AOPs Are Not Additive: On the Biogeo-Optical Modeling of the Diffuse Attenuation Coefficient

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Commonly we see the diffuse attenuation coefficient of downwelling irradiance (K_d) expressed as a sum of the contributions of various constituents. We show here that, both theoretically and numerically, because K_d is an apparent optical property (AOP), this approach is not consistent with radiative transfer. We further advocate the application of models of K_d developed in past decades that are not only consistent with radiative transfer but also provide more accurate estimates, in particular for coastal turbid waters.

Keywords: solar radiation, apparent optical properties, inherent optical properties, diffuse attenuation coefficient, optical additivity

BACKGROUND

Solar radiation is the energy source for the entire earth system. In aquatic environments, unlike terrestrial environments, solar radiation can penetrate to great depths to fuel photosynthesis and to heat up the upper layer (Zaneveld et al., 1981; Platt, 1986; Lewis et al., 1990). The propagation of solar radiation from surface to greater depths can be expressed as (Mobley, 1994)

$$E_d(z, \lambda) = E_d(0^-, \lambda)\, e^{-K_d(\lambda)\, z}. \tag{1}$$

Here E_d (W/m^2/nm) is the downwelling irradiance, z (m) is the depth from the surface (0^- for subsurface), K_d (m^{-1}) is the attenuation coefficient of downwelling irradiance between surface and depth z, and λ (nm) for wavelength. Since the variation of $E_d(0^-)$ is independent of water properties (except extremely turbid waters where the enhanced upwelling flux will result in significant contributions to $E_d(0^-)$ due to internal reflection), it is then imperative to describe the variation of K_d for various aquatic environments when quantifying the impact of water constituents on the heat budget (Morel and Antoine, 1994; Ohlmann et al., 2000), the feedback of oceanic systems on climate changes (Rochford et al., 2001; Gnanadesikan and Anderson, 2009), as well as the vertical variation of primary production (Sathyendranath and Platt, 1995).

Historically, with an objective of easy modeling and efficient calculation for large scale applications, K_d is commonly expressed as (Smith and Baker, 1978; Morel, 1988; Morel and Maritorena, 2001),

$$K_d(\lambda) = K_w(\lambda) + K_{bio}(\lambda), \tag{2}$$

with K_w the contribution of pure (sea)water, and K_{bio} the contributions of phytoplankton. In this expression, i.e., the so-called "Case-1" scheme (Morel and Prieur, 1977), the attenuation of pure

(sea)water is considered as a background, while other constituents that are actively changing, such as phytoplankton and suspended mineral solids, are considered as added contributions. In addition, the contributions of colored dissolved organic matter (CDOM) and organic detritus are considered as co-varying with phytoplankton, and lumped into the K_{bio} term. So their contributions are not ignored or omitted as might be implied by the equation, although its application is limited to "Case-1" waters.

In order to explicitly evaluate and understand the impact of constituents such as CDOM and/or suspended mineral particles or particulate inorganic matter (PIM) on the propagation of solar radiation, K_d in many studies is expanded as a sum of more components, although there are subtle variations among these models (Smith and Baker, 1978; Baker and Smith, 1982; Gallegos et al., 1990; Devlin et al., 2009; Kim et al., 2015),

$$K_d(\lambda) = K_w(\lambda) + K_{bio}(\lambda) + K_{CDOM}(\lambda) + K_{PIM}(\lambda). \quad (3)$$

Here K_{CDOM} and K_{PIM} are the diffuse attenuation coefficients resulted from CDOM and PIM, respectively. In essence, these biogeo-optical models of K_d effectively treat K_d, an apparent optical property (AOP) (Preisendorfer, 1976), as an inherent optical property (IOP) (Preisendorfer, 1976), which is not consistent with the definitions and the nature of variations of K_d (Stavn, 1988). The attitude of treating K_d as an IOP might stem from that K_d of "Case 1" water, after correcting for the sun angle effect, can be considered as a "quasi" IOP (Gordon, 1989). However, it was never claimed that this would work in any other water types than "Case 1" water. Many subsequent studies have, for the most part, somehow ignored these limitations in applications.

