Review Article

Light Scattering by Pure Water and Seawater: Recent Development

Xiaodong Zhang\(^1\) and Lianbo Hu\(^2\)

\(^1\)Division of Marine Science, School of Ocean Science and Engineering, The University of Southern Mississippi, USA
\(^2\)Ocean Remote Sensing Institute, Ocean University of China, China

Correspondence should be addressed to Xiaodong Zhang; xiaodong.zhang@usm.edu

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Light scattering by pure water and seawater is a fundamental optical property that plays a critical role in ocean optics and ocean color studies. We briefly review the theory of molecular scattering in liquid and electrolyte solutions and focus on the recent developments in modeling the effect of pressure, extending to extreme environments, and evaluating the effect of salinity on the depolarization ratio. We demonstrate how the modeling of seawater scattering can be applied to better understand spectral absorption and attenuation of pure water and seawater. We recommend future efforts should be directed at measuring the polarized components of scattering by pure water over a greater range of wavelengths, temperature, salinity, and pressure to constrain and validate the model and to improve our knowledge of the water’s depolarization ratio.

1. Introduction

As more than 70% of the earth surface is covered by the oceans, light scattering by water plays a critical role in ocean color studies. Our ability to model molecular scattering by water directly affects how well the particle field can be derived from the measurements, which unavoidably include contributions from particles as well as water. While light scattering fundamentally arises from the interaction between photons and molecules, the Rayleigh theory of scattering by individual molecules in gases [1] cannot be directly applied to liquid because molecules in liquid, unlike those in the gas phase, are subject to intermolecular bonding, and hence, the interference of light has to be considered [2]. Smoluchowski [3] and Einstein [4] developed the theory of fluctuation of density due to the thermal motions of molecules to explain the light scattering by a liquid. Applying this theory, Raman [5] estimated the scattering by pure water and attributed the blue color of the ocean to the combination of scattering and absorption by water molecules. In addition to density fluctuation, Einstein [4] also considered scattering due to fluctuation of concentration, a theory applicable to solutions, such as seawater. Zimm [2] developed an alternative theory by combining Rayleigh scattering for individual molecules with the statistical mechanics of molecules to treat the interference of scattering by all molecules. To the first approximation, his result is the same as that based on the theory of fluctuation.

Since the development of the Smoluchowski-Einstein density fluctuation theory more than one century ago, a great deal of progress has been made in our understanding and modeling of light scattering by pure water and seawater. Morel [6] reviewed the Smoluchowski-Einstein theory and its comparison with the measurements of light scattering by pure water and seawater. He found reasonable agreement between the theory and experiments, even though the agreement was better for liquids other than water. Morel [6] also reviewed the Smoluchowski-Einstein theory and its comparison with the measurements of light scattering by pure water and seawater. He found reasonable agreement between the theory and experiments, even though the agreement was better for liquids other than water. This is mainly because (1) purification is more difficult to accomplish for water than for other liquids and (2) relatively low scattering by water (in the order of \(10^{-5}–10^{-4} \text{m}^{-1} \text{sr}^{-1}\) depending on the wavelength) as compared to other liquids places stringent requirements on instrument calibration and control of stray light. Using the latest measurements of the thermodynamic variables and better representation of density fluctuation, Zhang and Hu [7] were able to predict the scattering by pure water that agrees with the measurements by Morel [8] within the experimental error of 2%. Zhang et al. [9] derived from concentration fluctuation an analytical expression of scattering as a function of salinity that agreed with the measurements very well. The Zhang et al. [9] model has been...
tested globally in a variety of waters [10]. Zhang [11] provided a comprehensive review of light scattering by water and its modeling.

In this study, we will review recent developments that have allowed the scattering by seawater to be modeled from 300 nm to 900 nm for nearly any water body in the oceans. Improved modeling of seawater scattering can also constrain the spectral absorption coefficient of water because attenuation is easier to measure than absorption. We will demonstrate an example of this application. We will conclude by discussing how our knowledge on scattering by seawater can be further improved in view of ocean color remote sensing. For self-completeness, we will start with a brief introduction to the fluctuation theory of light scattering.

