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Effects of inelastic radiative processes on the determination of water-leaving spectral radiance from extrapolation of underwater near-surface measurements

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Extrapolation of near-surface underwater measurements is the most common method to estimate the waterleaving spectral radiance, $L_w(\lambda)$ (where λ is the light wavelength in vacuum), and remote-sensing reflectance, $R_{\rm rs}(\lambda)$, for validation and vicarious calibration of satellite sensors, as well as for ocean color algorithm development. However, uncertainties in $L_w(\lambda)$ arising from the extrapolation process have not been investigated in detail with regards to the potential influence of inelastic radiative processes, such as Raman scattering by water molecules and fluorescence by colored dissolved organic matter and chlorophyll-a. Using radiative transfer simulations, we examine high-depth resolution vertical profiles of the upwelling radiance, $L_{\mu}(\lambda)$, and its diffuse attenuation coefficient, $K_{L_{i}}(\lambda)$, within the top 10 m of the ocean surface layer and assess the uncertainties in extrapolated values of $L_w(\lambda)$. The inelastic processes generally increase L_u and decrease K_{L_u} in the red and nearinfrared (NIR) portion of the spectrum. Unlike $K_{L_{x}}$ in the blue and green spectral bands, $K_{L_{x}}$ in the red and NIR is strongly variable within the near-surface layer even in a perfectly homogeneous water column. The assumption of a constant $K_{L_{\alpha}}$ with depth that is typically employed in the extrapolation method can lead to significant errors in the estimate of L_w . These errors approach ~100% at 900 nm, and the desired threshold of 5% accuracy or less cannot be achieved at wavelengths greater than 650 nm for underwater radiometric systems that typically take measurements at depths below 1 m. These errors can be reduced by measuring L_{u} within a much shallower surface layer of tens of centimeters thick or even less at near-infrared wavelengths longer than 800 nm, which suggests a requirement for developing appropriate radiometric instrumentation and deployment strategies. © 2016 Optical Society of America

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1. INTRODUCTION

Satellite ocean color measurements provide a means for studying the biogeochemical and ecological dynamics of the world's ocean over extended spatial and temporal scales that are not achievable by conventional oceanographic observations. Satellite images of ocean color have been used to produce regional and global maps of several data products of interest to the study of ocean biogeochemistry and ecology, such as chlorophyll-*a* concentration (Chl) [1,2], particulate organic carbon (POC) [3,4], particulate inorganic carbon [5,6], primary productivity [7,8], and optical properties of the upper ocean ([9] and references therein). The accuracy of spectral water-leaving radiance $L_w(\lambda)$ (λ stands for light wavelength in vacuum) or remote-sensing reflectance $R_{rs}(\lambda)$ derived from spaceborne ocean color sensors is critical for the success of these applications. $L_w(\lambda)$ is defined as the spectral upwelling radiance just above the water surface (i.e., at $z = 0^+$ where z is a symbol for depth), which is associated with light emerging from below the surface. $R_{rs}(\lambda)$ is defined as a ratio of $L_w(\lambda)$ to the spectral downward plane irradiance incident on the water surface, $E_d(z = 0^+, \lambda) \equiv E_s(\lambda)$. $R_{rs}(\lambda)$ is typically used as an ocean color quantity from which various data products characterizing water constituents or optical properties are derived through appropriate algorithms. In this paper we focus primarily on $L_w(\lambda)$, which is a component of $R_{rs}(\lambda)$ dependent on water constituents and optical properties as well as boundary conditions (e.g., sun position, sky conditions, sea surface state).

A longstanding goal in ocean color radiometry is to determine $L_w(\lambda)$ with an accuracy better than 5% [10,11]. Whereas such accuracy is very difficult to achieve from satellite measurements that are influenced by atmospheric effects and light reflection from the sea surface, in situ determinations of $L_w(\lambda)$ with such high accuracy are also difficult to achieve. Accurate in situ determinations of these quantities are important for ocean color algorithm development ([12] and references therein), validation of satellite-derived values of $L_w(\lambda)$ and $R_{\rm rs}(\lambda)$ [12,13], and post-launch on-orbit vicarious calibration of satellite ocean color sensors [11,14–16]. The most common approach for *in situ* determinations of $L_w(\lambda)$ is based on the extrapolation of near-surface underwater measurements of upwelling radiance, $L_u(z, \lambda)$, up to the sea surface [17]. The underlying assumption of this approach is that the unknown spectral diffuse attenuation coefficient for upwelling radiance, $K_{L_u}(z, \lambda)$, within the near-surface extrapolation layer is constant with depth and has the same value as the measured attenuation coefficient within some depth interval below the extrapolation layer [17,18]. Whereas this assumption has been generally recognized as a source of uncertainty in $L_w(\lambda)$, this problem and its potentially large quantitative consequences have not been investigated in detail, especially with regard to the effects of inelastic radiative processes in the red and near-infrared (NIR) spectral regions [13].

For the purpose of determining $L_w(\lambda)$, the underwater measurements of upwelling radiance $L_u(z, \lambda)$ are typically accomplished using one of the following approaches: (i) a surface float system that takes time-series measurements at just a single depth relatively close to the surface (typically ~20 cm or so), (ii) a profiling system that takes nonsimultaneous measurements at different depths as the instrument descends vertically through the water column, and (iii) a fixed multidepth system capable of taking simultaneous time-series measurements at a few preselected discrete depths. While each of these approaches has some advantages and limitations [19], it is the recognition of limitations that provides a main motivation for this study.

In the first approach the extrapolation layer is relatively thin (~20 cm) but there is no measurement of $K_{L_u}(\lambda)$ at all because $L_u(z, \lambda)$ is measured at a single depth. Therefore, speculative assumptions about the values of $K_{L_u}(\lambda)$ are needed to extrapolate the measured data to the surface. In the second profiling approach, measurements of $L_{\mu}(z, \lambda)$ are taken during the downcast of a profiling radiometer and begin typically at a depth of about 1 m or greater depending on environmental conditions. On rare occasions the acquisition of profiling data begins at shallower depths within the top 1 m layer (e.g., [18,20]). Typically, however, for the profiling approach the near-surface extrapolation layer with unknown $K_{I_{m}}(\lambda)$ is thicker than for the surface float approach. In addition, the values of $K_{L_{\alpha}}(\lambda)$ at depths below the extrapolation layer are obtained from nonsimultaneous measurements at different depths, which requires a careful accounting for possible changes in the light field incident upon the water surface during the underwater profiling measurement. In the third multidepth approach, the issue of nonsimultaneity of measurements is eliminated but in practice the available systems have a relatively thick extrapolation layer (1 m or more) and the values of $K_{L_u}(z, \lambda)$ below the extrapolation layer are obtained from two or more measurement depths within a depth interval that is also relatively thick, at least a few meters. Again, this approach imposes limitations caused by unknown values of $K_{L_u}(\lambda)$ within the near-surface extrapolation layer. Thus, when using any of these three approaches significant uncertainties in the estimates of $L_w(\lambda)$ can arise in situations when $K_{L_u}(z, \lambda)$ varies significantly with depth within the near-surface layer including the extrapolation layer.

The water-leaving radiance $L_w(\lambda)$ is normally calculated as

$$L_w(\lambda) = (t/n^2)L_u(z = 0^-, \lambda),$$
 (1)

where *t* is the transmittance for upwelling radiance across the water-air interface, *n* is the refractive index of water, and $L_u(z = 0^-, \lambda)$ is the upwelling radiance just below the water surface at $z = 0^-$. The factor t/n^2 is typically assumed to be a known constant [21] and $L_u(z = 0^-, \lambda)$ is estimated from underwater radiance measurements using an extrapolation method. Therefore, for the purpose of our discussion $L_u(z = 0^-, \lambda)$ and $L_w(\lambda)$ can be used interchangeably. Assuming that the underwater upwelling radiance, $L_u(z, \lambda)$, is measured at least at two discrete depths, z_1 and z_2 , $L_u(z = 0^-, \lambda)$ is estimated from

$$L_{u}(z = 0^{-}, \lambda) = L_{u}(z_{1}, \lambda) \exp[K_{L_{u}}(z_{1} - z_{2}, \lambda)z_{1}], \quad (2)$$

where $L_u(z_1, \lambda)$ is the measured upwelling radiance at depth z_1 and $K_{L_u}(z_1 - z_2, \lambda)$ is the effective diffuse attenuation coefficient of upwelling radiance within a depth layer bounded by the shallower depth z_1 and deeper depth z_2 . The depth z is positive downward so $z_1 < z_2$. We note that *in situ* measurements of $L_u(z, \lambda)$ are typically made with a sensor pointing directly downward. In this case $L_u(z, \lambda)$ is referred to as zenith radiance according to the direction of light propagation [22]. As our interest is in the extrapolation of $L_u(z, \lambda)$ measured at deeper depths to a shallower depth, we note that there is no usual negative sign before the term $K_{L_u}(z, \lambda)$ in Eq. (2). The effective diffuse attenuation coefficient within the layer bounded by depths z_1 and z_2 is determined from

$$K_{L_{u}}(z_{1}-z_{2},\lambda)=\frac{\ln L_{u}(z_{1},\lambda)-\ln L_{u}(z_{2},\lambda)}{z_{2}-z_{1}}.$$
 (3)

The main assumption underlying the application of Eq. (2) is that $K_{L_u}(z_1 - z_2, \lambda)$ is equal to the attenuation coefficient, $K_{L_u}(0^- - z_1, \lambda)$, within the extrapolation layer between $z = 0^-$ and z_1 . We note that this assumption is required for accurate underwater near-surface extrapolation for all types of in-water radiometric systems (i.e., surface float, profiling, and multidepth systems) regardless of the fact that different systems generally use different approaches to determine $K_{L_u}(z, \lambda)$. However, this assumption is not necessarily valid for all environmental situations and measurement scenarios (e.g., [18,20]). In addition, the extent to which this assumption is violated can depend strongly on light wavelength.

