Ocean Optics XIV CD-ROM, Kailua-Kona, Hawaii, 10-13 November 1998
(published by Office of Naval Research, November 1998)

ONE-PARAMETER MODEL OF SEAWATER OPTICAL PROPERTIES

Vladimir I. Haltrin

Naval Research Laboratory, Ocean Sciences Branch, Code 7331
Stennis Space Center, MS 39529-5004, USA.
Phone: 228-688-4528, fax: 228-688-5379

haltrin@nrlssc.navy.mil

INTRODUCTION

A one-parameter model of the inherent optical properties of seawater is proposed. The model is based on the results of *in situ* measurements of inherent optical properties that were conducted at different seas and oceans by Carder *et al.* [1], Clark *et al.* [2], Kopelevich [3], and Prieur and Sathyendranath [4]. The pure water optical properties are taken from works by Pope and Fry [5], and Morel and Prieur [6]. The results of these investigations are processed using radiative transfer simulations in order to force this model to satisfactory agree with a regression between the color index and the chlorophyll concentration proposed by Morel and Gordon [7, 8]. The resulting model couples two concentrations of colored dissolved organic matter (concentrations of humic and fulvic acids) and two concentrations of suspended scattering particles (concentrations of terrigenic and biogenic suspensions) with the chlorophyll content in the range of $0 \div 12 \; mg / m^3$.

The model is tested on the independently derived experimental regression, based on experimental data by Timofeyeva [9], that connects the diffuse attenuation coefficient with the single scattering albedo. For the range of chlorophyll concentrations ($0 \div 12 \; mg / m^3$) considered here the match is in the range of an experimental error, *i. e.* about 10%.

MODEL OF SEAWATER OPTICAL PROPERTIES

From the optical point of view, the seawater is an absorbing and scattering medium. The light energy, that propagates in water, is absorbed by the water molecules and dissolved organic matter (DOM) or yellow substance or “Gelbstoff”. By propagating the light is also elastically scattered by the thermal fluctuations in water (Rayleigh scattering) and by the hydrosol particles suspended in water (Mie scattering). The major portion of absorbed energy is transformed to the heat. The rest of the absorbed energy is re-emitted back with the increase in wavelength (Raman scattering and fluorescence). The elastic scattering occurs without the change in energy, only the direction of propagation changes.

All optical properties of seawater are divided on two groups: inherent optical properties and apparent optical properties. Inherent optical properties depend only on processes of absorption and single scattering in seawater. Apparent optical properties are determined by processes of radiative transfer in the sea. These properties depend on inherent optical properties, geometry of illumination, and processes of transmission and reflection by the sea surface and sea bottom.

There are only two major inherent optical properties: an absorption coefficient a and an angular scattering coefficient $\beta(\vartheta)$ (here ϑ is a scattering angle). All other inherent optical properties, the phase function of scattering $p(\vartheta) \equiv \beta(\vartheta) / b$, the scattering coefficient $b = 0.5 \int_0^{\pi} \beta(\vartheta) \sin\vartheta \, d\vartheta$, the beam attenuation coefficient $c = a + b$, the single scattering albedo $\omega_0 = b / c$, the backscattering coefficient $b_B = 0.5\int_{\pi/2}^{\pi} \beta(\vartheta)\sin\vartheta\, d\vartheta$, the probability of backscattering $B = 0.5\int_{\pi/2}^{\pi} p(\vartheta)\sin\vartheta\, d\vartheta$, and the Gordon's parameter $g = \omega_0\, B / (1 - \omega_0 + \omega_0\, B)$, are derivatives of the two major inherent optical properties.

The model presented here has been constructed and tested during more than a decade [12-14]. It represents an integrated entity constructed from a time-proven pieces proposed by different researchers.