2. Brief Review

2.1. The Smoluchowski-Einstein Fluctuation Theory of Light Scattering. Random thermal motion of molecules in a liquid causes the fluctuation in the number of molecules in a given volume element (Figure 1). The size of volume elements is small compared with the wavelength of light such that the light field inside the volume elements can be considered homogeneous, but big enough to contain a sufficient number of molecules for statistical thermodynamics to be applicable. As a reference, a volume element of linear size 50 nm would contain approximately 4 million water molecules.

For a liquid, such as pure water (Figure 1(a)), the microscopic fluctuation in the number of molecules leads to microscopic fluctuation in density ($\rho$; kg m$^{-3}$) and subsequently the microscopic fluctuation in the refractive index ($n$) that ultimately leads to the scattering of light. The volume scattering function ($\beta_d$; m$^{-1}$ sr$^{-1}$) due to density fluctuation is [3, 4]

$$\beta_d(\theta) = \frac{\pi^2 k_B T \beta_T}{2\lambda^4} \left( \frac{\partial n^2}{\partial \rho} \right)^2 (1 + \cos^2 \theta),$$

(1)

where $k_B$ is Boltzmann constant (=1.38 $\times$ 10$^{-23}$ m$^2$ kg s$^{-2}$ K$^{-1}$), $\lambda$ (m) is the wavelength of light in vacuum, $\beta_T$ (m s$^{-2}$ K$^{-1}$) is the isothermal compressibility, $T$ (K) is absolute temperature, and $\theta$ is the scattering angle.

For a solution, such as pure seawater that contains both water molecules and disassociated salt ions, the microscopic fluctuation in the number of molecules leads to two types of microscopic fluctuations, density (Figure 1(b)) and salt concentration (C; kg m$^{-3}$) (Figure 1(c)). Both fluctuations lead to microscopic fluctuation in the refractive index. For a solution, the volume scattering function due to density fluctuation is the same as Equation (1), and the volume scattering function due to concentration fluctuation ($\beta_c$) is [4, 12]

$$\beta_c(\theta) = \frac{\pi^2}{2N_A \lambda^4} \left( \frac{\partial n^2}{\partial \rho} \right)^2 \frac{CV_0'}{-\partial \ln a_0/\partial C} (1 + \cos^2 \theta),$$

(2)

where $a_0$ and $V_0'$ (m$^3$ mol$^{-1}$) are the activity and partial molar volume of water, respectively. The detailed derivation of Equations (1) and (2) can be found in Zhang [11]. For seawater, the concentration of salt is often expressed as salinity ($S$; g kg$^{-1}$). From Equation (2), Zhang et al. [9] deduced the volume scattering function due to salinity fluctuation ($\beta_s$):

$$\beta_s(\theta) = \frac{\pi^2 M_0}{2N_A \lambda^4} \left( \frac{\partial n^2}{\partial S} \right)^2 \frac{6 + 6\delta}{6 - 7\delta} (1 + \cos^2 \theta),$$

(3)

where $M_0$ is the molecular weight of pure water (18.01528 g mol$^{-1}$). Also note that $S$ in Equation (3) differs from the practical salinity unit $S$ (%) in both definition and values, $S$(g kg$^{-1}$) = (35.16504/35) $\times$ $S$(‰) [13].

2.2. Anisotropic Effect. Few molecules are isotropic, and the anisotropic nature of the molecules, including water molecules, affects the scattering in two ways [14]. The first effect is to increase the overall intensity of scattering, by an amount determined by the Cabannes factor ($f_c$):

$$f_c = \frac{6 + 6\delta}{6 - 7\delta},$$

(4)

where $\delta$ is the depolarization ratio, defined as the ratio between horizontally and vertically polarized components of the scattered light at 90 degrees with an incident, unpolarized light. The second effect is to alter the angular pattern of the volume scattering function, where the $1 + \cos^2 \theta$ term in Equations (1)–(3) becomes $1 + (1 - \delta)/(1 + \delta) \cos^2 \theta$. For a detailed derivation of the anisotropic effects, refer to Zhang [11].