We also note that data obtained from profiling measurements of $L_u(z, \lambda)$ for the purpose of extrapolation can vary depending on deployment strategy, for example, free fall versus wire-stabilized, depth resolution, which can range from less than 2 cm to over 10 cm, and the algorithm applied in the regression analysis, for example, linear versus nonlinear regression [18–20,23]. Data obtained from surface floats can vary depending on whether the required values of $K_{L_u}(z, \lambda)$ within the extrapolation layer are determined from models based on certain assumptions, for example, the assumption about surface Chl and its relation to $K_{L_u}(z, \lambda)$, or from independently measured profiles of $L_u(z, \lambda)$ [19]. The key point is that the use of $L_u(z, \lambda)$ data obtained with profiling or surface float systems can lead to different extrapolation results depending on the specific approach applied. The measurements of $L_u(z, \lambda)$ with multidepth systems equipped with two or more sensors taking simultaneous measurements at different preselected discrete depths potentially exhibit less variability in the extrapolation results.

Example multidepth systems providing measurements at discrete depths are the Marine Optical BuoY (MOBY) [11,24,25] and the Bouée pour l'acquisition de Séries Optiques à Long Terme (BOUSSOLE) [13], which have been used for vicarious calibration of satellite ocean color sensors, such as Sea-viewing Wide Field-of-view Sensor (SeaWiFS), Moderate Resolution Imaging Spectroradiometer (MODIS), and MEdium Resolution Imaging Spectrometer (MERIS). Although the requirement for very high accuracy of in situ determinations of water-leaving radiance $L_w(\lambda)$ is important, the depth configuration of these measurements may not ensure the highest possible accuracy of $L_w(\lambda)$ within some spectral ranges of interest to ocean color applications, especially the red and NIR ranges. The reasons for this include engineering and environmental considerations in the design of MOBY and BOUSSOLE. Specifically, MOBY has used three discrete depths of measurements, 1, 5, and 9 m. Accordingly, MOBY data can be used to estimate $L_u(z = 0^-, \lambda)$ and $L_w(\lambda)$ from measurements taken at one of the three pairs of depths: $z_1 =$ 1 m and $z_2 = 5$ m, $z_1 = 5$ m and $z_2 = 9$ m, or $z_1 = 1$ m and $z_2 = 9$ m. Thus, in the best case scenario the extrapolation layer is the top 1 m of the water column and $K_{L_u}(z_1 - z_2, \lambda)$ is obtained within the layer between 1 and 5 m.

It has been reported that whereas the satellite-derived data of $L_w(\lambda)$ are generally in good agreement with *in situ* determinations of $L_w(\lambda)$ from several data sources including MOBY and BOUSSOLE measurements in the blue and green spectral region (≤ 555 nm), the satellite estimates in the red spectral region (e.g., ~670 nm) are significantly higher than in situ estimates (e.g., [15,16]) or can even become negative for turbid waters with $Chl > 0.5 \text{ mg m}^{-3}$ [26]. The potential for large error in $L_w(670)$ has been explained by the relatively low signal in the red compared to that in the blue and green. Such explanation provides a good reason for why the uncertainty in satellite-derived $L_w(670)$ is often higher than that in the blue and green, but cannot explain why the satellitederived $L_w(670)$ is negative or often much higher than its in situ counterpart obtained from the underwater extrapolation method while no significant discrepancy is observed in the blue and green [15,16]. Although uncertainties in atmospheric correction and calibration of the satellite sensor can cause errors in satellite-derived values of $L_w(670)$, Antoine *et al.* [13] also suggested that large error can occur in the in situ determinations of $L_w(670)$ from the extrapolation method owing to the effects of inelastic radiative processes, in particular Raman

scattering by water molecules. These investigators reported that the effects of inelastic processes may produce an error in $L_w(670)$ of up to 50% when extrapolation to the surface is made from a depth of 4 m, and up to 30% when extrapolating from 2 m depth. As such errors greatly exceed the accuracy goal of 5%, further investigation is needed to address this issue.

The effects of inelastic processes on the vertical changes in underwater light-field characteristics and apparent optical properties including the diffuse attenuation coefficients have been demonstrated in the past [27-30]. For example, in the spectral regions where the effects of Raman scattering on the light field are significant, which is generally at light wavelengths longer than about 550 nm, the diffuse attenuation coefficients for radiance or irradiance can vary strongly with depth even within an optically uniform water column where the inherent optical properties (IOPs) are constant with depth [28,30]. Specifically, the diffuse attenuation coefficients in the red and NIR wavelengths will typically decrease considerably with depth until reaching an asymptotic regime [27-29]. This is because the contribution of Raman scattering to the light field in these spectral regions increases with depth, which generally acts to reduce the rate at which radiometric quantities are attenuated with depth. Such nonconstancy with depth, even for a perfectly homogeneous water column, is also expected for $K_{L_{\alpha}}(z, \lambda)$ within the top layer of about 10 m, which is most relevant to the extrapolation method [13]. Naturally, the assumption that $K_{L_u}(z_1 - z_2, \lambda) = K_{L_u}(0^- - z_1, \lambda)$, which is involved in Eq. (2), does not hold under such circumstances. The extrapolation from $L_{\mu}(z_1, \lambda)$ to just beneath the water surface using $K_{L_u}(z_1 - z_2, \lambda)$, which is smaller than $K_{L_u}(0^- - z_1, \lambda)$, will result in an underestimation of $L_u(z = 0^-, \lambda)$, and therefore also an underestimation of $L_w(\lambda)$ and $R_{rs}(\lambda)$. Such extrapolation errors caused by inelastic effects can be large, especially in the red and NIR spectral regions, which can affect the development and performance of ocean color algorithms that are developed with the use of *in situ* determinations of $R_{rs}(\lambda)$, validation of satellite retrievals of $L_w(\lambda)$ and $R_{rs}(\lambda)$ via the so-called matchup analysis between the *in situ* and satellite-derived data, as well as vicarious calibration of satellite sensors. A systematic investigation of this problem for the entire spectral range of relevance to ocean color applications from ultraviolet (UV) to NIR is needed. This is particularly important in view of planning future satellite ocean color missions, such as the US National Aeronautics and Space Administration's Plankton, Aerosol, Cloud, ocean Ecosystem (NASA PACE) mission that is expected to provide high spectral resolution measurements of water-leaving radiance from about 350 to 900 nm. Improved capabilities for *in situ* determinations of water-leaving radiance with consistently high accuracy across the entire spectral range is critical for pursuing scientific goals of missions such as PACE, which necessitate high radiometric accuracy and precision requiring high-quality calibration efforts as well as improved and new in-water ocean color algorithms requiring high-quality *in situ* radiometric determinations of $L_w(\lambda)$ and $R_{rs}(\lambda)$.

In this study, we present results from radiative transfer simulations to demonstrate the effects of inelastic radiative processes of Raman scattering by water molecules and fluorescence by chlorophyll-*a* and colored dissolved organic matter

(CDOM) on $L_u(z, \lambda)$ and $K_{L_u}(z, \lambda)$ within the top 10 m layer of the ocean for a broad range of water optical properties. Based on these results we assess the errors in $L_{\mu}(z=0^{-},\lambda)$ that result from the use of the extrapolation method within the nearsurface layer. The sole focus of this analysis is placed on errors caused by nonconstancy of $K_{L_{\mu}}(z, \lambda)$ within the longwavelength portion of the spectrum in the underwater nearsurface extrapolation layer, which is associated with the effects of inelastic processes. Whereas we recognize that other sources of uncertainties contribute to determinations of $L_{\mu}(z=0^{-},\lambda)$ from underwater measurements of $L_{\mu}(z, \lambda)$, the other sources of error are beyond the scope of this study. The effects of inelastic processes are expected to produce generally much larger error in extrapolated $L_{\mu}(z=0^{-},\lambda)$ in the red and NIR spectral region compared with other error sources. For example, it was reported that radiometric calibration, optical corrections (e.g., corrections for self-shading and bottom effects), and environmental factors result in uncertainty of ~3.5%-5% within the 412-683 nm spectral region for a profiling system [23] and less than 3.5% for a multidepth buoy system [31]. Although most discussion in this paper uses simultaneous multidepth measurements at a few discrete depths as an example source of $L_{\mu}(z, \lambda)$ data, the key considerations regarding the extrapolation issues are also applicable to other methods and radiometric systems for acquiring $L_u(z, \lambda)$ data. This is because the different methods for acquiring $L_{\mu}(z, \lambda)$ data share essentially the same principles with regard to determinations of $L_{\mu}(z=0^{-},\lambda)$ from extrapolation, albeit data processing and mathematical procedures involved might differ. In addition, our study is not intended to provide operational protocols for correcting for extrapolation errors because we focus specifically on demonstrating and quantifying the potential errors associated with the effects of inelastic processes alone. As an important outcome of this study we provide, however, recommendations for improved depth configuration of radiance sensors in the measurements of $L_{\mu}(z, \lambda)$ to ensure that the effects of inelastic processes do not produce errors that exceed the desired accuracy of 5% in determinations of $L_{\mu}(z = 0^{-}, \lambda), L_{\nu}(\lambda)$, and $R_{\rm rs}(\lambda)$ from the underwater extrapolation method regardless of other sources of uncertainties.

2. METHODS

The underwater light field in the ocean was simulated using the scalar radiative transfer model Hydrolight 5.1.4 from Sequoia Scientific, Inc. [22,32]. This model computes the full angular distribution of spectral radiance at each preselected output depth, from which other radiometric quantities (i.e., irradiances) and apparent optical properties are also derived. In this study, we focus on underwater upwelling zenith radiance $L_u(z, \lambda)$ and the diffuse attenuation coefficient of this radiance $K_{L_u}(z, \lambda)$. In Hydrolight, $K_{L_u}(z, \lambda)$ at depth z is computed based on a 1 cm depth layer between z and z + 1 cm and thus considered representative of depth z.

