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Beauty of Math in Ocean Optics: Two-Stream Equations of Åas

Lee Zhongping

State Key Lab of Marine Environmental Science, College of Ocean and Earth Sciences, Xiamen University, Xiamen 361102, Fujian, China

Abstract Solar radiation in the visible domain can penetrate aquatic environment, which drives photon-related processes including phytoplankton photosynthesis and heating of the upper water column. In addition, the scattered light in the water column can emerge (escape) from water, which forms the bases to sense properties in aquatic environments using sensors onboard satellites. Thus, an understanding of the processes and properties related to the propagation of solar radiation in-and-out of water is a basic requirement in ocean optics and ocean color remote sensing. The spatial (and spectral for inelastic scattering) variation of radiance is governed by the radiative transfer equation, which is not directly applicable to infer in-water optical properties or to describe the relationships between the optical properties measured in the field and inherent optical properties related to environmental properties. Through simple mathematical derivations, or manipulations, of the radiative transfer equation (RTE), Åas transferred the RTE into a set of two equations describing the change of upwelling and downwelling irradiance with depth, and further obtained concise analytical relationships between the apparent and inherent optical properties. These equations not only form the basic theoretical relationships in ocean optics, but also lay the foundation of semi-analytical algorithms in ocean color remote sensing.

Key words ocean optics; ocean color; radiative transfer; two-stream model; remote sensing; apparent optical properties; inherent optical properties

海洋光学中的优美代数表达: Åas 的两流模型

李忠平*

厦门大学近海海洋环境科学国家重点实验室,海洋与地球学院,福建厦门361102

摘要 太阳辐射(光)能够穿透水体,照耀水体的上层,驱动浮游植物的光合作用和加热水体。同时,水中物质对光的散射导致一部分光逃离水体并进入大气层,从而成为从卫星高度反演水中物质的含量、成分的信息源。因此,理解、刻画光在水中的传播形式以及其与水中物质的关系是海洋光学和水色遥感的最基础的要求和课题。光的空间变化由辐射传递方程决定,但该方程不能够直接用于遥感反演,也不能够直接表达表观光学量与固有光学量之间的关系。通过简单的数学推导,Åas 将辐射传递方程转换成一个优美的两流模式来描述上行和下行辐照度随深度的变化形式,并进一步推导出表观光学量与固有光学量之间的解析关系。该模型给出了海洋光学中最基本的关系式,为水色遥感的半解析算法的研发奠定了基础。

关键词 海洋光学;水色;辐射传输;两流模型;遥感;表观光学量;固有光学量

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1 Background

Ocean optics belongs to the category of

environmental optics. Compared to classical optics or laser optics, where the subject under study is an individual photon or a light beam, ocean optics

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通信作者: *zpli2015@xmu.edu.cn

studies light (or radiance) in a three-dimensional (3D) space, or the diffuse light. For a light beam, the size of a measurement sensor is significantly greater than the width of this light beam, but in ocean optics, it is completely the opposite where sensor's size is incomparable to the radiance environment; consequently, a completely different set of "laws" or relationships must be developed in order to adequately describe, and understand, the variation of radiance in this 3D space.

The quantities that can be adequately measured with a spectroradiometer in this 3D environment are radiance or irradiance, where the latter is an integration of radiance over a predefined angular range, which can also be viewed as a "broad-angle radiance." The propagation of radiance (*L*) is governed by the radiative transfer equation (RTE)^[1], and for radiance in the aquatic environment, it can be written as:

$$\frac{\mathrm{d}L(z,\theta,\varphi)}{\mathrm{d}z}\cos\theta = -c(z)L(z,\theta,\varphi) + \int \beta(z,\theta',\varphi' \to \theta,\varphi)L(z,\theta',\varphi')\,\mathrm{d}\Omega', \qquad (1)$$

where z (in m) is depth from surface and positive, θ is the zenith angle, φ is azimuth angle, and $d\Omega'$ is an infinitesimal solid angle around angle (θ' , φ'). c (in m⁻¹) is the beam attenuation

coefficient, with β (in m⁻¹ • sr⁻¹) for water's volume scattering function, and both c and β are inherent optical properties (IOPs)^[2]. Note that in this equation, it is assumed that there are no internal sources such as fluorescence and Raman scattering, otherwise a third term should be included for radiance from such processes. Also, the variable wavelength (λ) is omitted for brevity.