MODEL OF ABSORPTION

The absorption coefficient $a(\lambda)$, (m^{-1}) is taken to be:

$$a(\lambda) = a_w(\lambda) + a_c^0(\lambda)\left(C_c / C_c^0\right)^{0.602} + a_f^0\, C_f \exp(-k_f\, \lambda) + a_h^0\, C_h \exp(-k_h\, \lambda)\,, \qquad (1)$$

where $a_w(\lambda)$ is the pure water absorption coefficient in m^{-1}, λ is the vacuum wavelength of light in *nm*, $a_0^c(\lambda)$ is the specific absorption coefficient of chlorophyll in m^{-1} , C_c is the total concentration of chlorophyll in mg / m^3 $(C_c^0 = 1 mg / m^3)$, $a_f^0 = 35.959\, m^2 / mg$ is the specific absorption coefficient of fulvic acid (the first component of the DOM); $k_f = 0.0189\, nm^{-1}$; $a_h^0 = 18.828\, m^2 / mg$ is the specific absorption coefficient of humic acid (the second component of DOM); $k_h = 0.01105\, nm^{-1}$; C_f and C_h are, respectively, concentrations of fulvic and humic acids in mg / m^3. The values for $a_w(\lambda)$, and $a_0^C(\lambda)$ are given in Refs. [5, 4], and the values for DOM components are given in Refs. [1, 15].

MODEL OF SCATTERING

The scattering $b(\lambda)$ and backscattering $b_B(\lambda)$ coefficients are calculated according to Refs. [3, 10, 11, 14, 15]:

$$b(\lambda) \;=\; b_w(\lambda) + b_s^0(\lambda)\, C_s + b_l^0(\lambda)\, C_l\;, \qquad (2)$$

$$b_B(\lambda) \;=\; 0.5\, b_w(\lambda) + B_s\, b_s^0(\lambda)\, C_s + B_l\, b_l^0(\lambda)\, C_l\;, \qquad (3)$$

here

$$B_s = 0.5\int_{\pi/2}^{\pi} p_s(\vartheta)\sin\vartheta\, d\vartheta = 0.039, \quad B_l = 0.5\int_{\pi/2}^{\pi} p_l(\vartheta)\sin\vartheta\, d\vartheta = 6.4\cdot 10^{-4}, \qquad (4)$$

B_s is a probability of backscattering by small particles, B_l is a probability of backscattering by large particles, $b_w(\lambda)$ is the scattering coefficient by pure water in m^{-1}, $b_s^0(\lambda)$ and $b_l^0(\lambda)$ are, respectively, the specific scattering coefficients in m^2 / g for small and large particulate matter, C_s and C_l are, respectively ,concentrations in g / m^3 of small and large particles. The equation for $b_w(\lambda)$ is derived by interpolating the data published by Morel and Prieur [6]:

$$b_w(\lambda) \;=\; \left(5.826\cdot 10^{-3}\, m^{-1}\right)\left(\frac{400}{\lambda}\right)^{4.322}. \qquad (5)$$

The spectral dependencies for scattering coefficients of small and large particulate matter are given by the following equations [3, 10]:

$$b_s^0(\lambda) \;=\; \left(1.1513\, m^2 / g\right)\left(\frac{400}{\lambda}\right)^{1.7}, \tag{6}$$

$$b_l^0(\lambda) \;=\; \left(0.3411\, m^2 / g\right)\left(\frac{400}{\lambda}\right)^{0.3}. \tag{7}$$

Expressions for the phase functions of scattering by small and large particles, $p_s(\vartheta)$ and $p_l(\vartheta)$, are given below.

The phase function of scattering is derived earlier by O. Kopelevich from results of *in situ* measurements. This phase function was proposed in a tabular form in Ref. [3] as a part of a physical model of light scattering in seawater. The Kopelevich model expresses the total hydrosol scattering function as a linear combination of two phase functions p_s and p_l. The phase function p_s describes scattering by small terrigenic fraction of particles with the density $\rho_s = 2\,g / cm^3$. The phase function p_l describes scattering by large particles associated with a biogenic fraction of marine hydrosol with the density $\rho_l = 1\,g / cm^3$. The total hydrosol angular scattering coefficient is expressed as follows:

$$\beta_H(\lambda,\vartheta) = b_s^0(\lambda)\, p_s(\vartheta)\, C_s + b_l^0(\lambda)\, p_l(\vartheta)\, C_l. \tag{8}$$

The small- and large-component phase functions in Eq. (8) can be expressed by the following regressions [16]:

$$p_S(\vartheta) = 5.61746 \exp\left(\sum_{n=1}^{5} s_n\, \vartheta^{3n/4}\right), \quad p_L(\vartheta) = 188.381 \exp\left(\sum_{n=1}^{5} l_n\, \vartheta^{3n/4}\right), \tag{9}$$

here ϑ is the scattering angle in degrees. The coefficients s_n and l_n are given in Table 1.

