. Remote Sens.*, vol. 17, no. 16, pp. 3135–3155, 1996.

[2] Z. Lee, K. L. Carder, and K. Du, "Effects of molecular and particle scatterings on the model parameter for remote-sensing reflectance," *Appl. Opt.*, vol. 43, no. 25, p. 4957, 2004.

[3] H. R. Gordon *et al.*, "A semianalytic radiance model of ocean color," *J. Geophys. Res.*, vol. 93, no. D9, p. 10909, 1988.

[4] a Morel and B. Gentili, "Diffuse-Reflectance of Oceanic Waters. 2. Bidirectional Aspects," *Applied Optics*, vol. 32, no. 33. pp. 6864–6879, 1993.

[5] C. D. Mobley, L. K. Sundman, and E. Boss, "Phase function effects on oceanic light fields," *Appl. Opt.*, vol. 41, no. 6, p. 1035, 2002.

[6] Z. Lee, K. L. Carder, and R. A. Arnone, "Deriving inherent optical properties from

water color: a multiband quasi-analytical algorithm for optically deep waters.," *Appl. Opt.*, vol. 41, no. 27, pp. 5755–72, 2002.

[7] R. M. Pope and E. S. Fry, "Absorption spectrum (380 - 700nm) of pure water. II. Integrating cavity measurements," *Appl. Opt.*, vol. 36, no. 33, pp. 8710–8723, 1997.

[8] A. Morel, "Optical properties of pure water and pure sea water," *Optical aspects of oceanography*, vol. 1. pp. 1–24, 1974.

[9] Z. Lee, K. L. Carder, C. D. Mobley, R. G. Steward, and J. S. Patch, "Hyperspectral remote sensing for shallow waters. I. A semianalytical model.," *Appl. Opt.*, vol. 37, no. 27, pp. 6329–38, 1998.

[10] A. Bricaud, A. Morel, and L. Prieur, "Absorption by dissolved organic matter of the sea (yellow substance) in the UV and visible domains," *Limnol. Oceanogr.*, vol. 26, no. 1, pp. 43–53, 1981.

[11] K. L. Carder, S. K. Hawes, K. A. Baker, R. C. Smith, R. G. Steward, and B. G. Mitchell, "Reflectance Model for Quantifying Chlorophyll-a in the Presence of Productivity Degradation Products," *J. Geophys. Res.*, vol. 96, no. C11, pp. 20599–20611, 1991.

[12] C. S. Roesler and M. J. Perry, "In situ phytoplankton absorption, fluorescence emission, and particulate backscattering spectra determined from reflectance," *J. Geophys. Res.*, vol. 100, no. C7, p. 22767, 1995.

[13] Z. Lee, K. L. Carder, C. D. Mobley, R. G. Steward, and J. S. Patch, "Hyperspectral remote sensing for shallow waters. 2. Deriving bottom depths and water properties by optimization.," *Appl. Opt.*, vol. 38, no. 18, pp. 3831–43, 1999.

[14] S. Maritorena, D. A. Siegel, and A. R. Peterson, "Optimization of a semianalytical ocean color model for global-scale application Optimization of a semianalytical ocean color model for global-scale applications," *Appl. Opt.*, vol. 41, no. 15, pp. 2705–2714, 2002.

[15] A. Morel and H. Loisel, "Apparent optical properties of oceanic water: dependence on the molecular scattering contribution," *Appl. Opt.*, vol. 37, no. 21, p. 4765, 1998.

[16] P. J. Werdell and S. W. Bailey, "An improved in-situ bio-optical data set for ocean color algorithm development and satellite data product validation," *Remote Sens. Environ.*, vol. 98, no. 1, pp. 122–140, 2005.

[17] K. Levenberg, "A Method for the Solution of Certain Non-Linear Problems in Least," *Q. Appl. Math.*, vol. 2, no. 278, pp. 164–168, 1944.