Accounting for the anisotropic effects, Equation (1) becomes

$$\beta_d(\theta) = \frac{\pi^2 k_B T \beta_T}{2\lambda^4} \left( \frac{\partial n^2}{\partial \rho} \right)^2 \frac{6 + 6\delta}{6 - 7\delta} \left[ 1 + \frac{1 - \delta}{1 + \delta} \cos^2 \theta \right].$$

(5)

Equation (3) becomes

$$\beta_s(\theta) = \frac{\pi^2 M_0}{2N_A \lambda^4} \left( \frac{\partial n^2}{\partial S} \right)^2 \frac{6 + 6\delta}{6 - 7\delta} \left[ 1 + \frac{1 - \delta}{1 + \delta} \cos^2 \theta \right],$$

(6)

and the total volume scattering function by seawater ($\beta$) is

$$\beta(\theta) = \beta_d(\theta) + \beta_s(\theta).$$

(7)

3. Recent Development

The fluctuation theory for light scattering by pure water and seawater is well established. Among the variables that the model depends on, $k_B$, $M_0$, and $N_A$ are constants or assumed to be known (note however that light scattering had once been used to determine the value of the Avogadro number, $N_A$), and $T$, $S$, $\lambda$, and $\theta$ are independent variables. Therefore, further developments have been mainly achieved by better determination and/or parameterization of the remaining
variables, \(\beta_T, \rho, n, a_0\), and \(\delta\), and the partial derivative terms, \(\rho \partial n^2/\partial \rho, \delta n^2/\partial S\), and \(\partial \ln a_0/\partial S\).

3.1. Density Fluctuation. A critical development was that a better parameterization was found for the \(\rho \partial n^2/\partial \rho\) term in Equation (5) that led to a much-improved estimate of scattering due to density fluctuation [7]. Even though the refractive index \(n\) and density \(\rho\) are linked intimately by several classic formulae [15], including the Lorentz-Lorenz equation where \((n^2 - 1)/(n^2 + 2)\rho = \text{const}\) and \(\rho \partial n^2/\partial \rho = (n^2 - 1)/(n^2 + 2)/3\), the scattering estimates based on these classic formulae deviated significantly from the experiments [16]. Because of this, \(\rho \partial n^2/\partial \rho\) was replaced with

\[
\rho \frac{\partial n^2}{\partial \rho} = \frac{1}{\beta_T} \frac{\partial n^2}{\partial P},
\]

using the definition of isothermal compressibility \(\beta_T = \rho^{-1} \partial \rho/\partial P\).

Because the refractive index \(n\) has been measured under various pressures \(P\) [17, 18], Equation (8) allows the density fluctuation term to be approximated better than the classic Lorentz-Lorenz equation as demonstrated in Morel [6], Shifrin [19], and Buiteveld et al. [20]. For example, using Equations (5) and (8), we can estimate the scattering by pure water that agrees with the measurements [8, 21] with an average difference of 3.17% (Eq. (5)+Eq. (8) model in Figure 2).

In the meantime, the advancement in theoretical modeling of polarizability of liquid has improved the direct modeling of \(\rho \partial n^2/\partial \rho\) [22–24]. For example, from the general Lorentz-Lorenz theory, Proutiere et al. [24] deduced

\[
\rho \frac{\partial n^2}{\partial \rho} = \left( n^2 - 1 \right) \left[ 1 + \frac{2}{3} \frac{n^2 + 2}{n^2 - 1} \left( \frac{n^2 - 1}{3n} \right)^2 \right].
\]

Inserting Equation (10) into Equation (5), Zhang and Hu [7] were able to estimate the scattering by pure water that agreed with the measurements [8, 21] with an average difference of 0.67% (Eq. (5)+Eq. (9) model in Figure 2).

As discussed in Zhang and Hu [7], Equation (9) performs numerically better than Equation (8) in representing the density fluctuation because the uncertainty in modeling \(n\) is much less than the uncertainty in modeling \(\partial n/\partial P\).