Equation (1) provides a fundamental law regarding the loss and gain for radiance in a direction after an infinitesimal distance; but, due to its complexity, this equation is not directly applicable for the understanding of irradiance reflectance in water, nor for the inversion of water's inherent optical properties from a reflectance spectrum. A simplified relationship, but with a root in the radiative transfer equation, is required.

2 Simplification with clever algebraic derivations

To establish applicable relationships between apparent optical properties^[2] and IOPs, Åas^[3] worked on Eq. (1) by integrating both sides of Eq. (1) over the 4π solid angle. The left side becomes:

$$\frac{\mathrm{d}}{\mathrm{d}z} \int_{\Omega=0}^{4\pi} L(z,\theta,\varphi) \cos\theta \,\mathrm{d}\Omega = \frac{\mathrm{d}}{\mathrm{d}z} \left[\int_{\Omega=0}^{2\pi_{\mathrm{d}}} L(z,\theta,\varphi) \cos\theta \,\mathrm{d}\Omega - \int_{\Omega=0}^{2\pi_{\mathrm{u}}} L(z,\theta,\varphi) \left| \cos\theta \right| \mathrm{d}\Omega \right] = \frac{\mathrm{d}}{\mathrm{d}z} \left[E_{\mathrm{d}}(z) - E_{\mathrm{u}}(z) \right], \tag{2}$$

with $E_{\rm d}$ for downwelling irradiance, $E_{\rm u}$ for upwelling irradiance, and $2\pi_{\rm d}$ and $2\pi_{\rm u}$ for the solid angles in the downward and upward hemispheres, respectively. The vertical profiles of both $E_{\rm d}$ and

 $E_{\rm u}$ can be adequately measured with a planar irradiance spectroradiometer in the field.

The integration of the right side of Eq. (1) becomes:

$$-c\int_{\Omega=0}^{4\pi} L(z,\theta,\varphi) d\Omega + \int_{\Omega=0}^{4\pi} \left[\left[\beta(z,\theta',\varphi' \to \theta,\varphi) L(z,\theta',\varphi') d\Omega' \right] d\Omega = -cE_{o}(z) + \int_{\Omega'=0}^{4\pi} L(z,\theta',\varphi') \left[\left[\beta(\theta',\varphi' \to \theta,\varphi) d\Omega \right] d\Omega' = -cE_{o}(z) + bE_{o}(z), \right] d\Omega'$$
(3)

where E_o is the scalar irradiance, and b (in m⁻¹) is the scattering coefficient. Note that starting from

here, the variation of IOPs with z is omitted for simplicity.

Since the beam attenuation coefficient is a sum of the absorption coefficient (a) and b, i. e.,

$$c = a + b$$
, (4)

Eq. (2) and Eq. (3) suggest that:

$$\frac{\mathrm{d}}{\mathrm{d}z} \left[E_{\mathrm{d}}(z) - E_{\mathrm{u}}(z) \right] = -aE_{\mathrm{o}}(z). \tag{5}$$

This is the Gershun equation, which is significantly simpler than Eq. (1), but obtained completely differently many decades earlier ^[4]. This equation suggests that, if the three quantities $(E_{\rm o}, E_{\rm d}, {\rm and} E_{\rm u})$ can be accurately measured in the field, a profile of the absorption coefficient can then be calculated.

In a similar manner, but not integrating over the 4π solid angle, rather the upper and lower hemispheres separately, $\text{Åas}^{\text{[3]}}$ obtained a set of equations after introducing shape factors r_d and r_u :

$$\begin{split} \frac{\mathrm{d}E_{\mathrm{d}}(z)}{\mathrm{d}z} &= -\frac{a}{\mu_{\mathrm{d}}(z)} E_{\mathrm{d}}(z) - \\ \frac{r_{\mathrm{d}}(z)b_{\mathrm{b}}}{\mu_{\mathrm{d}}(z)} E_{\mathrm{d}}(z) + \frac{r_{\mathrm{u}}(z)b_{\mathrm{b}}}{\mu_{\mathrm{u}}(z)} E_{\mathrm{u}}(z), & (6) \\ \frac{\mathrm{d}E_{\mathrm{u}}(z)}{\mathrm{d}z} &= -\frac{a}{\mu_{\mathrm{u}}(z)} E_{\mathrm{u}}(z) - \\ \frac{r_{\mathrm{u}}(z)b_{\mathrm{b}}}{\mu_{\mathrm{u}}(z)} E_{\mathrm{u}}(z) + \frac{r_{\mathrm{d}}(z)b_{\mathrm{b}}}{\mu_{\mathrm{d}}(z)} E_{\mathrm{d}}(z), & (7) \end{split}$$