Fundamentally K_d is sun-angle dependent (Stavn, 1988; Mobley, 1994) (also weakly dependent on atmospheric properties). So, considering the model of Morel and Maritorena (2001), it is specifically stated that the model and the empirical coefficients (Equation 3 in Morel and Maritorena, 2001) are *valid just for low zenith sun angles*. But this restriction has in fact largely been ignored by the research community, which leads to inconsistent applications and errors. For instance, if we use this model for early morning or late afternoon situations, because of the likely large sun angle, this can easily result in 30% or greater errors in estimating K_d (Morel et al., 2002; Lee et al., 2005b). In the following, we demonstrate the non-additive nature of K_d theoretically and numerically.

THEORETICAL MODEL OF K_d

Based on radiative transfer, K_d is a function of IOPs (especially the absorption, a, and backscattering, b_b, coefficients) as (Lee et al., 2005b),

$$K_d = \frac{1}{\mu_d} a + \left(\frac{r_d}{\mu_d} - \frac{r_u R}{\mu_u} \right) b_b. \quad (4)$$

Here μ_d (μ_u) is the average cosine and r_d (r_u) is the shape factor for the downwelling (upwelling) light field (Stavn and

Weidemann, 1989), respectively. R is the irradiance reflectance (Gordon et al., 1975). Through numerical simulations via Hydrolight, it was found that the above expression could be simplified as (Lee et al., 2005b)

$$K_d(\lambda) = m_0 \, a(\lambda) + m_1 \left(1 - m_2 \, e^{-m_3 \, a(\lambda)} \right) b_b(\lambda), \quad (5)$$

with m_{0-3} constants that are independent of wavelength and water properties. Note that these model parameters vary weakly with depth (Lee et al., 2005b) due to changes of light field structure, consistent with the change of μ_d with depth (Stavn, 1988; Berwald et al., 1995; McCormick, 1995). Also note that for large zenith angles, the forward scattering coefficient will also contribute to the diffuse attenuation coefficient through its contribution to μ_d, μ_u, r_d and r_u (Stavn and Weidemann, 1989). Mathematically, Equation (5) can be rewritten as,

$$K_d(\lambda) = m_0 \, a(\lambda) + m_1 \, b_b(\lambda) - m_1 \, m_2 \, e^{-m_3 \, a(\lambda)} \, b_b(\lambda). \quad (6)$$

Consequently, although $a(\lambda)$ and $b_b(\lambda)$ are additive, a nature of IOPs, the interaction term between $a(\lambda)$ and $b_b(\lambda)$ (the third term on the right side of Equation 6) is *not* additive, thus K_d cannot be additive—a general nature of AOPs. This characteristic is further highlighted in details below.

For simplicity, let's consider a medium has just two constituents: pure seawater and suspended inorganic mineral particles (PIM). For pure seawater alone, following Equation (6), there is

$$K_w(\lambda) = m_0 \, a_w(\lambda) + m_1 \, b_{bw}(\lambda) - m_1 \, m_2 \, e^{-m_3 \, a_w(\lambda)} \, b_{bw}(\lambda). \quad (7)$$

Here $a_w(\lambda)$ and $b_{bw}(\lambda)$ are the spectral absorption and backscattering coefficients of pure seawater.

For suspended inorganic mineral particles alone,

$$K_{PIM}(\lambda) = m_0 \, a_{PIM}(\lambda) + m_1 \, b_{bPIM}(\lambda) \\ - m_1 \, m_2 \, e^{-m_3 \, a_{PIM}(\lambda)} \, b_{bPIM}(\lambda), \quad (8)$$

with a_{PIM} and b_{bPIM} being the absorption and backscattering coefficients of suspended mineral particles.