3.2. Uniformed Parameterization. The thermodynamic variables \(\beta_T\) [25], \(\rho\) [26], and \(a_0\) [27] have been measured and parameterized individually in the light scattering model for pure water [7] and seawater [9]. While all of them vary with temperature, salinity, and pressure, only the dependences on temperature and salinity were parameterized in the scattering models, and their ranges of applicability were 0 to 30°C for \(T\) and 0 to 40 g kg\(^{-1}\) for \(S\). Feistel [28, 29] developed specific Gibbs energy of seawater \(g(S, T, p)\) from experimental data of heat capacities, freezing points, vapor pressures, and mixing heats over an extended validity range of -12°C ≤ \(T\) ≤ 8°C, and -0.1 Pa ≤ \(p\) ≤ 100 MPa, where \(p\) is sea pressure in Pa, and the absolute pressure \(P = 101325 + p\). The unit for Gibbs energy \(g\) is J kg\(^{-1}\) or m\(^2\) s\(^{-2}\). From thermodynamic relationships [30], we have

\[
\rho = \frac{1}{g_p},
\]
\[ \beta_T = -\frac{g_p}{g_p}, \quad (11) \]
\[ \frac{\partial \ln a_0}{\partial S} = -\frac{M_0S}{N_k k_B T} \theta_{so}, \quad (12) \]

where \( g_p \) represents the first-order partial derivative of \( g \) with respect to \( p \) and \( g_{pp} \) and \( g_{ss} \) represent the second-order derivative of \( g \) with respect to \( p \) and \( S \), respectively.

Inserting Equation (11) into Equation (5) leads to
\[ \beta_d(\theta) = \frac{\pi^2 k_B T}{2\lambda^4} \left( -\frac{g_p}{g_p} \right) \left( \frac{\partial n^2}{\partial \rho} \right)^2 \frac{6 + 6\delta}{6 - 7\delta} \left( 1 + \frac{1 - \delta}{1 + \delta} \cos^2 \theta \right). \quad (13) \]

Inserting Equations (10) and (12) into Equation (6) leads to
\[ \beta_s(\theta) = \frac{\pi^2 k_B T}{2\lambda^4} \left( \frac{g_p}{g_p} \right) \left( \frac{\partial n^2}{\partial S} \right)^2 \frac{6 + 6\delta}{6 - 7\delta} \left( 1 + \frac{1 - \delta}{1 + \delta} \cos^2 \theta \right). \quad (14) \]

The use of specific Gibbs energy of seawater and its derivatives to represent the various thermodynamic variables has improved the modeling of seawater scattering in several aspects. First, it provides a uniform parameterization, where the thermodynamic variables \( \rho, \beta_T, \) and \( a_0 \) are all expressed using specific Gibbs energy. Second, this uniform parameterization ensures the internal consistency among the various thermodynamic variables, potentially lowering the uncertainty and improving the performance of the model. Third, the constructions of the model for scattering due to density (\( \beta_d \)) and salinity (\( \beta_s \)) fluctuations (i.e., the similarity between Equations (13) and (14)), which do not alter the underlying physical principle, do appear more consistent than those between Equations (5) and (6). Lastly and more importantly, it extends the applicability of the model to nearly any natural water body on earth. For example, with Equations (13) and (14), the light scattering at \( 3\times10^{-4} \) with an accuracy of \( 0.058\% \) for QF and 0.063\% for MS if restricted to temperature > -6°C (Figure 4(a)). Mayuk and Light [42] also measured the refractive index of water with salinities up to 121 g kg\(^{-1}\), which the QF and MS models can predict with an uncertainty of 0.015\% and 0.005\% at 590 nm, respectively (Figure 4(b)). Huibers [43] showed the QF model, which was developed using data from 400 to 700 nm, compared well with the measurements by Irvine and Pollack [44] that extended from 200 to 1100 nm. Comparison with the measurements by Irvine and Pollack [44] and Daimon and Masumura [45] showed that both QF and MS models can be applied to the UV region down to 260 nm with an uncertainty < 1.0\% and to the NIR region up to 1100 nm with an uncertainty < 0.1\% (Figure 4(c)).