The primary inputs required by Hydrolight are the vertical profiles of spectral IOPs of seawater, which include the spectral absorption coefficient, $a(z, \lambda)$, spectral scattering coefficient, $b(z, \lambda)$, and spectral scattering phase function $\tilde{\beta}(z, \psi)$, where ψ is the scattering angle (see [22] for definitions of IOPs

Table 1.	Description	of Radiative	Transfer	Simulation
Scenarios	S			

$Chl^a (mg m^{-3})$	0, 0.02, 0.2, 2
Solar Zenith Angle (°)	0, 30, 60
Cloud Cover	Clear sky
Wind Speed	5 m/s
Inelastic Processes ^b	(i) none, (ii) Raman scattering only,
	(iii) Raman scattering, CDOM and
	chlorophyll-a fluorescence
Spectral Range	300–900 nm at 5 nm intervals
Depth Resolution	0.01 m for 0-0.1 m, 0.05 m for
	0.1–1 m, and 0.1 m for 1–10 m
Bottom	Infinitely deep ocean

"When chlorophyll-*a* concentration (Chl) is 0, the ocean is assumed to consist of only pure seawater. For the remaining Chl cases, both uniform [29] and nearly uniform [33] profiles of Chl within top 10 m were simulated for each Chl.

^bFor the simulations of a pure seawater ocean, only cases (i) and (ii) apply.

and other quantities used in hydrologic optics). In this study, we examined three scenarios with IOPs associated with three different concentrations of chlorophyll-*a*, Chl, within the surface oceanic layer and one additional scenario with IOPs determined solely by pure seawater (see Table 1). Chlorophyll-*a* is a major pigment in phytoplankton and serves as a proxy for phytoplankton biomass.

To cover the typical range of phytoplankton biomass in the open ocean, surface Chl values of 0.02 mg m⁻³, 0.2 mg m⁻³, and 2 mg m⁻³ were assumed. For each Chl two sets of radiative transfer simulations were performed, one with uniform vertical profiles of Chl within the top 10 m based on Li et al. [29] and the other with nearly uniform profiles within the top 10 m based on Uitz et al. [33]. The nearly uniform profiles of Chl within the surface layer are referred to as profiles S1, S4, and S8 in Uitz et al. [33]. We rescaled these profiles to obtain the values of Chl just below the surface of 0.02, 0.2, and 2 mg m⁻³, respectively (Fig. 1). Although the uniform and nearly uniform Chl profiles are very similar within the top 10 m of the water column, these two scenarios of simulations differ significantly in terms of Chl profiles below the 10 m depth. Specifically, whereas the profiles based on the study of Li et al. [29] consist of three layers, i.e., the top uniform layer, the transition layer with Chl decreasing to zero, and the deep layer with no chlorophyll-a, the S1, S4, and S8 profiles from Uitz et al. [33] are described by Gaussian functions with a subsurface Chl maximum (see these references for more details).

Based on the profiles of Chl, the input IOPs of seawater were specified within the spectral range from 300 to 900 nm at 5 nm intervals. The total absorption coefficient $a(z, \lambda)$ was modeled as a sum of three component coefficients representing the molecular absorption of pure water, $a_w(\lambda)$, suspended particles, $a_p(z, \lambda)$, and colored dissolved organic matter, $a_q(z, \lambda)$:

$$a(z,\lambda) = a_w(\lambda) + a_p(z,\lambda) + a_q(z,\lambda).$$
(4)

Values of $a_w(\lambda)$ were obtained from the measurements such as Sogandares and Fry [34] and Pope and Fry [35] (see Hydrolight technical documentation [32] for more details). These values represent a water temperature of ~23°C and were assumed to be independent of depth. The coefficients $a_p(z, \lambda)$ and $a_g(z, \lambda)$ were calculated from Chl using the "New



Fig. 1. Depth profiles of chlorophyll-*a* concentration, Chl, within the upper 200 m of the water column for the three nearly uniform cases within the top 10 m layer. The value of surface Chl is indicated for each case. The depth of the Chl maximum is 115, 45, and 15 m for the surface Chl values of 0.02, 0.2, and 2 mg m⁻³, respectively. All subsequent figures and the results in Tables 2 and 3 represent the simulations based on the nearly uniform cases of Chl within the near-surface ocean depicted in this figure.

Case 1" bio-optical model embedded within Hydrolight [32]. In brief, the particulate absorption coefficient was determined from a power function of chlorophyll-*a* concentration

$$a_{p}(z,\lambda) = A(\lambda)[\operatorname{Chl}(z)]^{E(\lambda)},$$
(5)

where $A(\lambda)$ and $E(\lambda)$ are wavelength-dependent parameters determined from field studies [36,37]. The value of $a_g(z, \lambda)$ was calculated from the relationship

$$a_g(z,\lambda) = a_g(z,440)e^{-S(\lambda-440)} = 0.2a_p(z,440)e^{-S(\lambda-440)}$$
, (6)

where the spectral slope parameter S was set to 0.014 nm^{-1} .

The total spectral scattering coefficient, $b(z, \lambda)$, was calculated as the sum of component coefficients associated with pure seawater, $b_w(\lambda)$, and suspended particles, $b_p(z, \lambda)$:

$$b(z,\lambda) = b_w(\lambda) + b_p(z,\lambda).$$
(7)

Values of $b_w(\lambda)$ representing a typical oceanic salinity of 35‰ at a temperature of 20°C were obtained from Morel [38] and were assumed to be independent of depth. The values of $b_p(z, \lambda)$ were calculated as the difference between the particulate beam attenuation coefficient, $c_p(z, \lambda)$, and $a_p(z, \lambda)$. Values of $c_p(z, \lambda)$ were calculated according to Loisel and Morel [39]:

$$c_p(z,\lambda) = 0.407 [\text{Chl}(z)]^{0.795} \left(\frac{\lambda}{660}\right)^{\nu},$$
 (8a)

where the exponent ν was parameterized as

$$v = 0.5(\log_{10} \text{Chl} - 0.3)$$
 (8b)

The additional IOP required as input to radiative transfer simulations is the spectral scattering phase function characterizing the angular shape of the spectral volume scattering function [22]. The phase function of pure seawater, $\tilde{\beta}_w(\psi)$, and the Fournier-Forand phase function of particles [40], $\tilde{\beta}_p(z, \psi)$, were used. The Fournier-Forand phase function was parameterized in terms of the particulate backscattering fraction $\tilde{b}_{bp}(z)$ (i.e., the ratio of particulate backscattering to total particulate scattering). Values of $\tilde{b}_{bp}(z)$ were assumed to be related to Chl [41] and hence $\tilde{\beta}_p(z, \psi)$ for different Chl cases are slightly different. Note, however, that for any given Chl and depth z we used a single value of $\tilde{b}_{bp}(z)$ which is independent of light wavelength. Hence, for a given Chl we also used a single function $\tilde{\beta}_p(z, \psi)$ independent of wavelength. As an example of input IOPs, Fig. 2 depicts the spectra and vertical profiles of $a(z, \lambda)$, $b(z, \lambda)$, and backscattering coefficient $b_b(z, \lambda)$ for the nearly uniform profile of Chl = 0.2 mg m⁻³ within top 10 m.

In addition to IOPs, ancillary information about solar zenith angle, sky conditions, wind speed, and ocean bottom depth is required as input to the Hydrolight code. For each Chl scenario we performed the simulations for three solar zenith angles $(0^{\circ}, 30^{\circ}, \text{ and } 60^{\circ})$, clear sky conditions, wind speed of 5 m s⁻¹, and an infinitely deep ocean. We considered clear skies and relatively high positions of the sun because such conditions are relevant to satellite measurements of ocean color.

For each simulation scenario representing a specific Chl profile (hence IOPs within the water column) and solar zenith angle, three different Hydrolight runs were performed with different combinations of the presence or absence of inelastic radiative processes. These processes include Raman scattering by water molecules, fluorescence of chlorophyll-a, and fluorescence of CDOM. The three scenarios of simulations related to inelastic processes were: (i) no inelastic processes, (ii) the presence of Raman scattering only, and (iii) the presence of Raman scattering, fluorescence of chlorophyll-a, and fluorescence of CDOM. The description of how inelastic processes are computed in Hydrolight code can be found in [22]. In brief, Raman scattering is modeled by assuming a Raman scattering coefficient of 2.6×10^{-4} m⁻¹ at an excitation wavelength of 488 nm and the wavelength dependency of $\lambda^{-5.5}$, which is consistent with studies by Bartlett et al. [42] and Desiderio [43]. The Raman wavelength redistribution function is described by Eq. 5.94 in Mobley [22]. The modeling of chlorophyll-a fluorescence requires the phytoplankton spectral absorption coefficient, $a_{\rm ph}(z,\lambda)$, which is a product of Chl and Chl-specific absorption coefficient of phytoplankton according to [44]. The quantum efficiency of fluorescence is set to 0.02. Finally, the modeling of CDOM fluorescence requires CDOM absorption coefficients [Eq. (6)] and CDOM fluorescence quantum efficiency function. The CDOM fluorescence quantum efficiency function, which depends on excitation and emission wavelengths, is based on the experimental data of [45]. For all three inelastic processes, Hydrolight assumes an isotropic phase function, which is reasonable for fluorescence but may produce some (albeit inconsequential for the purposes of our study) uncertainty in Raman scattering ([29] and references therein). We note that there is some variability in the parameters describing the inelastic processes [22] and such variability may result in slight changes in the modeled $L_u(z, \lambda)$ and $K_{L_u}(z, \lambda)$. Nevertheless, we expect that the main conclusions describing the first-order effects associated with the presence versus absence of inelastic processes on the extrapolation of underwater measurements of $L_u(z, \lambda)$ within



Fig. 2. Spectra (top panels) at selected depths and vertical profiles within the upper 10 m (bottom panels) at indicated light wavelengths of (a),(d) the absorption coefficient $a(z, \lambda)$; (b),(e) the scattering coefficient $b(z, \lambda)$; and (c),(f) the backscattering coefficient $b_b(z, \lambda)$ for the scenario of nearly uniform depth profile of Chl = 0.2 mg m⁻³ within the top 10 m layer shown in Fig. 1.

the near-surface oceanic layer will remain similar, regardless of whether we use the "average" (standard) parameters of inelastic processes embedded within the Hydrolight code or some variation of these parameters.