Table 1. The coefficients in Eqs. (9) for two basic phase functions p_s and p_l.

n	1	2	3	4	5
s_n	-2.957089E-2	-2.782943E-2	1.255406E-3	-2.155880E-5	1.356632E-7
l_n	-1.604327	8.157686E-2	-2.150389E-3	2.419323E-5	-6.578550E-8

The seawater angular scattering coefficient is a linear combination of a Rayleigh phase function of scattering p_R and a hydrosol phase functions p_s and p_l:

$$\beta(\lambda,\vartheta) \;=\; b_w(\lambda)\, p_R(\vartheta) + b_s^0(\lambda)\, p_s(\vartheta)\, C_s + b_l^0(\lambda)\, p_l(\vartheta)\, C_l. \tag{10}$$

Equations (1)–(10) allow us to compute inherent optical properties of seawater a, b, b_B, and $\beta(\lambda,\vartheta)$ as functions of wavelength and five concentrations C_c, C_h, C_f, C_s, C_l of dissolved and suspended matter.

RELATIONSHIPS BETWEEN CONCENTRATIONS

Results of *in situ* measurements of seawater optical properties show that in a majority of cases any two formerly independent optical properties correlate with each other.

In experiments and *in situ* measurements by Timofeyeva [9, 17-20] the diffuse attenuation coefficient correlates with the single scattering albedo and the diffuse reflection coefficient. Processing of all Petzold phase functions [21, 16] shows that the parameters of these phase functions correlate with a scattering coefficient and a single scattering albedo. In papers by Morel and Gordon [7, 8] the following correlation is proposed to estimate the chlorophyll concentration C_r in the upper ocean layer:

$$C_r = 1.92\ I_c^{1.8}, \quad I_c = R(550)/R(440), \tag{11}$$

here $R(\lambda)$ is a diffuse reflectance at wavelength λ. All these dependencies indicate that we can choose a single parameter to characterize all inherent optical properties. The optical model given by Eqs. (1)-(10) depends on five parameters: C_c, C_h, C_f, C_s, C_l. One-parameter model implies that we can express any four of these concentrations through a chosen fifth one. It is convenient to choose the chlorophyll concentration C_c as our main parameter. To derive four dependencies that express four concentrations C_h, C_f, C_s, C_l. through a chlorophyll concentration C_c we minimized the following five-dimensional functional:

$$\Delta(C_c, C_f, C_h, C_s, C_l) = \left|C_c - C_r\right| \equiv \left|C_c - 1.92\left[\frac{R_\infty(550)}{R_\infty(440)}\right]^{1.8}\right|. \tag{12}$$

The dependence of $R = R_\infty$ on a and b_B in Eq. (12) is taken from Ref. [12]. Two stabilizing relationships: $C_h/(C_h + C_f) = 0.1$ [1, 13] and $C_s + C_l = 0.5C_c^{0.75}$ [2] have been used to restrict a number of solutions. The statistical software package Data Desk® was used to solve this problem. For chlorophyll concentrations in the range of $0 \le C_c \le 12\,mg/m^3$ a number of solutions have been found. The single physically meaningful solution to this problem is presented below in a form of the four dependencies:

$$\left.\begin{aligned}
C_f &= 1.74098 \cdot C_c \cdot \exp\left(0.12327 \cdot C_c\right),\\
C_h &= 0.19334 \cdot C_c \cdot \exp\left(0.12343 \cdot C_c\right),\\
C_s &= 0.01739 \cdot C_c \cdot \exp\left(0.11631 \cdot C_c\right),\\
C_l &= 0.76284 \cdot C_c \cdot \exp\left(0.03092 \cdot C_c\right).
\end{aligned}\right\} \tag{13}$$

These dependencies allow us to calculate concentrations of dissolved organic matter (C_f, C_h) and concentration of particles (C_s, C_l) through the concentration of chlorophyll C_c. Dependencies (13) with Eqs. (1)-(10) constitute a one-parameter model of seawater optical properties.