where $b_{\rm b}$ (in m⁻¹) is the backscattering coefficient, and $\mu_{\rm d}$ and $\mu_{\rm u}$ are the average cosine of downwelling and upwelling irradiance, respectively. Shape parameters $r_{\rm d}$ and $r_{\rm u}$ are defined as:

$$r_{\rm d}(z) = \frac{1}{b_{\rm b}E_{\rm od}(z)} \times \int_{\Omega'=0}^{2\pi_{\rm d}} \left[\int_{\Omega=0}^{2\pi_{\rm u}} \beta(\theta', \varphi', \theta, \varphi) d\Omega \right] L(z, \theta', \varphi') d\Omega', (8)$$
$$r_{\rm u}(z) = \frac{1}{b_{\rm b}E_{\rm ou}(z)} \times$$

$$\int_{\Omega'=0}^{2\pi_{\rm u}} \left[\int_{\Omega=0}^{2\pi_{\rm d}} \beta(\theta', \varphi', \theta, \varphi) \,\mathrm{d}\Omega \right] L(z, \theta', \varphi') \,\mathrm{d}\Omega', \quad (9)$$

with $E_{\rm od}$ and $E_{\rm ou}$ for the downwelling and upwelling scalar irradiance, respectively. Basically $r_{\rm d}$ and $r_{\rm u}$ reflects normalized reflectance coefficients of downward and upward scalar

irradiance, respectively. For chlorophyll concentration in a range of 0.01–10.0 mg/m³ and assume the optical properties of other constituents co-vary with that of chlorophyll, the values of $r_{\rm d}$ and $r_{\rm u}$ were found in a range of \sim 1.2–20, with $r_{\rm u}/r_{\rm d}$ ratio of roughly 1.4–2.2^[5].

Equation (6) and equation (7) are the famous two-stream equations that describe the vertical variations of $E_{\rm d}$ and $E_{\rm u}$, which show that the consequence of absorption is always a loss for both $E_{\rm d}$ and $E_{\rm u}$, but the backscattering affects both positively (gain) and negatively (loss) for the propagation of these irradiances. Considering that the solar radiation comes from above the sea surface, $E_{\rm u}$ would be 0 (or waters will be black) if there is no backscattering. More importantly, the variations of the four radiance-distribution-related parameters ($\mu_{\rm d}$, $\mu_{\rm u}$, $r_{\rm d}$, and $r_{\rm u}$) vary in a much narrow range in natural aquatic environments^[5-6], which leave the change of $E_{\rm d}$ and $E_{\rm u}$ mainly governed by a and $b_{\rm b}$.

3 Applications of two-stream equations

Define the diffuse attenuation coefficient of downwelling irradiance ($K_{\rm d}$) and irradiance reflectance (R), respectively, as:

$$K_{\rm d} = -\frac{1}{E_{\perp}} \frac{\mathrm{d}E_{\rm d}}{\mathrm{d}z},\tag{10}$$

$$R = \frac{E_{\mathrm{u}}}{E_{\mathrm{d}}},\tag{11}$$

where K_d and R (as well as remote sensing reflectance described below) are the most important AOPs in ocean optics. Divide both side of Eq. (6) by E_d , we can get:

$$K_{d}(z) = \frac{a}{\mu_{d}(z)} + \left[\frac{r_{d}(z)}{\mu_{d}(z)} - \frac{r_{u}(z)R(z)}{\mu_{u}(z)} \right] b_{b},$$
(12)

which, for simplicity, maybe written as:

$$K_{d}(z) = m(z)a + \nu(z)b_{h}.$$
 (13)

This shows that, conceptually, since the four distribution parameters vary in a narrow range^[5-6], the variation of K_d is mainly driven by a and b_b . Further, in principle, since the two scaling parameters (m, ν) of a and b_b to K_d do not equal, Eq. (12) and Eq. (13) indicate that the

weightings of a and b_b to K_d are not the same, contrary to commonly adopted approximations.