All scenarios of radiative transfer simulations included in this study are summarized in Table 1. Overall we obtained results from 60 simulations. Specifically we ran 54 simulations representing three Chl scenarios, each with two profile types, three solar zenith angles, and three scenarios of inelastic processes. For pure seawater we ran six simulations as we have three solar zenith angles and two scenarios of inelastic processes (i.e., no inelastic processes and Raman scattering only) for each solar zenith angle. On the basis of these simulations our analysis is focused on $L_{\mu}(z, \lambda)$ and $K_{L_{\mu}}(z, \lambda)$ within the top 10 m of the water column. Importantly, as our primary interest is in this near-surface layer, we examine the behavior of these quantities with depth using results calculated with fine depth resolution, i.e., 1 cm intervals between the surface and 0.1 m depth, 5 cm intervals between 0.1 and 1 m depth, and 10 cm intervals between 1 and 10 m depth. The chosen scheme for output depths of Hydrolight simulations is also listed in Table 1. We also note that we restrict the presentation of simulation results to the spectral range 350–900 nm, although the simulations included the range 300-350 nm to properly account for the contributions of inelastic processes at wavelengths longer than 350 nm. All results presented are for Chl profiles that are nearly uniform within the top 10 m and have a subsurface Chl maximum. This is because $L_u(z, \lambda)$ and $K_{L_u}(z, \lambda)$ within the top 10 m from

these simulations were very similar to those obtained for the scenario of the three-layer Chl profiles with uniform top layer (not shown). This similarity indicates that the differences in the vertical profiles of IOPs below 10 m depth have little influence on the near-surface values of $L_u(z, \lambda)$ and $K_{L_u}(z, \lambda)$ for the two types of Chl profiles examined in this study.

As our primary interest in this study is to evaluate the reduced accuracy of the extrapolation method owing to depth variations in $K_{Lu}(z, \lambda)$ within the near-surface layer, the relative error, ϵ_r , in extrapolated values of $L_u(z = 0^-, \lambda)$ caused by uncertainty associated with depth-dependent $K_{L_u}(z, \lambda)$ can be determined from

$$\epsilon_r = \frac{L_u^{\text{extr}}(z=0^-,\lambda) - L_u^{\text{true}}(z=0^-,\lambda)}{L_u^{\text{true}}(z=0^-,\lambda)},$$
(9)

where $L_u^{\text{true}}(z = 0^-, \lambda)$ represents the values computed with Hydrolight simulations and $L_u^{\text{extr}}(z = 0^-, \lambda)$ represents the extrapolated values of $L_u(z = 0^-, \lambda)$ determined from Eq. (2) using $L_u(z_1, \lambda)$ and $K_{L_u}(z_1 - z_2, \lambda)$ from Hydrolight simulations.

3. RESULTS AND DISCUSSION

A. L_u and K_{L_u} Within the Near-Surface Layer

For the sake of simplicity in presentation of results, hereafter the dependence of optical quantities on depth z and light wavelength λ will be dropped unless full symbols are required to avoid ambiguity. Figure 3 shows the near-surface vertical profiles of L_u at selected wavelengths (450, 550, 650, and 850 nm) for a hypothetical pure seawater ocean, different Chl cases, and different scenarios of inelastic processes. These results are for the nearly uniform Chl profiles within the top 10 m as shown in Fig. 1 and the solar zenith angle of 0° .

With no inelastic processes included in the simulations, the vertical profiles of L_u are nearly straight lines on the semilogarithmic graphs regardless of light wavelength and IOPs within the water column. This indicates that $K_{L_{u}}$ is nearly constant with depth. However, this scenario is unrealistic in aquatic environments because inelastic processes are always present. When inelastic processes were included in the simulations, the semilogarithmic plots of L_u profiles exhibit significant curvature in the near-surface layer for wavelengths in the red and NIR spectral regions (e.g., 650 and 850 nm). This curvature indicates that K_{L_u} varies with depth owing to inelastic processes, with the highest values close to the surface. This result is observed for all Chl cases as well as for the hypothetical case of a perfectly homogeneous ocean consisting of pure seawater. In the latter case the only inelastic process is Raman scattering. In the three Chl cases, fluorescence of chlorophyll-a and CDOM are also present in addition to Raman scattering.

Our simulations show that the strong effects of inelastic processes on the L_u profiles in the red and NIR (e.g., 650 and 850 nm) are associated primarily with Raman scattering as the curves with only Raman scattering included in the

simulations are virtually indistinguishable from those with Raman scattering and fluorescence. We note, however, that chlorophyll-*a* fluorescence can have an important effect around 685 nm where fluorescence is maximum (not shown). All results presented in Fig. 3 also indicate that the inelastic processes generally lead to an increased magnitude of near-surface L_u when compared to the hypothetical case without inelastic processes, the relative difference in L_u between cases with and without inelastic processes becomes smaller at the same wavelength and depth for higher Chl, and the effects of inelastic processes are small within the short-wavelength portion of the spectrum.

Figure 4 illustrates how the vertical changes in the attenuation of L_u within the top 10 m layer affect the extrapolation to obtain the upwelling radiance just below the surface. These results are from the same simulations as shown in Fig. 3, but solely for example wavelengths from the red and NIR spectral regions (650 and 850 nm) and one intermediate case of $Chl = 0.2 \text{ mg m}^{-3}$. The depicted vertical profiles of L_u (solid black lines) represent a realistic situation with the presence of Raman scattering and fluorescence. As indicated earlier these inelastic processes, mainly Raman scattering, are responsible for the curvature of the semilogarithmic plot of L_u , which reflects vertical changes in K_{L_u} . In Figs. 4(a) and 4(c) the dotted lines illustrate the extrapolation of L_u from simulation data



Fig. 3. Depth profiles of the upwelling radiance L_u at selected wavelengths for different simulation scenarios and a solar zenith angle of 0°. (a) Profiles for pure seawater ocean. (b),(c), and (d) Profiles corresponding to scenarios of surface chlorophyll-*a* concentration of 0.02, 0.2, and 2 mg m⁻³, respectively. For each scenario, the depicted results include simulations with only elastic processes (E), simulations which include Raman scattering (R), and simulations which include Raman scattering and the fluorescence of both chlorophyll-*a* and CDOM (R + F). The latter simulation is not applicable for the pure seawater scenario.



Fig. 4. Example illustrating errors in extrapolated values of spectral upwelling radiance just below the water surface, $L_u(z = 0^-, \lambda)$, which are associated with the effects of inelastic radiative processes. The left column illustrates the example simulations of a two-depth system, and the right column is for an example of a profiling system. For light wavelength of 650 nm (a) and (b), the extrapolated values of $L_u(z = 0^-, \lambda)$ using simulated measurements taken at shallower depths, 1 and 5 m for the two-depth system and 0.3–1 m for the profiling system, are shown as solid diamonds and at deeper depths, 5 and 9 m for two-depth system and 1 to 5 m for profiling system, are shown as solid squares. For light wavelength of 850 nm (c) and (d), the extrapolated values of $L_u(z = 0^-, \lambda)$ using simulated measurements taken at shallower depths, 0.3 to 1 m for the profiling system, are also shown as solid diamonds, and at deeper depths, 1 and 2 m for the two-depth system and 1–2 m for the profiling system, are shown as solid squares. The true values of $L_u(z = 0^-, \lambda)$ are shown as solid triangles. The simulated measurements of L_u by a two-depth system at indicated depths are shown as open circles in (a) and (c), and the simulated measurements of L_u by a profiling system with 0.1 m depth resolution are shown as the open diamonds (red) and squares (green) in (b) and (d). The red and green solid lines are the regression lines for the profiles of L_u in the corresponding color using the nonlinear regression approach. The results represent the simulation scenario for the surface Chl of 0.2 mg m⁻³, solar zenith angle of 0°, and inclusion of all three inelastic processes.

representing measurements at two depths indicated by open circles. At 650 nm, in one case the extrapolated value of surface radiance $L_u(z = 0^-, \lambda)$ is obtained under the assumption that measurements were taken at 1 and 5 m, and in the other case the extrapolation is based on measurements taken at 5 and 9 m. At 850 nm, the extrapolation is illustrated assuming that simulated measurements were taken at 1 and 2 m. This illustration demonstrates that the extrapolated values of $L_u^{\text{extrr}}(z = 0^-, \lambda)$ can differ significantly from the true value of $L_u^{\text{extrr}}(z = 0^-, \lambda)$ obtained from simulations. At 650 nm, $L_u^{\text{extrr}}(z = 0^-, 650)$ is underestimated by 3.4% and 33.4% for the measurement scenarios of 1–5 m and 5–9 m, respectively. At 850 nm the extrapolation errors are much larger reaching 87.4% for the measurement scenario of 1–2 m. The underestimation can also be illustrated for extrapolation based on L_u simulations that represent data taken at a 0.1 m depth resolution with a profiling system. The symbols and line in the red are for the extrapolation of L_u based on data between 0.3 and 1 m [Figs. 4(b) and 4(d)] and the green ones are for extrapolation of L_u based on data between 1 and 5 m at 650 nm [Fig. 4(b)] or between 1 and 2 m at 850 nm [Fig. 4(d)]. For this illustration a nonlinear regression approach was used. For such profiling data, $L_u^{\text{extr}}(z = 0^-, 650)$ is underestimated by 0.2% and 4.2% for the extrapolation scenarios of 0.3–1 m and 1–5 m, respectively, while $L_u^{\text{extr}}(z = 0^-, 850)$ is underestimated by 40.4% and 89.9% for the extrapolation scenarios of 0.3–1 m and 1–2 m, respectively.