VALIDATION

To validate a one-parameter model of seawater optical properties, two separate tests have been made:

1) The dependence between a color index $I_c(R)$ and chlorophyll concentration C_c was calculated using the proposed optical model. For the calculation of the color index I_c the following more general equation for diffuse reflectance under combined illumination by sun and sky have been used [12, 22]:

$$R = \frac{R_\infty + \mu_s\, q\, R_s}{1 + \mu_s\, q} \qquad (14)$$

where

$$R_\infty = \left(\frac{1-\bar{\mu}}{1+\bar{\mu}}\right)^2, \quad R_s = \frac{(1-\bar{\mu})^2}{1+\bar{\mu}\,\mu_s\,(4-\bar{\mu}^2)}, \qquad (15)$$

$$\bar{\mu} = \sqrt{\frac{a}{a+3b_B+\sqrt{b_B\,(4a+9b_B)}}}, \quad \mu_s = \sqrt{1-\left(\frac{\cos h_s}{n_w}\right)^2}, \qquad (15)$$

here $0 \le q \le 10$ is a ratio of illumination by sun to the illumination by sky [22], h_s is a solar elevation angle, $n_w \approx 4/3$ is the water refraction index. The computations have been made for all ranges of q's, chlorophyll concentrations $0 \le C_c \le 12\, mg/m^3$, and solar elevation angles $5° \le h_s \le 90°$. The computed regression ideally coincides with the left hand side of Eq. (11) and is shown in Fig. 1.

2) Using the presented model and the theory of Ref. [12] linked arrays of a single-scattering albedo and asymptotic diffuse attenuation coefficients were calculated for the range of chlorophyll concentrations $0 \le C_c \le 12\, mg/m^3$. The computed dependence between diffuse attenuation coefficient and single-scattering albedo and the similar experimental dependence published in Ref. [9] are shown in Fig. 2. These dependencies are very close and lie in the 10% error range.

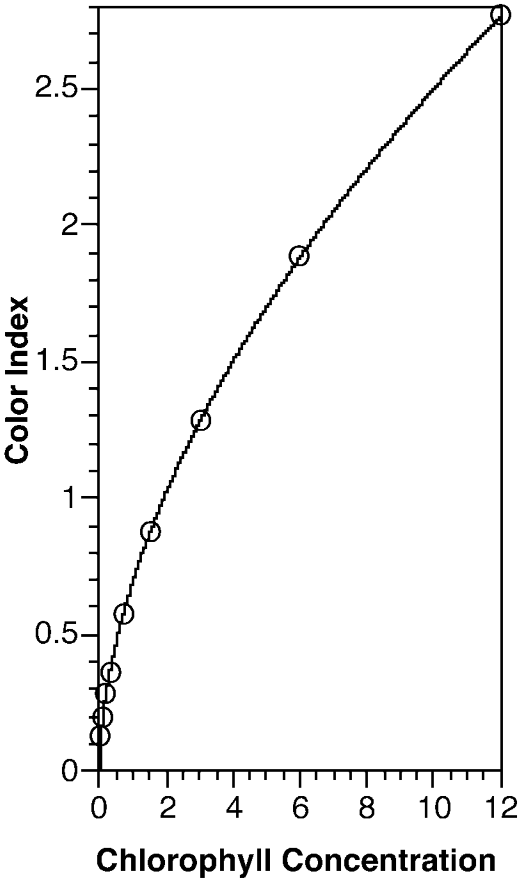
It is possible to conclude now that the presented one-parameter optical model of seawater inherent optical properties gives a good description of optical properties for the chlorophyll concentrations up to $12\, mg/m^3$. It is applicable to the open ocean waters and to the biologically pure coastal waters where clay, quartz and detritus correlate with a chlorophyll content.

CONCLUSION

A one-parameter model of the inherent optical properties of seawater is proposed. The model expresses spectral absorption, spectral scattering and spectral angular scattering coefficients of seawater through the concentration of chlorophyll.