### 3.3. Refractive Index of Water

The refractive index of seawater varies with temperature, salinity, pressure, and wavelength. To the best of our knowledge, there are no theoretical models for the refractive index of seawater, and empirical models have been developed based on the measurements. The Quan and Fry [36] (QF) empirical equation for the index of refraction of seawater was used in Zhang and Hu [7, 31] and Zhang et al. [9]. Because the QF model does not include pressure effect, the Millard and Seaver [37] (MS) model was used in Hu et al. [34] for investigating the effect of pressure on light scattering by seawater. The MS model was developed from four datasets, including Tilton and Taylor [38] providing the index of pure water as a function of wavelength and temperature at atmospheric pressure with an accuracy of \( 6 \times 10^{-7} \); Mehu and Johannin-Gilles [39] providing the dependence of the index of seawater on temperature, salinity, and wavelength at atmospheric pressure with an accuracy of \( 3 \times 10^{-5} \); Stanley [40] providing the dependence on temperature, pressure, and wavelength at 35\% salinity with an accuracy \( 6 \times 10^{-7} \); and Wadler et al. [18] providing the dependence on temperature, pressure, and wavelength for pure water with an accuracy of \( 1 \times 10^{-4} \). The QF model was developed from composite data that Austin and Halikas [41] compiled from the first two datasets of the four that MS used after applying quality control and screening. Both QF and MS models agree with the measurements within the experimental uncertainties. The original ranges of validity for the QF model are \( 0-30°C \) for \( T \), 0-35\% for \( S \), and 400-700 nm for \( \lambda \); for the MS model are \( 0-30°C \) for \( T \), 0-40\% for \( S \), 500-700 nm for \( \lambda \), and 0-11,000 dbar (approximately 10,000 meters) for \( p \).

Comparison with an independent data set by Mayuk and Light [42] showed that both QF and MS models can also be extended to subzero temperature down to -23°C [33] with an uncertainty of 0.058\% for QF and 0.063\% for MS if restricted to temperature > -6°C (Figure 4(a)). Mayuk and Light [42] also measured the refractive index of water with salinities up to 121 g kg\(^{-1}\), which the QF and MS models can predict with an uncertainty of 0.015\% and 0.005\% at 590 nm, respectively (Figure 4(b)). Huibers [43] showed the QF model, which was developed using data from 400 to 700 nm, compared well with the measurements by Irvine and Pollack [44] that extended from 200 to 1100 nm. Comparison with the measurements by Irvine and Pollack [44] and Daimon and Masumura [45] showed that both QF and MS models can be applied to the UV region down to 260 nm with an uncertainty < 1.0\% and to the NIR region up to 1100 nm with an uncertainty < 0.1\% (Figure 4(c)).

### 3.4. Depolarization Ratio

The current uncertainty in the values of the depolarization ratio of pure water is at least \( \pm 0.5\% \), whereas the uncertainties of the other fundamental parameters used to compute the scattering by water are on the order of 0.1\% or less. 50\% uncertainty in \( \delta \) translates to approximately 3.5\% uncertainty in the scattering coefficient (Figure 5(a)). Several factors contribute to the greater uncertainty in \( \delta \). First, it is challenging to measure \( \delta \) for pure water because the horizontal component of the scattered light by water is so small and to measure it accurately
requires highly sensitive detectors and great care in eliminating stray light contamination. Consequently, only a few measurements have been conducted. Zhang et al. [46] reviewed these early efforts and various values that have been determined for δ. The current value of 0.039 was based on the measurement by Farinato and Rowell [47] and is the smallest among the values that have been reported. Zhang [11] found that the measured spectral values of δ are inconsistent in terms of spectral variation, with the data by Raman and Rao [48] and Cohen and Eisenberg [49] decreasing with wavelength and those by Kratohvil et al. [50] and Pethica and Smart [51] increasing with wavelength. There had been no study on how δ varies with salinity even though the depolarization ratio of several aqueous salt solutions at various concentrations was measured [52]. Therefore, we still do not know if and how the depolarization ratio of water changes spectrally or with salinity. Relatively large uncertainty in δ and its variation with salinity and wavelength have been recognized as one of the knowledge gaps that the ocean color community should address [10].

Zhang et al. [46] measured the depolarization ratio of water and its variation with salinity using a DAWN EOS multiangle light scattering instrument (Wyatt Technologies) equipped with a laser source at 532 nm. To alleviate the low signal-to-noise ratio for measuring the horizontal component of the scattering, they used five methods to estimate the depolarization ratio and found a mean value of 0.0038 ± 0.002 for pure water, consistent with the value of 0.039 that was measured by Farinato and Rowell [47] and is adopted for the current use [10].