Fig. 5. Spectra of diffuse attenuation coefficient of upwelling radiance, K_{L_u} , at selected depths (top panels) and depth profiles of K_{L_u} at selected light wavelengths (bottom panels) for simulations with a solar zenith angle of 0°. Panels (a) and (d) represent a pure seawater ocean. Panels (b) and (e) depict results obtained using a scenario of surface Chl = 0.2 mg m⁻³, and panels (c) and (f) surface Chl = 2 mg m⁻³. The wavelength of 685 nm, near the center location of the chlorophyll-*a* fluorescence peak, is indicated in (a)–(c) by vertical dotted lines. The depth of 1 m is indicated in (d)–(f) by horizontal dotted lines. The notation of R, F, and E is described in Fig. 3.

Interestingly, the extrapolation errors for the two-depth and profiling scenarios of data acquisition are very close to each other as long as the measurement depth interval is the same; for example, 3.4% versus 4.2% for the measurement depth interval of 1-5 m at 650 nm and 87.4% versus 88.7% for the measurement depth interval of 1-2 m at 850 nm. These results indicate that the extrapolation errors for a two-depth or a profiling radiometric system can exceed greatly an accuracy goal of 5% if $K_{L_{e}}$ changes with depth. The key to avoid or minimize the extrapolation errors is to identify the depth range of the near-surface layer within which K_{L_u} remains constant or nearly constant and make measurements within this layer, or to take into account the inelastic processes during data reduction. For the purposes of determining the thickness of the near-surface layer with nearly constant K_{L_u} and thus depth requirements for minimizing the effects of inelastic processes on extrapolation of L_{μ} , the following analysis will be mainly focused on data obtained at a few discrete depths that correspond to the use of a multidepth radiometric system. This is an effective way of presenting our results which are essentially applicable also to other scenarios of acquisition of underwater upwelling radiance data because the basic principles of the extrapolation method are the same.

The spectra of K_{L_u} at selected depths and vertical profiles of K_{L_u} at selected wavelengths within the top 10 m layer are

shown in Fig. 5 for the same simulation scenarios as in Fig. 3. For the scenario of a pure seawater ocean, Raman scattering was included in the simulations but there is obviously no fluorescence by chlorophyll-a and CDOM in this scenario. For the two Chl cases presented, Raman scattering and fluorescence processes were included. For comparison, the simulation results for the scenario without inelastic processes are also shown. The most remarkable feature of K_{L_u} spectra is a considerable decrease of the K_{L_u} values in the long-wavelength portion of the spectrum, which is caused primarily by Raman scattering and also chlorophyll-a fluorescence in the red band around 685 nm [Figs. 5(a)-5(c)]. In the short-wavelength portion of the spectrum, however, the effects of inelastic processes are much weaker so the $K_{L_{\mu}}$ values are quite close to the hypothetical case with no inelastic processes. Owing to inelastic processes the values of $K_{L_{u}}$ can be even smaller than the pure water absorption coefficient (not shown) and this result can be observed in the long-wavelength portion of the spectrum in various water types ranging from very clear to turbid waters with relatively high Chl [30]. In pure seawater ocean, the comparison of K_{L_u} between the simulated cases with and without inelastic processes in Figs. 5(a) and 5(d) indicates that K_{L_u} in the red and NIR is clearly smaller than pure water absorption already at 1 cm depth. As depth increases, K_{L_u} in this spectral region, regardless of Chl, continues to decrease and is reduced by up to an order of magnitude at about 10 m when compared to the surface value or the case with no inelastic processes [Figs. 5(d)– 5(f)]. The relative decrease of K_{L_u} in the red and NIR with depth is smaller for higher Chl cases, similar to the results obtained by [30], except around 685 nm where chlorophyll-*a* fluorescence is maximum.

In contrast to the red and NIR spectral region, K_{L_u} in the blue and green (e.g., 450 and 550 nm) varies weakly with depth in the near-surface layer [Figs. 5(d)-5(f)]. This is also the case in the UV (not shown). However, when Chl is relatively high (e.g., 2 mg m⁻³), $K_{L_{a}}$ in the blue and green exhibits a noticeable increase with depth, especially below 1 m [Fig. 5(f)]. Note that this change is in the opposite direction to the effect caused by inelastic processes. It is also worth noting that this increase of K_{L_u} cannot be explained by the slightly nonuniform profiles of Chl (and hence the IOPs) within the top 10 m layer (see Figs. 1 and 2) which were used as input to the Hydrolight simulations. This is because similar results were also obtained from the simulations with perfectly homogeneous profiles of Chl and IOPs within the top 10 m (not shown). Thus, this vertical change of $K_{I_{m}}$ in the blue and green is most likely associated with the angular distribution of the light field, which is one of the factors known to affect apparent optical properties. The consequence for the application of the extrapolation method is that special caution is required not only in the red and NIR but also in the blue and green for relatively turbid waters with $\text{Chl} \geq 2 \text{ mg m}^{-3}$, even though the effects of inelastic processes are very small or negligible in this short-wavelength portion of the spectrum. Qualitatively similar features and behavior of the diffuse attenuation coefficients of underwater radiometric quantities were reported in an earlier radiative transfer study [20].

The example vertical profiles of K_{L_u} in Fig. 5 provide direct insight into the limitations of the extrapolation method. We recall that the extrapolation can be error free only when K_{L_u} (at a given wavelength) is constant within the near-surface extrapolation layer and the same value of K_{L_u} remains also constant in the underlying layer within which the measurements are done. Figure 5 indicates that K_{L_u} in the NIR spectral region stays nearly constant only within the top 10-20 cm. This layer extends to about 1 m depth for the red spectral region and to a few meters or more for shorter wavelengths. Thus whenever the measurements used for the extrapolation are not made within this near-surface layer of constant K_{L_u} , an error will arise in the extrapolated value $L_u^{\text{extr}}(z = 0^-, \lambda)$. For example, the vertical decrease of $K_{L_{u}}$, which is typically observed in the red and NIR owing mainly to Raman scattering, will result in an underestimation of $L_{\mu}^{\text{true}}(z=0^{-},\lambda)$, whereas the generally slight vertical increase of K_{L_u} in the blue and green will lead to slight overestimation of $L_u^{\text{true}}(z = 0^-, \lambda)$. It is thus not surprising that previous studies reported dramatic underestimation of $L_w(\lambda)$ in the red spectral region in conjunction with the use of underwater radiometric systems providing measurements of upwelling radiance at depths below 1 m [15,16]. The extrapolation error is evaluated in greater detail in Section 3.C.

B. Effects of Solar Zenith Angle on $K_{L_{\mu}}$

As $K_{L_{u}}$ is an apparent optical property of a water body it depends not only on the IOPs of water but also the boundary conditions, including sky conditions and sun position (e.g., [22]). Figure 6 depicts results from radiative transfer simulations that illustrate the effect of solar zenith angle under clear sky conditions on the vertical profile of $K_{L_{u}}$ in the near-surface layer. With regard to water IOPs, the same simulation scenarios as in Fig. 5 are presented, namely a pure seawater ocean, $Chl = 0.2 \text{ mg m}^{-3}$, and $Chl = 2 \text{ mg m}^{-3}$, and all the inelastic processes were included. The results show that K_{L_u} at a given light wavelength and depth increases with increasing solar zenith angle (θ_s) and this observation is consistent with earlier studies (e.g., [30]). $K_{L_{u}}$ also tends to increase to a lesser extent with increasing θ_s when the sun is high in the sky (see results for $\theta_{\rm s}$ varying between 0° and 30° in Fig. 6) compared with lower positions of sun (θ_s between 30° and 60°). From the point of view of the extrapolation method it is important to note that the vertical shapes of $K_{L_{u}}$ profiles are nearly the same within the top 10 m layer for the examined range of solar zenith angles. Therefore, the extrapolation accuracy is not expected to be



Fig. 6. Depth profiles of K_{L_u} at the indicated light wavelengths for solar zenith angles of 0° (solid lines), 30° (dashed-dotted lines), and 60° (dashed lines). All three inelastic processes were included in these simulations. From left to right, the results depict simulations of a pure seawater ocean, and two scenarios of surface Chl, 0.2 and 2 mg m⁻³.

affected significantly by the solar position for θ_s ranging from 0° to at least 60°, which was also suggested by Antoine *et al.* [13]. The discussion in Sections 3.C–3.E is focused on the simulation results obtained with the solar zenith angle of 0°.

C. Evaluation of Extrapolation Errors

To evaluate the extrapolation errors in greater detail we assume that underwater measurements of upwelling radiance are made at three discrete depths: 1, 5, and 9 m. This assumption is consistent with the design of an instrument such as MOBY, a radiometric system that has been used for vicarious calibration of satellite ocean color sensors [11,25]. In the case of MOBY measurements the extrapolation to obtain $L_{\mu}(z = 0^-, \lambda)$ is typically made starting with measured $L_u(z_1 = 1, \lambda)$ and using measured $K_{L_u}(z_1 - z_2, \lambda)$, where $z_1 = 1$ m and $z_2 = 5$ m. Occasionally, when the measurement of L_u at 1 m depth is not available, the extrapolation utilizes the measured $L_u(z_1 = 5, \lambda)$ and $K_{L_u}(z_1 - z_2, \lambda)$, where $z_1 = 5$ m and $z_2 = 9$ m. We evaluate the extrapolation errors for both cases of measurements taken at these discrete depths, although it is important to emphasize that this analysis is not intended to evaluate the performance of any specific radiometric system such as MOBY.