Separately, based on Eq. (5), after expanding $E_{\rm o}$ to $E_{\rm od}$ and $E_{\rm ou}$, and omitting the vertical variation of R with depth (for homogeneous waters), there is:

$$R = \frac{\mu_{\mathrm{u}}}{\mu_{\mathrm{d}}} \left(\frac{K_{\mathrm{d}}\mu_{\mathrm{d}} - a}{a + \mu_{\mathrm{u}}K_{\mathrm{d}}} \right). \tag{14}$$

Further, since Eq. (12) indicates $K_{\rm d} \, \mu_{\rm d} - a$ is proportional to $b_{\rm b}$, the above expression indicates that there is:

$$R = \frac{\mu_{\rm u}}{\mu_{\rm d}} \left(1 - \frac{\mu_{\rm d}}{\mu_{\rm u}} \frac{r_{\rm u}}{r_{\rm d}} R \right) \frac{r_{\rm d} b_{\rm b}}{a + \mu_{\rm u} K_{\rm d}}.$$
 (15)

Considering the ratio $r_{\rm u}/r_{\rm d}$ is in a narrow range^[5-6] and the value of R is small (generally less than a few percent for oceanic waters), the above equation approximates:

$$R \approx \frac{\mu_{\rm u}}{\mu_{\rm d}} \frac{r_{\rm d}b_{\rm b}}{a + \mu_{\rm u}K_{\rm d}},\tag{16}$$

or,

$$R \propto \frac{b_{\rm b}}{xa + yb_{\rm b}}.\tag{17}$$

This is an important and basic relationship in ocean optics that is achieved completely from the radiative transfer equation, which is echoed by Sathyendranath and Platt^[7] through a quasi-singlescattering approximation. This relationship shows that to the first order, irradiance reflectance is proportional to the ratio of $b_b/(a+b_b)$ (after model parameters x and y are approximated as equal), with b_b appearing in both nominator and denominator to reflect its positive and negative effects in the propagation of the two streams of irradiance. One important implication of b_b in both nominator and denominator is that when b_b is significantly greater than a (for instance, at some wavelengths for waters with extremely high load of suspended sediments), R will approach an increasing asymptotic value, instead of proportionally (linear or nonlinear) with the increase of concentrations of suspended sediments.

4 Extension to remote sensing reflectance

In a similar fashion and focusing on the upwelling radiance pointing to zenith $[L_u(z, 0, 0)]$, a quantity can be measured by a remote sensor, and Zaneveld^[8] separated the integration term in the right side of Eq. (1) into the upper and lower hemispheres, which becomes:

$$\int_{\Omega'=0}^{4\pi} \beta(\theta', \varphi' \to 0, 0) L(z, \theta', \varphi') d\Omega' =$$

$$\int_{\varphi'=0\theta'=0}^{2\pi} \int_{0}^{\pi/2} \beta(\theta', \varphi' \to 0, 0) L(z, \theta', \varphi') \sin \theta' d\theta' d\varphi' +$$

$$\int_{\varphi'=0\theta'=\pi/2}^{2\pi} \int_{0}^{\pi} \beta(\theta', \varphi' \to 0, 0) L(z, \theta', \varphi') \sin \theta' d\theta' d\varphi'.$$
(18)

Basically, in the right side of Eq. (18), the first integration is over radiance going downward, i.e., it is the backscattering of downwelling radiance contributing to $L_{\rm u}(z,0,0)$. The second integration of the right side of Eq. (18), on the other hand, is over the radiance going upward, i.e., it is the forward scattering of upwelling radiance contributing to $L_{\rm u}(z,0,0)$. Further, Zaneveld^[8] utilized the observations that the volume scattering function in the backscattering domain and the upwelling radiance do not vary greatly for different angles, and then wrote Eq. (18) as:

$$\int_{\Omega'=0}^{4\pi} \beta(\theta', \varphi' \to 0, 0) L(z, \theta', \varphi') d\Omega' =$$

$$f_{b}(z, 0, 0) b_{b} \int_{\varphi'=0\theta'=0}^{2\pi} \int_{\pi/2}^{\pi/2} L(z, \theta', \varphi') \sin \theta' d\theta' d\varphi' +$$

$$f_{L}(z, 0, 0) L_{u}(z) \int_{\varphi'=0\theta'=0}^{2\pi} \beta(\theta', \varphi' \to 0, 0) \sin \theta' d\theta' d\varphi',$$
(19)

with parameters $f_{\rm b}$ and $f_{\rm L}$ defined as (note that here $f_{\rm b}$ has no 2π in the nominator, which then has a unit as ${\rm sr}^{-1}$ and is different from the original $f_{\rm b}$ in Zaneveld, but the essence is the same):