The model is based on the results of *in situ* measurements of inherent optical properties that were conducted at different seas and oceans by a number of researchers. The results of these investigations are processed n order to force this model to satisfactory agree with the well-known regression $C_c = 1.92\, I_c^{1.8}$ [7, 8] between the color index I_c and the chlorophyll concentration C_c. The resulting model couples two concentrations of colored dissolved organic matter (concentrations of humic and fulvic acids) and two concentrations of suspended scattering particles (concentrations of terrigenic and biogenic suspensions) with the chlorophyll content.

The model is tested on the independently derived experimental regression, that connects the asymptotic diffuse attenuation coefficient with the single scattering albedo. For the range of chlorofyll concentrations ($0 \le C_c \le 12\, mg/m^3$) the match is in the range of an experimental error. This one-parameter model of seawater optical properties is applicable to the open ocean waters and to the biologically pure coastal waters where clay, quartz and detritus correlate with a chlorophyll content.



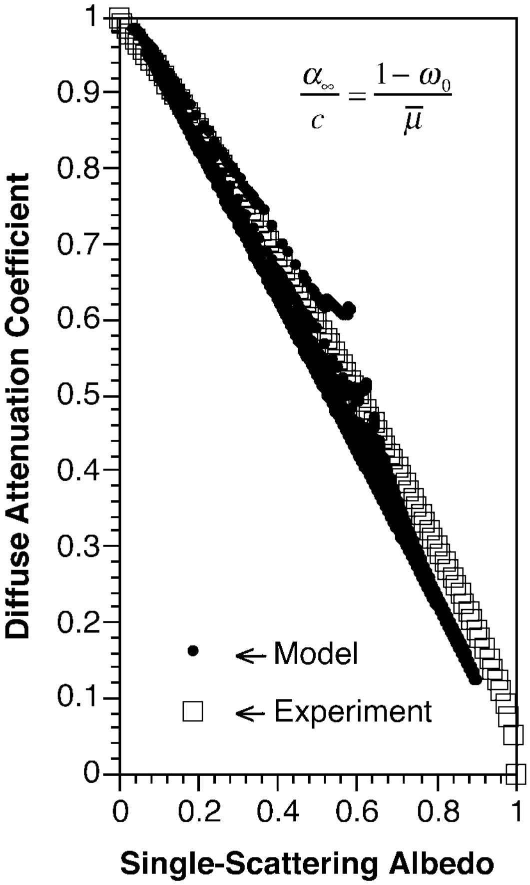


Figure 1 (left). The regression between the color index $I_c = R(550)/R(440)$ and the chlorophyll concentration C_c computed for different types of illumination (symbols) as compared to the regression $C_c = 1.92\, I_c^{1.8}$ (solid line).

Figure 2 (right). The computed, using Eqs. (14)-(15) and the model given by Eqs. (1)-(10), and the experimental [9] regressions between the asymptotic diffuse attenuation coefficient α_∞ (in units of the beam attenuation coefficient c) and the single-scattering albedo ω_0.

ACKNOWLEDGMENT

The author thanks continuing support at the Naval Research Laboratory through the Littoral Optical Environment (LOE 6640-08) and Optical Oceanography (OO 73-5051-08) programs. He also is grateful to Dr. Alan D. Weidemann for help. This article represents NRL contribution PP/7331–98–0017.

REFERENCES

1. K. L. Carder, R. G. Stewart, G. R. Harvey, and P. B. Ortner, “Marine humic and fulvic acids: Their effects on remote sensing of ocean chlorophyll,” *Limnol. Oceanogr*. **34**, 68-81 (1989).