Figures 7(a)-7(c) compare the spectra of $K_{L_u}(z_1, \lambda)$ with the spectra of $K_{L_u}(z_1 - z_2, \lambda)$ for the two extrapolation cases, namely the first case with $z_1 = 1$ m and $z_2 = 5$ m and the second case with $z_1 = 5$ m and $z_2 = 9$ m. These results were



Fig. 7. Assessment of errors in the extrapolation of $L_u(z = 0^-, \lambda)$ by a MOBY-like system for a solar zenith angle of 0° and the three surface Chl scenarios of 0.02 mg m⁻³ (left column), 0.2 mg m⁻³ (middle column), and 2 mg m⁻³ (right column). All three inelastic processes were included in the simulations. (a)–(c) Spectra of the reference K_{L_u} at 1 m (solid line) and 5 m (dotted–dashed line) as well as layer-effective K_{L_u} calculated from simulated L_u at 1 and 5 m (dashed line) and that at 5 and 9 m (dotted line). (d)–(f) Spectra of true $L_u(z = 0^-, \lambda)$ (solid line), extrapolated $L_u(z = 0^-, \lambda)$ from L_u at 1 m using $K_{L_u}(z_1 - z_2, \lambda)$ where $z_1 = 1$ m and $z_2 = 5$ m (dashed line), and that from L_u at 5 m using $K_{L_u}(z_1 - z_2, \lambda)$ where $z_1 = 5$ m and $z_2 = 9$ m (dotted line). (g)–(i) Extrapolation errors computed by Eq. (9) for the two extrapolation scenarios in (d)–(f). Negative errors imply underestimation of $L_u^{\text{true}}(z = 0^-, \lambda)$ and positive errors indicate overestimation.

obtained from radiative transfer simulations for the three scenarios of Chl profiles as shown in Fig. 1. For low and intermediate Chl, $K_{L_u}(z_1 - z_2, \lambda)$ is smaller than $K_{L_u}(z_1, \lambda)$ for light wavelengths longer than ~580 nm. For Chl = 2 mg m⁻³ this result holds for wavelengths longer than ~635 nm. We also note that in this long-wavelength portion of the spectrum $K_{L_u}(z_1 - z_2, \lambda)$ is also smaller than $K_{L_u}(z, \lambda)$ at other depths $z < z_1$ (not shown), which means that it is smaller than $K_{L_u}(0^- - z_1, \lambda)$ within the near-surface extrapolation layer.

Because $K_{L_u}(z_1 - z_2, \lambda)$ differs from $K_{L_u}(0^- - z_1, \lambda)$ the extrapolation error associated with change in $K_{L_u}(z, \lambda)$ arises in Eq. (2). According to Eq. (9), the extrapolated values $L_u^{\text{extr}}(z = 0^-, \lambda)$ are underestimated relative to $L_u^{\text{true}}(z = 0^-, \lambda)$ when using the underestimated values of K_{L_u} within the extrapolation layer. This underestimation of surface radiance in the red and NIR spectral regions is illustrated in Figs. 7(d)-7(f)for the two cases of extrapolation. For both cases the values of $L_u^{\text{extr}}(z = 0^-, \lambda)$ are clearly smaller than $L_u^{\text{true}}(z = 0^-, \lambda)$ in these spectral regions. As expected, the underestimation of surface radiance is larger when the extrapolation toward the surface starts at a deeper depth. In our example results, this situation occurs when the extrapolation starts at 5 m using the values of $K_{I_{m}}(z_1 - z_2, \lambda)$ representing the layer between $z_1 = 5$ m and $z_2 = 9$ m. However, as shown in Figs. 7(d)–7(f), the surface radiance is also significantly underestimated when the extrapolation starts at 1 m using $K_{L_{u}}(z_1 - z_2, \lambda)$ with $z_1 = 1$ m and $z_2 = 5 \text{ m}.$

Figures 7(g)-7(i) depict the percentage error in extrapolated values of $L_u(z = 0^-, \lambda)$ caused by uncertainty associated with the error in $K_{L_n}(0^- - z_1, \lambda)$, which was calculated from Eq. (9) using data of $L_u^{\text{extr}}(z = 0^-, \lambda)$ and $L_u^{\text{true}}(z = 0^-, \lambda)$ from Figs. 7(d)-7(f). The error is comparatively small in the blue-green spectral region and begins to increase sharply with increasing wavelength at the transition from the green to red portion of the spectrum. This transition occurs roughly between 580 and 630 nm depending on the extrapolation case and the Chl scenario. The extrapolation errors are larger when the extrapolation begins at 5 m depth compared with 1 m depth. At the longest wavelength examined, $\lambda = 900$ nm, $L_{\mu}(z = 0^{-}, \lambda)$ is underestimated by as much as 80% for $Chl = 0.02 \text{ mg m}^{-3}$ [Fig. 7(g)] and 98% for $Chl = 2 \text{ mg m}^{-3}$ [Fig. 7(i)]. At shorter NIR wavelengths, for example at 750 nm, the errors are also very large, about 67% and 97% for the lowest and highest Chl cases, respectively. At an example wavelength from the red portion of the spectrum, $\lambda = 670$ nm, $L_{\mu}(z = 0^{-}, \lambda)$ is underestimated by ~10% when extrapolation starts at 1 m and ~55% when extrapolation starts at 5 m for the cases of relatively low Chl $\leq 0.2 \text{ mg m}^{-3}$. Overall, our analysis presented in Fig. 7 indicates that the extrapolation errors in the red and NIR caused by inelastic processes typically reach the levels of tens of percent. Thus these errors exceed significantly the accuracy goal of 5% in the derived values of water-leaving radiance [10,11]. Our results also explain the issues in the estimation of $L_w(670)$ observed by Franz *et al.* [15] and Bailey *et al.* [16].

In addition to the issues in the red and NIR, noticeable overestimation of $L_u(z = 0^-, \lambda)$ is observed at wavelengths shorter than 600 nm for the case of Chl = 2 mg m⁻³ when extrapolation starts at 5 m using $K_{L_u}(z_1 - z_2, \lambda)$ with $z_1 = 5$ m and $z_2 = 9$ m [Fig. 7(i)]. This overestimation ranges between 2.6% at 370 nm and 5.7% at 585 nm. These errors are associated with the increase of K_{L_u} with depth in the blue and green spectral regions as discussed above in relation to Figs. 5(d)–5(f). For lower Chl this overestimation is, however, small or negligible (within 0.2% for Chl = 0.02 mg m⁻³ and 1% for Chl = 0.2 mg m⁻³).

While our results demonstrate that the desired accuracy goal of 5% in the derived value of water-leaving radiance is not achievable at wavelengths longer than ~650 nm with the underwater radiometric measurement systems that measure L_u at depths greater than about 1 m, the large errors in satellitederived ocean color data within the long-wavelength portion of the spectrum can also have detrimental effects on the accuracy of satellite-derived $L_w(\lambda)$ at shorter wavelengths through the atmospheric correction [14]. This is because accurate measurements in NIR bands are essential to atmospheric correction of satellite measurements of ocean color across the entire spectrum [46]. The current NASA standard atmospheric correction for ocean color sensors assumes a perfect calibration of the sensor at 865 nm, and also makes the initial assumption that the ocean is black in the NIR, i.e., L_w or $L_u(z = 0^-)$ is zero at NIR wavelengths.

The "black pixel" assumption in the NIR may lead to invalid negative water-leaving reflectance in the blue bands (e.g., [26,47]). These studies reported that the accuracy of retrieved water-leaving reflectance from satellite measurements was much improved by adopting a nonzero L_w in the NIR derived from bio-optical modeling using an iterative process, especially in water bodies with $Chl \ge 0.5 \text{ mg m}^{-3}$. In addition, Turpie et al. [48] suggested that a 0.3% calibration error around 748 and 869 nm in the satellite sensors could lead to significant errors in the blue and green bands and thus more than a 20% change in the satellite-derived Chl. In spite of the fact that the magnitude of $L_{\mu}(z = 0^{-})$ in the NIR is small, the black pixel assumption can cause significant issues, and assessment of these effects require accurate in situ determinations of $L_u(z = 0^-)$ in the NIR. However, if underwater radiometric systems do not provide measurements of L_u at very shallow depths within the top 1 m layer, the use of such systems does not yield accurate determinations of $L_{\mu}(z=0^{-})$ in the NIR. As indicated in Fig. 7, $L_u^{\text{true}}(z = 0^-)$ can be more than 1 order of magnitude larger than $L_u^{\text{extr}}(z = 0^-)$ at NIR wavelengths, which implies that the use of underwater radiometric systems with optimal depth configuration is essential to accurately extrapolate the water-leaving radiance in the NIR from in situ measurements. Such accurate determinations are needed for the in situ validation of black pixel assumption in various waters and development of ocean color algorithms that involve NIR bands.