Therefore, a sum ($K_d^{sum}(\lambda)$) of the two contributions to K_d following Equations (2) and (3) resulted in,

$$K_d^{sum}(\lambda) = m_0(a_w(\lambda) + a_{PIM}(\lambda)) + m_1(b_{bw}(\lambda) + b_{bPIM}(\lambda)) \\ - m_1 \, m_2 \left(e^{-m_3 \, a_w(\lambda)} \, b_{bw}(\lambda) + e^{-m_3 \, a_{PIM}(\lambda)} \, b_{bPIM}(\lambda) \right). \quad (9)$$

However, when the medium is composed of both pure seawater and suspended mineral particles, its K_d following radiative transfer (Equation 6) is

$$K_d(\lambda) = m_0(a_w(\lambda) + a_{PIM}(\lambda)) + m_1(b_{bw}(\lambda) + b_{bPIM}(\lambda)) \\ - m_1 \, m_2 \left(e^{-m_3 \, a_w(\lambda) - m_3 \, a_{PIM}(\lambda)} \right) (b_{bw}(\lambda) + b_{bPIM}(\lambda)). \quad (10)$$

Clearly, as shown above, when there are more constituents, because the light field is determined by the bulk properties (Stavn, 1988; Stavn and Weidemann, 1989; Lee et al., 2005b), a_w and a_{PIM} will affect the contribution of both b_{bw} and b_{bPIM} to K_d. However, when K_d is treated as an additive property of K_w and K_{PIM}, the effect of a_w on the contribution of b_{bPIM} and the effect of a_{PIM} on the contribution of b_{bw} are excluded.

NUMERICAL DEMONSTRATION

To demonstrate the above point numerically, **Figure 1** compares K_d spectra from Hydrolight (Mobley and Sundman, 2013) simulations with K_d^{sum}, where the two component spectra (K_w and K_{PIM}) were also obtained from Hydrolight simulations using the same constituents as for K_d. Specifically, spectral (400–800 nm, 10 nm interval) $E_d(z)$ were simulated with Hydrolight, and K_d between surface and z is calculated following

$$K_d(\lambda) = \frac{1}{z} \ln \left(\frac{E_d(0^-, \lambda)}{E_d(z, \lambda)} \right) \qquad (11)$$

For the derivation of K_w from Hydrolight, all other constituents were held to 0 except for the properties of pure seawater. Values of a_w are a combination of Lee et al. (2015) and Pope and Fry (1997) while values of b_{bw} are those of Morel (1974). For the derivation of K_{PIM} from Hydrolight, PIM was set as 10 g/m^3 and the default optical model parameters for suspended minerals included in Hydrolight were used to get the absorption and scattering coefficients of PIM. Note that this PIM concentration is just a low-medium value for turbid coastal waters (Babin et al., 2003; Doxaran et al., 2009). For this simulation, an idealized "transparent pure seawater" was used where very low values of a_w (0.1 × 10^{-4} m^{-1}) and b_{bw} (0.5 × 10^{-5} m^{-1}) were employed. With such a setup the contribution of this "transparent pure seawater" to the calculated K_d (Equation 11) is then negligible, and the resultant K_d from Hydrolight simulations can be considered as K_{PIM}. The sun angle for all simulations for both K_w and K_{PIM} was set as 30° from zenith along with a clear sky.