Their measurements also showed an approximately 10% increase of δ with a 40 PSU increase in salinity. However, they found that the measured scattering became increasingly greater than the modeled scattering as salinity increases, an indication of potential contamination by nanoparticles in the prepared seawater samples. Because of this, their result on the change of δ with salinity is inconclusive.

As all light detectors have a finite acceptance angle, Zhang et al. [46] examined the effect of a sensor’s field of view (FOV) on measuring δ (Figure 5(b)). As expected, the error increases with the FOV. For the DAWN EOS instrument mentioned above, however, the FOV is 2.2° and hence has a negligible effect of <0.2% on deriving δ. Even though defined as the ratio of the horizontal to vertical components of scattered light at 90°, δ can be measured at other angles, which have an advantage of a reduced effect of FOV as compared to only using 90° measurements to estimate δ. This should be considered in future efforts in measuring δ of water.

4. New Applications

Our improved ability to model the scattering by pure water and seawater can also constrain the spectral absorption by water because attenuation is easier to measure than absorption, which can be derived as the difference between the attenuation and the scattering.

4.1. Absorption of Pure Water at UV Spectral Region. With future satellite missions, such as PACE, observing the oceans

Figure 3: The volume scattering function calculated at scattering angle 90° β(90) as a function of (a) temperature (T), (b) salinity (S), and (c) sea pressure (p). The variations are normalized by β(90) at T = 15°C (T₀), S = 0 g kg⁻¹ (S₀), and p = 0 MPa (p₀).
with hyperspectral capability from UV to NIR, the knowledge of spectral absorption of water in the UV is critical [10]. The measurement of the spectral absorption coefficient of water in the UV spectral region has been mainly conducted using spectrophotometry [53, 54]. In other words, it is the attenuation coefficient \( c \) (m \(^{-1} \)) that was measured, and to obtain the absorption coefficient \( a \) (m \(^{-1} \)), the scattering coefficient \( b \) (m \(^{-1} \)) due to water needs to be subtracted, i.e.,

\[
a(\lambda) = c(\lambda) - b(\lambda). \tag{15}
\]

The scattering coefficient \( b \) for pure water

\[
b = 2\pi \int_0^{\pi} \beta_d(\theta) \sin \theta d\theta = \frac{8\pi}{3} \beta_d(90) \left[ \frac{2 + \delta}{1 + \delta} \right], \tag{16}
\]

where \( \beta_d(90) \) represents the volume scattering function due to density fluctuation at scattering angle 90° and can be calculated using either Equation (5) or Equation (13). Note that \( b \) calculated from Equation (16) is only for pure water; for pure
seawater, replace $\beta_a(90)$ with $\beta_a(90) + \beta_s(90)$, where $\beta_s(90)$ can be calculated using either Equation (6) or Equation (14).

Both Quickenden and Irvin [54] and Kröckel and Schmidt [53] have corrected the scattering due to water in their estimates of the absorption coefficient. However, their estimate of pure water scattering used Equation (8), which as shown in Figure 2 has greater uncertainty than Equation (9). Also, Quickenden and Irvin [54] used a value of 0.051 for the depolarization ratio $\delta$ [47] and Kröckel and Schmidt [53] used a value 0.108 for $\delta$ [50]. As we have discussed in Section 3.4, the currently accepted value for $\delta$ is 0.039. As a result, both Quickenden and Irvin [54] and Kröckel and Schmidt [53] underestimated the scattering by water compared with the Zhang et al. [9] model (Figure 6(a)). Consequently, their estimates of the spectral absorption coefficient by water in the UV were overestimated (Figure 6(b)). The latest pure water absorption coefficients in the UV and visible region were measured by Mason et al. [55] using a specialized integrating cavity equipped with a newly developed diffuse reflector with high reflectivity in the UV region. This measurement was also considered most accurate thus far [10]. Both Quickenden and Irvin [54] and Kröckel and Schmidt [53] absorption coefficients corrected with the Zhang et al. [46] model agree well with Mason et al. [55] at wavelengths between 250 and 280 nm but are greater than Mason et al. [55] at wavelengths from 290 to 340 nm. It is also interesting to note that the Kröckel and Schmidt [53] data using the Zhang et al. [9] model for scattering correction approach the Mason et al. [55] value at 350 nm.