$$f_{b}(z,0,0) = \frac{1}{b_{b}E_{cd}(z)} \int_{e'=0\theta'=0}^{2\pi} \int_{e'=0}^{\pi/2} \beta(\theta',\varphi' \rightarrow 0,0) L(z,\theta',\varphi') \sin\theta' d\theta' d\varphi', \tag{20}$$

$$f_{L}(z,0,0) = \frac{1}{b_{f}L_{u}(z,0,0)} \int_{\varphi'=0\theta'=\pi/2}^{2\pi} \int_{-\pi/2}^{\pi} \beta(\theta',\varphi' \rightarrow 0,0)L(z,\theta',\varphi') \sin\theta' d\theta' d\varphi'. \tag{21}$$

Based on the definition of E_{od} and forward scattering coefficient (b_f) , Eq. (19) leads to:

$$\int_{\Omega'=0}^{4\pi} \beta(\theta', \varphi' \to 0, 0) L(z, \theta', \varphi') d\Omega' = f_{b}(z, 0, 0) b_{b} E_{od}(z) + f_{L}(z, 0, 0) L_{u}(z, 0, 0) b_{f}.$$
(22)

Thus, for upwelling radiance going to zenith $[L_u(z,0,0)]$, applying both Eq. (1) and Eq. (22), there is:

$$-\frac{\mathrm{d}L_{\mathrm{u}}(z,0,0)}{\mathrm{d}z} = -cL_{\mathrm{u}}(z,0,0) + f_{\mathrm{b}}(z,0,0)b_{\mathrm{b}}E_{\mathrm{od}}(z) + f_{\mathrm{L}}(z,0,0)L_{\mathrm{u}}(z,0,0)b_{\mathrm{f}}.$$
(23)

Define ratio (r_s , in sr^{-1}) of upwelling radiance to downwelling scalar irradiance and the diffuse attenuation coefficient of upwelling radiance (K_{Lu}), respectively, as:

$$r_{s}(z,0,0) = \frac{L_{u}(z,0,0)}{E_{od}(z)},$$
 (24)

$$K_{Lu}(z,0,0) = -\frac{\mathrm{d}L_{u}(z,0,0)}{L_{u}(z,0,0)\mathrm{d}z},$$
 (25)

and r_s can then be written as

$$r_{s}(z,0,0) = \frac{f_{b}(z,0,0)b_{b}}{K_{Lu}(z,0,0) + c - f_{L}(z,0,0)b_{f}}.$$
(26)

Further, as $c=a+b=a+b_{\rm b}+b_{\rm f}$, and consider the diffuse attenuation coefficient is in general a function of a and $b_{\rm b}$ [see Eq. (13)], we get:

$$r_{s}(z,0,0) = f_{b}(z,0,0)b_{b} = \frac{f_{b}(z,0,0)b_{b}}{(1+m')a + (1+v')b_{b} + [1-f_{L}(z,0,0)]b_{f}}.$$
(27)

Furthermore, since downwelling scalar irradiance can be converted to downwelling planar irradiance through the average cosine of downwelling irradiance (μ_d), the in-water remotesensing reflectance ($r_{\rm rs}$), defined as the ratio of upwelling radiance to downwelling planar irradiance, is:

$$r_{\rm rs}(z) = \frac{1}{\mu_{\rm d}(z)} \frac{f_{\rm b}(z)b_{\rm b}}{(1+m')a + (1+v')b_{\rm b} + [1-f_{\rm L}(z)]b_{\rm f}}. \tag{28}$$

Again, this is simply a mathematical re-write of the RTE, as Zaneveld^[8] pointed out, "it is an exact solution". What remain unknown are the values of the modeling parameters (f_b , f_L , m', v'). Further, these parameters vary in a narrow range, such as f_L being in a range of 1.0–1.1^[9], and thus the physics meaning of this formulation is very clear: remote sensing reflectance is mainly driven by the absorption and backscattering coefficients.