There are distinct differences in K_d (at least for this case) in the longer wavelengths (~10–15% for the 600–800 nm range), where a_w makes significant contributions to the total a; and this contribution, when there are sediments, to K_d is not represented in the additive descriptions of K_d (the red curve). For the shorter wavelengths (<~500 nm), because most (>~98%) of the contributions to K_d comes from PIM, the sum of the two terms match the bulk results well. Certainly the impact of the non-additive nature of K_d depends on the values of both a and b_b. For "Case-1" waters or waters where the scattering coefficients are relatively small, it might be applicable, without great errors, to treat $K_d(\lambda)$ as an additive property. However, this will depend on the validity of the above-mentioned assumptions. While not based on any assumptions of "Case-1" conditions or dependencies, the modeled K_d spectrum following Equation 5 is in an excellent agreement with the Hydrolight K_d spectrum
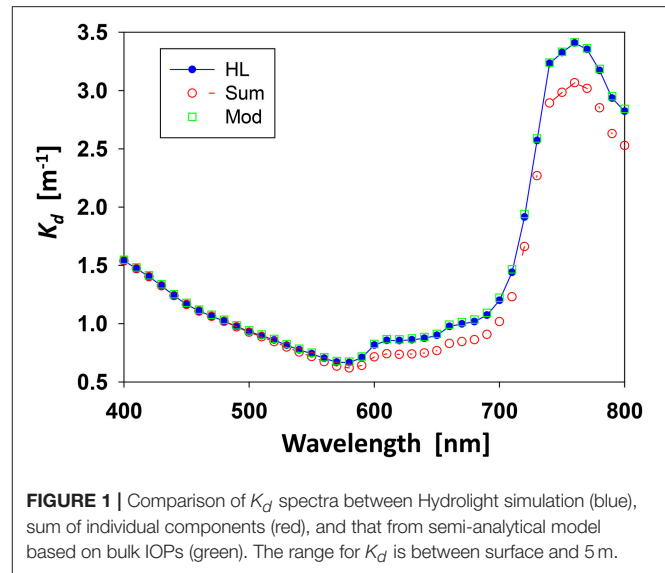
FIGURE 1 | Comparison of K_d spectra between Hydrolight simulation (blue), sum of individual components (red), and that from semi-analytical model based on bulk IOPs (green). The range for K_d is between surface and 5 m.

(~1% differences, see **Figure 1**), which highlights the much wider applicability of models based on radiative transfer. And, the robust performance of this model was also demonstrated in Zimmerman et al. (2015) for the quite turbid Chesapeake Bay waters.

Historically (Lorenzen, 1972; Smith and Baker, 1978; Woodruff et al., 1999; Gallegos, 2001; Devlin et al., 2008), there are also studies that treat the attenuation coefficient (K(PAR)) of the photosynthetic available radiation (PAR) as being additive of the contributions of individual constituents,

$$K(PAR) = K_w(PAR) + K_{bio}(PAR) + K_x(PAR), \qquad (12)$$

with K_x(PAR) for contributions except phytoplankton and pure (sea)water. Following the above logic and discussion regarding spectral K_d, we easily observe that this model is not consistent with radiative transfer either (Morel, 1988). In particular, it is ambiguous of the light spectra that should be used for the calculation of K_w(PAR) or K_{bio}(PAR). Further, because K(PAR) is the attenuation coefficient of solar radiation of a wide spectral range (400–700 nm, i.e., the PAR spectral range), while the spectral quality of $E_d(z)$ changes significantly from surface to depths, which then causes K(PAR) to change greatly (as much as a factor of 4) from surface to depth (Lee et al., 2005a; Lee, 2009). Consequently, the applicability of such biogeo-optical models for K(PAR) is ambiguous at the very least.

CONCLUSIONS

Because the interaction term (the third term on the right side of Equation 6) of $K_d(\lambda)$ (or K(PAR)) depends on the values of both a and b_b, the contribution of this term to K_d is not always small or negligible. Also, this interaction term is not a linear function of a and b_b. Therefore, for consistency with radiative transfer and for more accurate estimation, and also to incorporate advancements in ocean optics of recent decades, it is better to

get bulk IOPs first from biogeochemical properties, and then to calculate K_d based on IOPs. In short, IOPs are additive, but AOPs are not.

AUTHOR CONTRIBUTIONS

All authors contributed to the hypothesis and overall discussions regarding diffuse attenuation of solar radiation. ZL drafted the manuscript and both SS and RS commented and edited the manuscript before submission.

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