4.2. Salinity and Temperature Correction for AC Meter. The commercial spectral/hyperspectral absorption and attenuation meter (WET Labs Inc.; http://www.SeaBird.com) measures $a$ and $c$ that are contributed by nonwater substance by subtracting the corresponding values due to pure water. The pure water values are measured in the lab during calibration. Because measurements taken in the field typically have temperatures and salinities different from the lab condition, the changes of pure water absorption and attenuation due to changes of temperature and salinity have to be accounted for [56]. For the absorption channel of the AC meter, the change of absorption by pure water due to changes in temperature (from $T_0$ to $T$) and in salinity (from 0 to $S$), $\Delta a_{\text{meas}}$, is

$$\Delta a_{\text{meas}} = \Psi_T(T - T_0) + \Psi_S S + b_{42-180}(T, S) - b_{42-180}(T_0, 0),$$

and for the attenuation channel of the AC meter, the corresponding change of attenuation, $\Delta c_{\text{meas}}$, is

$$\Delta c_{\text{meas}} = \Psi_T(T - T_0) + \Psi_S S + b(T, S) - b(T_0, 0).$$

Here, $\Psi_T$ (m$^{-1}$·C$^{-1}$) is the temperature dependence of absorption by water and $\Psi_S$ (m$^{-1}$·S$^{-1}$) and $\Psi_{S,c}$ (m$^{-1}$·S$^{-1}$) are the salinity dependence of absorption by water for the a- and c-channels of the AC meter, respectively [56–58]. Because the a-channel of the AC meter also collects the scattered light from 0 to $\sim 42^\circ$, the absorption coefficient derived from the AC meter includes the contribution of scattering from 42 to 180°, which is represented by $b_{42-180}$ in Equation (17). The c-channel of the AC meter has an acceptance angle of $\sim 0.9^\circ$, and strictly speaking, only the scattering from 0.9 to 180° contributes to the measured attenuation coefficient. For
pure water, however, the difference of scattering from 0.9 to 180° and the total scattering from 0 to 180° is negligible, and hence, the total scattering \( b \) is used in Equation (18).

Currently, the temperature and salinity corrections applied to AC meter data only involve the absorption (i.e., the first two) terms in Equations (17) and (18) [56–58], and

![Figure 6: (a) Comparison of the scattering coefficient of pure water \((b, \text{m}^{-1})\) calculated by Quickenden and Irvin [54] (QI), Kröckel and Schmidt [53] (KS), and Zhang et al. [9] (ZHH). (b) Comparison of the absorption coefficient of pure water \((a, \text{m}^{-1})\) that is derived by subtracting \( b \) values in (a) from the attenuation coefficients \((c, \text{m}^{-1})\) measured by Quickenden and Irvin [54] and by Kröckel and Schmidt [53]. For each attenuation dataset, two sets of absorption coefficients are shown: one is the original values (QI and KS) and the other is the values updated using the ZHH model for scattering (QI-ZHH and KS-ZHH). The absorption coefficients of pure water measured by Mason et al. [55] (MCF) were also overlaid.](image)