5 Numerical parameterizations

The above expressions provide a general guidance between AOPs and IOPs, and it is necessary to parameterize the formulations for the purpose to derive IOPs from AOPs or to estimate from the measurement of Unfortunately, this parameterization could not be derived from the RTE, and must rely on data or numerical simulations. Using data simulated from Hydrolight[10-11], Carlo or approximations or numerical parameterizations have been proposed, which include:

1) Irradiance reflectance

Equation (16) or (17) has been commonly simplified to:

$$R = f \frac{b_{\mathrm{b}}}{a + b_{\mathrm{b}}},\tag{29}$$

with f approximated as 0. 33 in Ref. [12], while Morel and Gentili^[13] developed a Look-Up-Table (LUT) for "Case-1" waters. On the other hand, from more than 22000 Hydrolight simulations, Albert and Mobley^[14] proposed a formulation for R as:

$$R = p_1 (1 + p_2 u + p_3 u^2 + p_4 u^3) \times \left(1 + p_5 \frac{1}{\cos \theta}\right) (1 + p_6 U) u, \tag{30}$$

with u for

$$u = \frac{b_b}{a + b_b},\tag{31}$$

where U represents surface wind speed, and θ_s represents subsurface solar zenith angle. Values of p_1-p_6 can be found in Table 3 in Ref. [14].

Separately, for reflectance at a wavelength where b_b is much greater than a (roughly > 2, i. e., high scattering, weak absorption condition)^[15], it is found that the Kubelka-Munk model is also applicable^[16], where R is described as

$$R = \frac{b_{\rm b}/a}{1 + b_{\rm b}/a + \sqrt{1 + 2b_{\rm b}/a}}.$$
 (32)

However, because the absorption coefficient of aquatic environment is highly spectrally dependent, even for waters with high load of sediments, only some wavelengths meet this $b_{\rm b}\!>\!2a$ condition, and thus Eq. (32) may not work well to model an R spectrum from the spectra of $b_{\rm b}$ and $a^{[17]}$.

2) Remote sensing reflectance

Based on Eq. (28), also for simple parameterization, r_{rs} has been commonly approximated as a function of u:

$$r_{\rm rs} = gu, \qquad (33)$$

with the variation of g further expressed as a function of u by Gordon $et\ al.$ ^[18]:

$$g = g_0 + g_1 u. (34)$$

For nadir-viewing $r_{\rm rs}$, values of g_0 and g_1 are found as 0.0949 sr⁻¹ and 0.0794 sr⁻¹ through Monte Carlo simulations^[18]. In addition to this quadratic formulation for $r_{\rm rs}$, Albert and Mobley^[14] proposed to use 4-th order polynomials:

$$r_{\rm rs} = p_1 (1 + p_2 u + p_3 u^2 + p_4 u^3) \times \left(1 + p_5 \frac{1}{\cos \theta_s}\right) (1 + p_6 U) \left(1 + p_7 \frac{1}{\cos \theta_v}\right) u,$$
(35)

where values of p_1-p_7 can be found in Table 3 of Albert and Mobley^[14], with θ_v for sensor's viewing angle in water.

To account for the different phase functions of molecular scattering and particle scattering, it was proposed to express r_{rs} using two separate terms,

$$r_{rs}(\lambda,\Omega) = g_{w}(\Omega) \frac{b_{bw}(\lambda)}{a(\lambda) + b_{b}(\lambda)} + g_{p}(\lambda,\Omega) \frac{b_{bp}(\lambda)}{a(\lambda) + b_{b}(\lambda)},$$
(36)

with

$$g_{\text{w}} = 0.113, g_{\text{p}} = 0.197 \left[1 - 0.636 \exp\left(-2.552 \frac{b_{\text{bp}}}{a + b_{\text{b}}}\right) \right], (37)$$

for nadir-viewing $r_{\rm rs}$ after Hydrolight simulations^[19]. Here $b_{\rm bw}$ and $b_{\rm bp}$ are the backscattering coefficients of pure (sea) water and particles, respectively ($b_{\rm b}=b_{\rm bw}+b_{\rm bp}$), while $g_{\rm w}$ and $g_{\rm p}$ represent different weightings of molecule and particle backscatterings contributing to $r_{\rm rs}$.

3) Diffuse attenuation coefficient of downwelling irradiance

The formulation for K_d [Eq. (12) and Eq. (13)] indicates that this property also varies with depth (light field) even for homogeneous waters. For the averaged attenuation between surface and a depth where 10% of surface solar radiation remains, Lee *et al.* [20] proposed the following approximation:

$$\bar{K}_{d} = (1 + 0.005\theta_{a})a +$$

 $4.26(1-0.265\eta_{\rm w})(1-0.52{\rm e}^{-10.8a})b_{\rm b}$, (38) with $\eta_{\rm w}$ for the ratio of $b_{\rm bw}/b_{\rm b}$, $b_{\rm bw}$ for the backscattering coefficient of pure (sea) water, and $\theta_{\rm a}$ for solar zenith angle in air (in degree).