[18] D. W. Marquardt, "An Algorithm for Least - Squares Estimation of Nonlinear Parameters," *J. Soc. Indust. Appl. Math*, vol. 11, no. 2, pp. 431–441, 1963.

[19] J. A. Nelder and R. Mead, "A Simplex Method for Function Minimization," *Comput. J.*, vol. 7, no. 4, pp. 308–313, 1965.

[20] H. Zhan, Z. Lee, P. Shi, C. Chen, and K. L. Carder, "Retrieval of Water Optical Properties for Optically Deep Waters Using Genetic Algorithms," *IEEE Trans. Geosci. Remote Sens.*, vol. 41, no. 5, pp. 1123–1128, 2003.

[21] W. H. Slade, H. W. Ressom, M. T. Musavi, and R. L. Miller, "Inversion of Ocean

Color Observations Using Particle Swarm Optimization," *IEEE Trans. Geosci. Remote Sens.*, vol. 42, no. 9, pp. 1915–1923, 2004.

[22] S. Kirkpatrick, C. D. Gelatt, and J. M. Vecchi, "Optimization by Simulated Annealing," *Science (80-. ).*, vol. 220, no. 4598, pp. 671–680, 1983.

[23] J. Kennedy and R. Eberhart, "Particle swarm optimization," *Neural Networks, 1995. Proceedings., IEEE Int. Conf.*, vol. 4, pp. 1942–1948 vol.4, 1995.

[24] M. Erik, H. Pedersen, and M. E. H. Pedersen, "Good parameters for particle swarm optimization," *Tech. Rep. HL1001, Hvass Lab.*, vol. HL1001, pp. 1–12, 2010.

[25] E. Mezura-Montes and C. A. Coello Coello, "Constraint-handling in nature-inspired numerical optimization: Past, present and future," *Swarm Evol. Comput.*, vol. 1, no. 4, pp. 173–194, 2011.

[26] B. N. Seegers, R. P. Stumpf, B. A. Schaeffer, K. A. Loftin, and P. Jeremy Werdell, "Performance metrics for the assessment of satellite data products: An ocean color case study," *Opt. Express*, vol. 26, no. 6, pp. 7404–7422, 2018.

[27] P. J. Werdell *et al.*, "Generalized ocean color inversion model for retrieving marine inherent optical properties," *Appl. Opt.*, vol. 52, no. 10, p. 2019, 2013.

Table 1: Number of spectra for NOMAD subset datasets

| IOP | NOMAD6w |
|---|---|
| $a_{\phi}(443)$ | 327 |
| $a_{dg}(443)$ | 307 |
| $bb_{p}(555)$ | 129 |
| $a_{tot}(443)$ | 307 |
| $bb_{tot}(555)$ | 129 |

Table 2: Bounds used for variables in Particle Swarm Optimization

| Parameter ($m^{-1}$) | Minimum constraint | Maximum constraint |
|---|---|---|
| $a_{\phi}(443)$ | 0.001 | 1.5 |
| $a_{dg}(443)$ | 0.001 | 3 |
| $bb_{p}(555)$ | 0.001 | 0.02 |

Table 3: Multiplicative Bias and MAE values obtained for IOPs using SAA5v and SAA3V for NOMAD6w dataset

| Dataset | Model | $a_{\phi}$ (443) | $a_{dg}$ (443) | $b_{bp}$ (555) | $a_{tot}$ (443) | $bb_{tot}$ (555) |
|---|---|---|---|---|---|---|
| NOMAD6w | | **Multiplicative Bias** | | | | |
| | **SAA5v** | 0.79 | 0.69 | 1.38 | **0.79** | **1.27** |
| | **SAA3V** | 0.64 | 0.78 | 1.45 | 0.77 | 1.32 |
| | | **Multiplicative MAE** | | | | |
| | **SAA5v** | 1.71 | 1.68 | 1.42 | **1.40** | **1.30** |
| | **SAA3V** | 1.91 | 1.58 | 1.48 | 1.42 | 1.34 |