![Figure 7: Changes in absorption \((\Delta a)\) and scattering coefficient \((\Delta b_{42-180} \text{ for a-channel and } \Delta b \text{ for c-channel})\) of pure water that would be measured by AC meter a-channel (a) and c-channel (b) when water temperature decreases from 20°C in the lab condition to 10°C in the field and salinity increases from 0 to 34 g kg\(^{-1}\) in the field. \(\Delta a + \Delta b_{42-180}\) and \(\Delta a + \Delta b\) are the total temperature and salinity correction that should be applied to the AC meter’s a- and c-channel, respectively. The dash lines are the typical precision (±0.001 m\(^{-1}\)) of the AC meter at a 4 Hz sampling rate.](image)
the changes of scattering (the last two terms in Equations (17) and (18)) have not been accounted for. Actually, Sullivan et al. [57] used Equations (17) and (18) to estimate the values of $\Psi_T$, $\Psi_{S,a}$, and $\Psi_{S,c}$ by subtracting the calculated scattering terms from their AC meter measurements of pure water at different temperatures and of NaCl solution at a concentration of 100 $\text{g kg}^{-1}$. Therefore, it is logical to include the scattering terms when applying the temperature and salinity corrections. Figure 7 compares the change of absorption and change of scattering that would be measured by an AC meter in a hypothetical case, where temperature decreases from a lab condition of 20°C to 10°C in the field and salinity increases from 0 to 34 $\text{g kg}^{-1}$ in the field. The change in scattering due to temperature and salinity (blue lines in Figure 7) has a magnitude comparable or greater than the change in absorption (black lines in Figure 7) at the spectral ranges 400 to 570 nm and 640 to 670 nm. These spectral ranges are just outside the absorption shoulders centered at approximately 600 and 750 nm. The total change in both absorption and scattering for this hypothetical case is on the order 0.001–0.002 $\text{m}^{-1}$ and hardly detectable with the precision of the AC meter. Theoretically, the temperature and salinity corrections include the corresponding effect on the scattering. But with the current precision of the AC meter ($\pm 0.001 \text{ m}^{-1}$ at 4 Hz), the scattering effect is negligible.

5. Future Work

The modeling of scattering by pure water and pure seawater has been well developed. Among the variables involved in modeling the molecular scattering by water and sea salts, refractive index and Gibbs free energy were modeled with very high accuracy with uncertainties on the order of 0.1% or less. The largest uncertainty up to ±50% comes from the depolarization ratio, which can lead to about 3.5% uncertainty on estimating the scattering coefficient of pure water or pure seawater. The current values of 0.039 that have been adopted by the ocean color community were based on the measurement conducted in 1976 [47] for pure water and were recently confirmed [46]. However, we still need to improve our knowledge on the spectral variability of $\delta$ of pure water and its possible variation with salinity. In addition to the depolarization ratio, more studies are needed to measure the scattering of pure seawater over a greater range of wavelengths, temperatures, salinities, and pressures to constrain and validate the developed models. The current pure seawater scattering data that have been used for validating the models were measured by Morel [6] half a century ago and only at the ambient temperature and pressure, five wavelengths, and one salinity. As pointed out by Morel [6], there are three challenges for measuring scattering of pure seawater including (1) absolute calibration and high sensitivity of the scattering meter, (2) minimizing stray light, and (3) purification of seawater. These three challenges still remain nowadays. For example, current commercial scattering meters such as ECO-BB (Sea-Bird Scientific), DAWN EOS (Wyatt Technologies), or LISST-VSF (Sequoia Scientific) have the sensitivity of $1 \times 10^{-4} - 1 \times 10^{-5} \text{ m}^{-1} \text{sr}^{-1}$ and are therefore not adequate to resolve pure water or seawater scattering in the longer wavelengths or the horizontal component of the scattering in depolarization ratio determination. Therefore, special experimental setups with sensitivity at least on the order of $\sim 1 \times 10^{-6} \text{ m}^{-1} \text{sr}^{-1}$ and strictly controlling the stray light are needed in the future to conduct the precise scattering measurements of pure seawater.

Biogeochemical-Argo (BGC-Argo) profiling floats typically include measurements of backscattering [59] at depths up to 2000 m, and future Deep Biogeochemical Argo floats will descent to 6000 m [60]. These in situ measurements of scattering are subject to the effect of pressure. In the current data processing scheme for the backscattering data (Version 1.4) [61], the scattering due to seawater is computed using the Zhang et al. [9] model, which does not consider the effect of pressure and hence is only applicable to the surface waters. For BGC-Argo, this could lead to an underestimation of backscattering by particles by up to 10% [34]. Therefore, we recommend the BGC-Argo community to reprocess the backscattering data by accounting for the effect of pressure on the scattering by seawater.

Data Availability

The MATLAB code for light scattering by pure seawater is available at https://sites.google.com/view/xiaodongzhangmarineopticslab/programs.

Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this article.

Authors’ Contributions

XZ drafted the manuscript; LH analyzed data and provided figures.

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