Based on Hydrolight simulations and for the subsurface diffuse attenuation coefficient of downwelling irradiance $[K_d(0)]$, Albert and Mobley^[14] obtained:

$$K_{\rm d}(0) = 1.055 \, \frac{a + b_{\rm b}}{\cos \theta_{\rm c}},$$
 (39)

which is similar to that found by $\operatorname{Gordon}^{[21]}$ from Monte Carlo simulations. In this kind of formulations, however, the weightings of a and b_b are considered equal, which is not exactly matching that derived from the radiative transfer equation [see Eq. (12)], although a numerical estimation of K_d may not differ much.

6 Contributions from chlorophyll fluorescence and Raman scattering

The above discussions, including Eq. (1), omitted the contributions from inelastic processes, such as those of chlorophyll fluorescence and Raman scattering. While these two are generally small in the surface layer of the ocean compared to the downwelling irradiance from the Sun and sky, they can be significant for some wavelengths and some waters in the upwelling radiance, and thus can be detected for sensors in remote platforms. For chlorophyll fluorescence induced by solar radiation and considering the water column is homogeneous and focusing on the emission wavelength (λ_{em}), after some approximations, Huot *et al.* [22] obtained a relationship of radiance due to chlorophyll fluorescence (L_f) as:

$$L_{\rm f}(\lambda_{\rm em}) = \frac{1}{4\pi} \frac{\phi Q_{\rm a}^*(\lambda_{\rm em})}{C_{\rm f}(\lambda_{\rm em})} \int_{\lambda=400}^{700} \frac{a_{\rm ph}(\lambda) E_{\rm o}(\lambda,0)}{K(\lambda) + a_{\rm f}(\lambda_{\rm em})} d\lambda,$$

(4(

where ϕ is the quantum yield of chlorophyll fluorescence, Q_a^* is the portion of emitted fluorescence not reabsorbed within the cell, $C_{\rm f}$ is the proportionality factor that converts fluorescence at $\lambda_{\rm em}$ to the whole fluorescence band, $a_{\rm ph}$ is the absorption coefficient of phytoplankton, K is the diffuse attenuation coefficient of scalar irradiance, and $a_{\rm f}$ is the attenuation coefficient of upwelling fluorescence radiance. Ratio of $L_{\rm f}$ to $E_{\rm d}(0^-)$ provides the subsurface remote sensing reflectance due to fluorescence radiance.

Further, for radiance from Raman scattering and applying a single scattering approximation along with an assumption of homogeneous water, Westberry *et al.* [23] obtained a formulation for nadir-viewing remote sensing reflectance due to Raman scattering as:

$$\begin{split} R_{\rm rs,Raman}(\lambda_{\rm em}) &= \\ \frac{t^2}{n^2} \frac{\beta_{\rm r}(\theta_{\rm s} \to \pi) b_{\rm r}(\lambda_{\rm em}) E_{\rm d}(0^+, \lambda_{\rm ex})}{[K_{\rm d}(\lambda_{\rm ex}) + K_{\rm L}(\lambda_{\rm em})] E_{\rm d}(0^+, \lambda_{\rm em})} \times \\ \left\{1 + \frac{b_{\rm b}(\lambda_{\rm ex})}{\mu_{\rm u}[K_{\rm d}(\lambda_{\rm ex}) + \kappa(\lambda_{\rm ex})]} + \frac{b_{\rm b}(\lambda_{\rm em})}{2\mu_{\rm u}\kappa(\lambda_{\rm em})}\right\}, \end{split}$$

where t is the transmittance across the air-water interface, n is the refractive index of water, β_r is the Raman phase function, b_r is the Raman scattering coefficient, K_L is the attenuation coefficient for upwelling radiance at emission wavelength, $\lambda_{\rm ex}$ is the excitation wavelength, and κ is the diffuse attenuation coefficient for radiance backscattered at a depth propagating towards the surface [24].

7 Concluding remarks

Through pure algebraic derivations, Åas[3] and Zaneveld[8] obtained relationships that show the fundamental dependence of AOPs (irradiance reflectance, diffuse attenuation coefficient, and remote sensing reflectance) on IOPs (in particular, absorption and backscattering coefficients). Although the exact values of the introduced variables could not be derived from the radiative transfer equation, these relationships provide a clear physics guide on the most important properties and the way of dependences. While it appears today that more and more practices use data or "big data" to answer science questions, the algebraic manipulations presented by Aas and Zaneveld highlight the power of math and physics in finding the core relationships governing properties in the natural environment.