2. D. K. Clark, E. T. Backer, and. A. E. Strong, “Upwelled spectral radiance distribution in relation to particular matter in water,” *Boundary-Layer Meteorol.*, **18**, 287-298 (1980).
3. O. V. Kopelevich, “Small-Parametric Model of the Optical Properties of Seawater,” in *Ocean Optics*, ***I****: Physical Ocean Optics*, A. S. Monin, ed., (Nauka Publishing, Moscow, 1983), 208-234, in Russian.
4. L. Prieur, and S. Sathyendranath, “An Optical Classification of Coastal and oceanic waters based on the specific spectral absorption curves of phytoplankton pigments, dissolved organic matter, and other particulate materials,” *Limnol. Oceanogr.*, **26**, 671-689 (1981).
5. R. M. Pope, and E. S. Fry, “Absorption spectrum (380-700 nm) of pure water: II. Integrating cavity measurements,” *Appl. Optics*, **36**, 8710-8723 (1997)
6. A. Morel, and L. Prieur, “Analysis of Variations in Ocean Color,” *Limnol. Oceanogr.*, **22**, 709–722 (1977).
7. A. Morel, “In-water and remote measurement of ocean color,” *Boundary-Layer Meteorol.*, **18**, 177-201 (1980).
8. H. R. Gordon, and A. Morel, *Remote assessment of ocean color for interpretation of satellite visible imagery*, A Review, (Springer Verlag, 1983).
9. V. A. Timofeyeva, “Optical characteristics of turbid media of the seawater type,” *Izv. Atmos. Ocean Physics*, **7**, 863-865, (1971).
10. V. I. Haltrin (*a.k.a.* В. И. Халтурин), “Propagation of Light in the Sea Depth,” in *Optical Remote Sensing of the Sea and the Influence of the Atmosphere*, V. A. Urdenko and G. Zimmermann, eds., (German Democratic Republic Academy of Sciences Institute for Space Research, Berlin, 1985), 20-62, in Russian.
11. V. I. Haltrin, G. W. Kattawar, and A. D. Weidemann, “Modeling of elastic and inelastic scattering effects in oceanic optics,” in SPIE **2963**, *Ocean Optics XIII*, S. G. Ackleson and R. Frouin, eds., Bellingham, WA, USA, 597-602, (1997).
12. V. I. Haltrin, “Self-consistent approach to the solution of the light transfer problem for irradiances in marine waters with arbitrary turbidity, depth and surface illumination,” *Appl. Optics*, **37**, 3773-3784 (1998).
13. S. K. Hawes, K. L. Carder, and G. R. Harvey, “Quantum fluorescence efficiencies of fulvic and humic acids: effect on ocean color and fluorometric detection”, in SPIE, **1750**, *Ocean Optics XI*, Gary D. Gilbert, ed., 212-223 (1992).
14. V. I. Haltrin, and G. W. Kattawar, *Effects of Raman Scattering and Fluorescence on Apparent Optical Properties of Seawater*, Report, No #, (Department of Physics, Texas A&M University, College Station, Texas, 1991).
15. V. I. Haltrin, and G. W. Kattawar, “Self-consistent solutions to the equation of transfer with elastic and inelastic scattering in oceanic optics: I. Model,” *Appl. Optics*, **32**, 5356-5367, (1993).
16. V. I. Haltrin, “Theoretical and empirical phase functions for Monte Carlo calculations of light scattering in seawater,” in *Proceedings of the Fourth International Conference Remote Sensing for Marine and Coastal Environments*, **I**, No ed., (Envir. Res. Inst. of Michigan, Ann Arbor, MI, 1997), 509-518.
17. V. A. Timofeyeva, “The diffuse reflection coefficient and its relation to the optical parameters of turbid media,” *Izv. Atmos. Ocean Physics*, **7**, 467-469, (1971).
18. V. A. Timofeyeva, “Relation between the optical coefficients in turbid media,” *Izv. Atmos. Ocean Physics*, **8**, 654-656, (1972).
19. V. A. Timofeyeva, “Relation between light field parameters and between scattering phase function characteristics of turbid media, including sea water,” *Izv. Atmos. Ocean Physics*, **14**, 843-848, (1978).
20. V. A. Timofeyeva, “Determination of Light-Field parameters in the depth regime from irradiance measurements,” *Izv. Atmos. Ocean Physics*, **15**, 774-776, (1979).
21. T. J. Petzold, *Volume Scattering Functions for Selected Ocean Waters*, SIO Ref. 72-78, (Scripps Institute of Oceanography, Visibility Laboratory, San Diego, CA, 1972).
22. V. I. Haltrin, “Apparent optical properties of the sea illuminated by Sun and sky: case of optically deep sea,” *Appl. Optics*, **38**, 8336-8340, (1999).