D. Measurement Requirements for Achieving Desired Extrapolation Accuracy

The results of extrapolation error analysis based on radiative transfer simulations that included the inelastic radiative processes for the three Chl scenarios (as shown in Fig. 1) and the solar zenith angle of 0° are summarized in Fig. 8. The primary purpose of this figure is to illustrate the various combinations of depth pairs z_1 and z_2 (where $z_2 > z_1$) such that the

measurements taken at these two depths ensure the desired accuracy of extrapolated surface radiance with an error less than 5%. Specifically, Fig. 8 illustrates the absolute values of the percent error calculated from Eq. (9) for all combinations of depth pairs z_1 and z_2 in the range from 0.01 to 10 m, which were included in the output results from simulations. These results are presented for five example wavelengths between 450 and 850 nm. The area in the green color (both dark and light green) indicates the domain of depth pairs z_1 and z_2 that satisfy the accuracy goal of 5%. The area in the light green color corresponds to the error less than 2%. The areas in the yellow and red colors indicate the domain with the error exceeding 5%.

As illustrated in the figure, in the blue and green spectral regions (450 and 550 nm) nearly all combinations of z_1 and z_2 within the top 10 m layer satisfy the accuracy goal of 5%. For low Chl cases (0.02 and 0.2 mg m⁻³) the even higher accuracy of errors less than 2% is achieved. Only for the high Chl case, and when both z_1 and z_2 are near 10 m, is the error somewhat higher than 5% (see a small area in yellow color in the upper right corner of relevant graphs for Chl = 2 mg m⁻³).

In contrast, with increasing wavelength into the red and NIR portions of the spectrum the domain of depth pairs z_1 and z_2 satisfying the accuracy goal of 5% becomes more and more restricted to smaller depths. This is indicated by the

yellow-red area in Fig. 8, which expands from the upper right corner of the graphs toward smaller values of z_1 and z_2 . This is naturally accompanied by the corresponding decrease in the size of the green area within the range of relatively small values of z_1 and z_2 . For example, it is clear that for $\lambda = 750$ nm and 850 nm the accuracy goal is not met for the depth pair of $z_1 = 1$ m and $z_2 = 5$ m regardless of the simulation scenario. In these spectral regions, z_1 must be less than 1 m and z_2 less than 5 m or even less than 1 m in certain combinations with z_1 . We also note that the rightmost corner of the green areas in Fig. 8 defines the maximum depth $z_1 (\equiv z_{1 \text{ max}})$ and the corresponding slightly deeper depth z_2 , which ensure that the accuracy goal of 5% is met. For example, for the simulation scenario of $Chl = 0.2 \text{ mg m}^{-3}$ this specific pair of depths for $\lambda = 650$ nm is: $z_{1 \text{ max}} = 2.8$ m and $z_{2} = 2.9$ m. For 750 nm, $z_{1 \text{ max}} = 0.3 \text{ m}$ and $z_{2} = 0.35 \text{ m}$, and for 850 nm, $z_{1 \text{ max}} = 0.15 \text{ m}$ and $z_{2} = 0.2 \text{ m}$. This example indicates that to ensure that the extrapolation error is within 5% at all light wavelengths up to 850 nm, the shallowest radiance sensor would have to be placed no deeper than 15 cm below the water surface. For the longest wavelength examined in this study, $\lambda = 900$ nm (not shown in Fig. 8), $z_{1 \text{ max}} = 0.1$ m and $z_2 = 0.15$ m, which points to a need for the shallowest depth of measurement of 10 cm only.



Fig. 8. Illustration of the extrapolation error at light wavelengths of 450, 550, 650, 750, and 850 nm resulting from all possible combinations of depth pairs z_1 and $z_2(z_1 < z_2)$ within the upper 10 m layer of the ocean. Results depict simulations at solar zenith angle of 0° with all three inelastic processes included. Three surface Chl scenarios of 0.02 (top), 0.2 (middle), and 2 mg m⁻³ (bottom) are shown. The color scale indicates the absolute values of errors in $L_{\mu}(z = 0^-, \lambda)$ as computed by Eq. (9).

The green area restricted to the range of small near-surface depths for the long-wavelength bands of the spectrum in Fig. 8 points to the inadequacy of measurement systems and deployment strategies that obtain L_u data at depths greater than 1 m for achieving the accuracy goal of the extrapolation method in the red and NIR spectral regions. We also emphasize that the challenge for achieving the accuracy goal of 5% in the *in situ* determinations of surface upwelling radiance from underwater measurements is further reinforced by the fact that the extrapolation error associated with depth variations in $K_{L_{n}}(\lambda)$ discussed in this paper is not the sole source of uncertainty, as indicated briefly in Section 1. Therefore, to ensure that the total error does not exceed 5% the safe strategy would be to keep the extrapolation errors discussed in this paper below 5%. For example, to keep the extrapolation error below 2% the acceptable depth pairs z_1 and z_2 would have to be chosen from the light green areas in Fig. 8. This reemphasizes the challenge for designing the measurement systems capable of taking measurements at very small near-surface depths within the top 1 m of the water column.

To provide more detailed insight into the measurement requirements that ensure small extrapolation errors in the most demanding long-wavelength portion of the spectrum, one example graph from Fig. 8 is replotted in Fig. 9 with additional information depicting example depth pairs z_1 and z_2 which ensure that the extrapolation error is less than 5% (dark green area) or less than 2% (light green area). Specifically, Fig. 9 shows the results for $\lambda = 750$ nm obtained with simulations for Chl = 0.2 mg m⁻³ [same data as in Fig. 8(i)]. As mentioned above, for this case the shallowest depth of measurement



Fig. 9. Similar to Fig. 8, but for the specific scenario of surface $Chl = 0.2 \text{ mg m}^{-3}$ and a light wavelength of 750 nm. The color scale indicates the absolute values of errors in $L_u(z = 0^-, \lambda)$ caused by extrapolation as computed by Eq. (9). The feasible solution domain for extrapolation error less than or equal to 5% is bounded by the left *y*-axis, the upper *x*-axis, and the black solid line. The black points within the dark green shaded area indicate examples of three feasible depth pairs (z_1, z_2) that achieve extrapolation accuracy better than 5%, and the three additional depth pairs located within the light green shaded area exhibit accuracy better than 2%.

must be located no deeper than 30 cm below the water surface to keep the extrapolation error below 5%. This is indicated by the data point in the rightmost corner of the green area in Fig. 9 with $z_1 \equiv z_{1 \text{ max}} = 0.3 \text{ m}$ and $z_2 = 0.35 \text{ m}$. Note, however, that this particular depth configuration requires the deeper depth of measurement that is just 5 cm below the shallower depth of measurement. Figure 9 also shows five additional example configurations of depth pairs that fall within the green area of the accuracy goal. Two of these example configurations ensure the extrapolation errors less than 5% and have larger separation between z_1 and z_2 than 5 cm. These configurations are $z_1 = 0.2$ m and $z_2 = 0.5$ m and $z_1 = 0.1$ m and $z_2 = 0.7$ m. The three remaining examples ensure the extrapolation errors less than 2%. These configurations are $z_1 = 0.1$ m and $z_2 = 0.4$ m, $z_1 = 0.15$ m and $z_2 = 0.35$ m, and $z_1 = 0.1$ m and $z_2 = 0.15$ m. We note that the configurations with a depth separation of tens of centimeters appear to provide more practical and desirable depth settings for field measurements with a two-depth (or multidepth) radiometric system compared with the separation by 5 cm only. Apart from potential practical issues in the design of field instrumentation, somewhat larger (but not too large) separation between the two depths than 5 cm can be beneficial in terms of producing larger differences in the measured radiance L_u at two depths, and hence more accurate determinations of desired values of K_{L_u} within the near-surface layer. On the basis of analysis of data in Fig. 9 a reasonable first option choice for the depth pair ensuring the extrapolation error less than 5% at 750 nm is $z_1 = 0.2$ m and $z_2 = 0.5$ m. For the error less than 2% this choice is $z_1 = 0.15$ m and $z_2 = 0.35$ m.

Such first option choices of z_1 and z_2 , accompanied with the transmittance of radiance between these two depths, are listed in Table 2 for several wavelengths from the red and NIR spectral region on the basis of similar analysis of simulation results for the scenarios of $Chl = 0.2 \text{ mg m}^{-3}$ and $Chl = 2 \text{ mg m}^{-3}$. The results for $Chl = 0.2 \text{ mg m}^{-3}$ are also applicable to waters that are optically clearer than those described by the scenario of $Chl = 0.2 \text{ mg m}^{-3}$. Note that more turbid waters $(Chl = 2 \text{ mg m}^{-3})$ allow the use of slightly larger depths of z_1 and z_2 compared with clearer waters. However, regardless of water optical properties, the key conclusion emphasized by the data presented in Table 2 is that measurements of upwelling radiance within the top layer of tens of centimeters (~50 cm) of the water column are required to ensure that the extrapolation error in the derived values of water-leaving radiance in the red (>650 nm) and NIR spectral regions is smaller than 5%. At present, this requirement is not met in most field experiments when underwater radiometric measurements are done, except a very limited number of experiments such as Wire-Stabilized Profiling Environmental Radiometer (WiSPER) [18,23] and Remotely Operated Vehicle (ROV) [49]. Therefore, there is a need for developing improved radiometric systems and refined deployment strategies that meet the depth requirements suggested above, in order to ensure more accurate in situ determinations of water-leaving radiance, especially in the red and NIR spectral regions. We also note that although our analysis is focused on just two depths representing the minimum requirement for determining K_{L_u} , which in turn is needed

	$Chl \le 0.2 \text{ mg m}^{-3}$					$Chl = 2 \text{ mg m}^{-3}$						
		$\leq 2\%$ $\leq 5\%$			$\leq 2\%$			≤ 5 <i>%</i>				
λ(nm)	z_1 (m)	z_2 (m)	Т	z_1 (m)	z_2 (m)	Т	z_1 (m)	z_2 (m)	Т	z_1 (m)	z_2 (m)	Т
650	1.0	3.0	0.56	1.5	4.5	0.44	2.5	5.5	0.34	3.0	7.5	0.21
700	0.4	1.2	0.72	0.8	1.5	0.77	0.5	1.1	0.81	0.8	1.8	0.73
750	0.15	0.35	0.66	0.2	0.5	0.55	0.2	0.55	0.35	0.3	0.8	0.32
800	0.15	0.5	0.53	0.3	0.65	0.54	0.35	0.75	0.44	0.5	1.0	0.37
850	0.1	0.2	0.68	0.1	0.3	0.47	0.1	0.35	0.34	0.2	0.45	0.35
900	0.05	0.1	0.74	0.1	0.15	0.75	0.1	0.2	0.52	0.15	0.25	0.52

Table 2. Recommended Depth Pairs z_1 and $z_2(z_2 > z_1)$ That Ensure the Accuracy of Extrapolated Values of $L_u(z = 0^-, \lambda)$ within 2% or 5% of the True Value^a

"Results are given at six selected light wavelengths λ for two Chl cases as indicated. The transmittance of L_u over the depth range from z_1 to z_2 , $T = L_u(z_2, \lambda)/L_u(z_1, \lambda)$, is also provided.

for extrapolation of L_u within the near-surface layer, in practice the deployment of radiometric systems capable of taking measurements at more than two depths has obvious benefits.