Reference

- [1] Chandrasekhar S. Radiative transfer [M]. New York: Dover, 1960.
- [2] Preisendorfer R W. Hydrologic optics [M]. Seattle: NOAA Pacific Marine Environmental Laboratory, 1976.
- [3] Åas E. Two-stream irradiance model for deep waters [J]. Applied Optics, 1987, 26(11): 2095-2101.
- [4] Gershun A. The light field [J]. Journal of Mathematics and Physics, 1939, 18(1/2/3/4): 51-151.
- [5] Stavn R H, Weidemann A D. Shape factors, twoflow models, and the problem of irradiance inversion in estimating optical parameters [J]. Limnology and Oceanography, 1989, 34(8): 1426-1441.
- [6] Kirk J T O. Volume scattering function, average cosines, and the underwater light field [J].

- Limnology and Oceanography, 1991, 36(3): 455-467.
- [7] Sathyendranath S, Platt T. Analytic model of ocean color[J]. Applied Optics, 1997, 36(12): 2620-2629.
- [8] Zaneveld J R V. A theoretical derivation of the dependence of the remotely sensed reflectance of the ocean on the inherent optical properties [J]. Journal of Geophysical Research: Oceans, 1995, 100 (C7): 13135-13142.
- [9] Ronald J, Zaneveld V. Remotely sensed reflectance and its dependence on vertical structure: a theoretical derivation [J]. Applied Optics, 1982, 21(22): 4146-4150.
- [10] Mobley C D, Sundman L K. HydroLight 5.2 user's guide M. Bellevue: Sequoia Scientific, Inc., 2013.
- [11] Mobley C D. Light and water: radiative transfer in natural waters [M]. New York: Academic Press, 1994: 592.
- [12] Gordon H R, Brown O B, Jacobs M M. Computed relationships between the inherent and apparent optical properties of a flat homogeneous ocean [J]. Applied Optics, 1975, 14(2): 417-427.
- [13] Morel A, Gentili B. Diffuse reflectance of oceanic waters: its dependence on sun angle as influenced by the molecular scattering contribution [J]. Applied Optics, 1991, 30(30): 4427-4438.
- [14] Albert A, Mobley C. An analytical model for subsurface irradiance and remote sensing reflectance in deep and shallow case-2 waters [J]. Optics Express, 2003, 11(22): 2873-2890.
- [15] Vargas W E, Niklasson G A. Applicability conditions of the Kubelka-Munk theory [J]. Applied Optics, 1997, 36(22): 5580-5586.
- [16] Sandoval C, Kim A D. Deriving Kubelka-Munk theory from radiative transport [J]. Journal of the

- Optical Society of America A, 2014, 31(3): 628-636.
- [17] Lee Z P, Shang S L, Lin G, et al. On the modeling of hyperspectral remote-sensing reflectance of high-sediment-load waters in the visible to shortwave-infrared domain[J]. Applied Optics, 2016, 55(7): 1738-1750.
- [18] Gordon H R, Brown O B, Evans R H, et al. A semianalytic radiance model of ocean color [J]. Journal of Geophysical Research Atmospheres, 1988, 93(D9): 10909.
- [19] Lee Z P, Carder K L, Du K P. Effects of molecular and particle scatterings on the model parameter for remote-sensing reflectance [J]. Applied Optics, 2004, 43(25): 4957-4964.
- [20] Lee Z P, Hu C M, Shang S L, et al. Penetration of UV-visible solar radiation in the global oceans: insights from ocean color remote sensing [J]. Journal of Geophysical Research: Oceans, 2013, 118 (9): 4241-4255.
- [21] Gordon H R. Can the Lambert-Beer law be applied to the diffuse attenuation coefficient of ocean water?[J]. Limnology and Oceanography, 1989, 34(8): 1389-1409.
- [22] Huot Y, Brown C A, Cullen J J. New algorithms for MODIS sun-induced chlorophyll fluorescence and a comparison with present data products [J]. Limnology and Oceanography: Methods, 2005, 3 (2): 108-130.
- [23] Westberry T K, Boss E, Lee Z P. Influence of Raman scattering on ocean color inversion models[J]. Applied Optics, 2013, 52(22): 5552-5561.
- [24] Philpot W D. Radiative transfer in stratified waters: a single-scattering approximation for irradiance [J]. Applied Optics, 1987, 26(19): 4123-4132.