E. Estimation of Surface Radiance from a Single-Depth Measurement

The spectral upwelling radiance at the surface, $L_u(z = 0^-, \lambda)$, can be estimated with desired accuracy from a single-depth near-surface measurement without a need for extrapolation or

knowledge of $K_{L_u}(z, \lambda)$ provided that this measurement is made at sufficiently small depth [49]. Such single-depth measurements very close to the surface can be made with surface float systems, such as a commercial system called Hyperspectral Tethered Spectral Radiometer Buoy (Hyper-TSRB, Satlantic Inc.). These measurements are typically made at a depth of ~20 cm or so. The most critical question for such single-depth deployments of radiometers concerns the maximum depth z_{max}



Fig. 10. Illustration of the absolute values of error in $L_u(z = 0^-, \lambda)$ at light wavelengths of 450, 550, 650, 750, and 850 nm when utilizing $L_u(z, \lambda)$ at a single depth *z* within the upper 10 m as the estimate of $L_u(z = 0^-, \lambda)$. Results depict simulations at solar zenith angle of 0° with all three inelastic processes included for three surface Chl scenarios of 0.02 (top), 0.2 (middle), and 2 mg m⁻³ (bottom). The color scale indicates the absolute values of error in percentage computed from the expression in the y-axis label. The error values of 2% and 5% are indicated by the light and dark green dotted lines, respectively.

	Chl = 0.0	12 mg m^{-3}	Chl = 0.	2 mg m^{-3}	$Chl = 2 mg m^{-3}$		
λ(nm)	$\leq 2\%$	≤ 5 <i>%</i>	$\leq 2\%$	≤ 5 <i>%</i>	$\leq 2\%$	\leq 5%	
450	1.00 m	2.6 m	0.5 m	1.2 m	0.15 m	0.45 m	
550	0.35 m	0.95 m	0.3 m	0.8 m	0.2 m	0.55 m	
650	0.07 m	0.15 m	0.06 m	0.15 m	0.05 m	0.1 m	
750	0.01 m	0.02 m	<0.01 m	0.02 m	<0.01 m	0.02 m	
850	<0.01 m	0.01 m	<0.01 m	0.01 m	<0.01 m	0.01 m	

Table 3. Maximum Depth z_{max} That Permits an Estimation of $L_u(z = 0^-, \lambda)$ Within the Listed Error Criteria of 2% and 5% from the Simulated Value of $L_u(z, \lambda)$ Taken at a Single Depth $z \le z_{max}$

that permits an estimation of $L_u(z = 0^-, \lambda)$ in terms of the measured value of $L_u(z, \lambda)$ taken at a single depth $z \leq z_{\max}$ with an error that meets the accuracy goals of 2% or 5%. Note that when posing this question we imply that no assumption is made or needed about $K_{L_u}(\lambda)$ within the near-surface layer between the surface and z_{\max} . Figure 10 addresses this question on the basis of our radiative transfer simulations for the three Chl scenarios and five selected light wavelengths ranging from the blue to NIR spectral bands. Specifically, this figure illustrates the absolute percent error in $L_u(z = 0^-, \lambda)$ caused by the assumption that the measured $L_u(z, \lambda)$ taken at a single depth zcan be used as an estimate of $L_u(z = 0^-, \lambda)$. Based on data presented in Fig. 10, Table 3 lists the values of z_{\max} that satisfy the accuracy goals of 2% and 5%.

In ultraoligotrophic waters with very low Chl of 0.02 mg m^{-3} , these accuracy goals in the blue spectral region can be achieved with a single-depth measurement taken at depths down to z_{max} of about 1 m and 2.6 m for the 2% and 5% errors, respectively (Table 3). As Chl increases z_{max} decreases so that the measurement within the top 45 cm is required to meet the accuracy goal of 5% in the blue spectral band when Chl is 2 mg m⁻³. At longer light wavelengths, in particular in the red and NIR spectral regions, z_{max} is reduced to very small values of 15 cm or less regardless of Chl. For example, to ensure the error of 5% or less at a wavelength of 650 nm in waters with $Chl = 0.2 \text{ mg m}^{-3}$, a single-depth measurement has to be taken at a depth of 15 cm or less. For the NIR wavelengths of 750 and 850 nm, such measurement would have to be taken just below the surface at 2 cm and 1 cm, respectively. These extremely small values of $z_{\rm max}$ indicate that the implementation of a single-depth measurement for estimating the water-leaving radiance in the NIR with sufficiently high accuracy is highly challenging and rather impractical under most environmental conditions. The use of multiple-depth measurements within the top layer of tens of centimeters along with the extrapolation to the surface as described in Section 3.D appears to be more feasible and hence preferable. We note that although accurate radiometric measurements at such shallow near-surface depths have been rarely attempted in the past, recently there have been specific efforts to develop new radiometric systems for acquiring high-quality optical data very close to the sea surface. These efforts include, for example, the development of an improved commercial freefalling profiler providing higher stability and depth resolution of measurement in the near-surface water column compared to previous profiling systems [50] and a multidepth spectroradiometer system for near-surface measurements [51].

4. CONCLUSIONS

Measurements of underwater upwelling radiance with a purpose of estimating the spectral water-leaving radiance often ignore the importance of the effects of inelastic radiative processes, especially Raman scattering by water molecules, which can produce large errors in the estimated water-leaving radiance in the red and NIR spectral regions from extrapolation of measurements throughout the near-surface layer of the water column. In this study, we present results from radiative transfer simulations that demonstrate that the inelastic processes produce strong depth dependence of the diffuse attenuation coefficient of upwelling radiance in the red and NIR spectral regions within the nearsurface layer. This depth dependence of the attenuation coefficient, which can be observed even within an optically homogeneous water column, poses a challenging problem for the extrapolation method. Specifically, if the extrapolation of underwater radiance measurements from a certain depth to the surface assumes incorrect values of the attenuation coefficient within the near-surface extrapolation layer, significant errors arise in the derived surface values of radiance. Many profiling and multidepth underwater radiometric systems acquire measurements at depths below 1 m and this limitation can lead to large extrapolation errors in the red and NIR.

We evaluated the extrapolation errors associated with depth dependence of the attenuation coefficient for several environmental scenarios through simulations with a radiative transfer model. Specifically, we demonstrated and quantified these errors for an example scenario when the water-leaving radiance is estimated from underwater measurements of L_{μ} taken at or below 1 m using either a two-depth system or a profiling system. We show that large extrapolation errors exceeding the accuracy goal of 5% are produced in the red and NIR spectral regions in both measurement scenarios. Generally, our finding is that when the measurements taken between 1 and 5 m are used in the extrapolation, the accuracy goal of 5% for the derived values of surface upwelling radiance can be achieved only at wavelengths shorter than about 650 nm. At longer wavelengths this accuracy goal is generally not met even when the extrapolation is made using measurements between 1 and 2 m and the derived surface radiance can be underestimated by tens of percent and by as much as nearly 100% in the NIR wavelengths approaching 900 nm.

Although a number of routinely used ocean color algorithms are based on the blue and green bands, for example chlorophyll-*a* and POC algorithms (e.g., [1,2,4]), ensuring high accuracy of *in situ* determinations of water-leaving radiance in the red and NIR wavelengths is equally important as in the blue and green. The satellite-derived values of water-leaving radiance or remote-sensing reflectance in the blue and green are prone to atmospheric correction errors that depend on the accuracy of measurements and validity of the black pixel assumption in the NIR bands (e.g., [46]). The validation of this assumption requires accurate *in situ* determinations of water-leaving radiance in the NIR. The high accuracy of water-leaving radiance in the red and NIR is also important because the bands from this spectral region are used directly in some ocean color algorithms, especially to derive data products in coastal and inland waters, such as concentrations of algal pigments (e.g., [52–56]) and suspended particles [57–61]. Some inversion algorithms to obtain IOPs from remote-sensing reflectance [62–65] also utilize the red and/or NIR bands.

The radiometric systems and deployment strategies along with the extrapolation schemes that do not meet the depth requirements suggested in this study do not ensure that the waterleaving radiance is derived with an error less than 5% in the red and NIR spectral regions (λ longer than about 650 nm). This is because the measurements are not taken at sufficiently small depths within the near-surface layer. The results presented in this study point to the necessity of making measurements at very shallow depths within the top layer of tens of centimeters. This is a highly challenging requirement from the engineering standpoint and also for the deployment of instrumentation and acquiring meaningful data in the near-surface layer, especially in view of the action of waves, currents, and turbulence at very small depths in oceanic environments. However, this challenge should not deter us from pursuing a goal toward developing improved capabilities for in situ determinations of water-leaving radiance in the red and NIR spectral regions.

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