Transmission across the water-air interface: resolving the impact of multiple interactions at the sea surface

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Abstract: A series of Monte Carlo and HydroLight radiative transfer simulations are used to demonstrate that the traditional form of the Fresnel transmission across the water-air interface is accurate. This contradicts assertions to the contrary in a recent paper [Opt. Express 25, 27086 (2017)] that suggested that the impact of multiple surface interactions had previously been ignored and that the transmission factor was dependent upon the turbidity of the water.

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1. Introduction

Transmission of light from below the sea surface into air is a key process in the formation of ocean colour remote sensing signals. The prevailing physical model of this transition, based on well-established Fresnel reflectance and transmission calculations and the equally well-established n^2 law for radiances has been used to predict emergent light fields for many decades with further work developing more robust approaches to deal with practical considerations such as the effect of wind-roughened surfaces.

Recently Dev and Shanmugam (D&S) [1] presented a new analysis of this process that challenges the established order and suggested that previous analyses had missed (i) a particulate contribution to the refractive index (RI) of seawater and (ii) multiple interactions of the upwelling photons with the water-air interface. The net effect of these alleged omissions was that the community had systematically underestimated water leaving radiances by as much as 33% in highly scattering waters.

Unsurprisingly such a dramatic assertion on such a fundamental point of radiative transfer simulation attracted interest and within a short period a response to the original article was published by Gordon and Voss (G&V) that challenged the theoretical basis of the proposed new model for water-air transmission [2]. The basis for the challenge was to propose a thought experiment using a simplified scenario and to show that the underlying radiative transfer theory could be explained in such a way that the original formulation of the water-air transition remained intact. The suggestion that particulate refractive index influenced the water-air transition was also challenged.

In their response to this challenge [3], D&S reiterated their conviction that the traditional approach failed to deal with multiple interactions at the sea surface but, based on their own experimental observations, noted that any contribution to the refractive index from particles was sufficiently small that it could effectively be ignored.

The current situation, therefore, is that the revised D&S model [3] for water-air transmission is available as an alternative approach to this key aspect of radiative transfer in the ocean. Researchers operating in this area will be left in doubt as to which model to use. Indeed, our

motivation for this short study was a need to consider this aspect of the system for a couple of different applications involving forward modelling and interpretation of ocean colour signals.

Here we approach the problem from a different perspective. The basis for our approach is to exploit results from our own Monte Carlo code which explicitly includes multiple interactions at the sea surface. This allows us to investigate the relationship between above and below surface radiance for a wide range of optical conditions. We compare results with equivalent simulations using the HydroLight (Sequoia Scientific) radiative transfer software which also resolves multiple surface interactions.

2. Theoretical arguments

2.1. Standard formulation for reflectance with multiple surface interactions

The total upwards radiance immediately beneath the sea surface, $L_u(\lambda, 0^-)$, can be described as the sum of contributions from multiple interactions at the water-air interface, $L_{ux}(\lambda, 0^-)$, such that

$$L_u(\lambda, 0^-) = L_{u1}(\lambda, 0^-) + L_{u2}(\lambda, 0^-) + L_{u3}(\lambda, 0^-) + \dots$$
 (1)

At each interaction with the sea-air interface a fraction of the upwards radiance is transmitted into air, $L_{wx}(\lambda, 0^+)$. For each interaction the transition is determined by the Fresnel relationship

$$L_{wx}(\lambda, 0^+) = \tau_{w,a} L_{ux}(\lambda, 0^-) \tag{2}$$

where $\tau_{w,a}$ is the upwards radiance transmission at the water-air interface and is given by

$$\tau_{w,a}(\lambda) = \frac{1 - \rho_{w,a}}{n_w^2} \tag{3}$$

and where n_w is the refractive index of seawater and $\rho_{w,a}$ is the Fresnel reflectance coefficient for the water-air interface. The total radiance transmitted into air, $L_w(\lambda, 0^+)$, can also be described as the sum of contributions from each interaction at the water-air interface

$$L_w(\lambda, 0^+) = L_{w1}(\lambda, 0^+) + L_{w2}(\lambda, 0^+) + L_{w3}(\lambda, 0^+) + \dots$$
(4)

substituting (2) into (4) gives

$$L_{w}(\lambda, 0^{+}) = \tau_{w,a} L_{u1}(\lambda, 0^{-}) + \tau_{w,a} L_{u2}(\lambda, 0^{-}) + \tau_{w,a} L_{u3}(\lambda, 0^{-}) + \dots$$
 (5)

Rearranging and using (1) gives the classic version of the radiance transmission function from water into air:

$$L_w(\lambda, 0^+) = \tau_{w,a} L_u(\lambda, 0^-) = \frac{1 - \rho_{w,a}}{n_w^2} L_u(\lambda, 0^-)$$
 (6)

Thus it is clear that it is perfectly feasible to describe the transmission of upwards radiance from water into air using the standard formulation of the n^2 – law for radiances and for it to take into account multiple interactions at the water-air interface. In this paper we will show that Eq. (6) holds for a standard format Monte Carlo model that specifically includes multiple interactions at the water-air interface. We will further show that the HydroLight radiative transfer model, a model which includes infinite orders of interaction by design [4], is consistent with the MC model. Finally, and very importantly, as the measured sub-surface upwards radiance, $L_u(\lambda, 0^+)$, is the sum of all contributions to the upwards radiance and is equivalent to the LHS of Eq. (1), we are able to conclude that there is no need for any modification of Eq. (6) for *in situ* measurements.

2.2. Critique of the D&S argument

In [1] D&S present an argument based on conservation of energy to derive a new expression for the water-air transmission that is claimed to account for previously overlooked multiple interactions. In the original paper they also claimed an additional term associated with impact of particle refractive index, but this was subsequently deemed to be insignificant in their rebuttal [3] of [2] so we do not refer to it further. The D&S consideration of energy conservation leads to the following expression for water-air transmission which varies with the upwards mean cosine, μ_u , and the single scattering albedo, ω :

$$\tau_{w,a} = \tau_{pw,a} + \mu_u \omega \tau_{pw,a} (1 - \tau_{pw,a}) + \mu_u \omega \tau_{pw,a} (1 - \tau_{pw,a})^2 + \mu_u \omega \tau_{pw,a} (1 - \tau_{pw,a})^3 + \dots$$
(7)

and where $\tau_{pw,a}$ is the partial transmission of originally incident radiance. Subsequent terms on the RHS of Eq. (7) refer to transmission of later interactions at the sea surface. Crucially, each of the terms on the RHS of Eq. (7) must operate on $L_{u1}(\lambda, 0^-)$ as it describes the progressive diminution of remaining upwards radiance through multiple interactions starting with $L_{u1}(\lambda, 0^-)$. However, by identifying a Maclaurin series within the expression [1] Eq. (7) simplifies to

$$\tau_{w,a} = \tau_{pw,a}(1 - \mu_u \omega) + \mu_u \omega \tag{8}$$

and in their rebuttal to [2] this is used to generate a final expression for the water leaving radiance

$$L_w(\lambda, 0^+) = \frac{1 - \rho_{w,a}}{n_w^2} \left[(1 - \mu_u \omega) + \frac{\mu_u \omega n_w^2}{(1 - \rho_{w,a})} \right] L_u(\lambda, 0^-).$$
 (9)

Equation (9) operates on the total upwards radiance beneath the sea surface, $L_u(\lambda, 0^-)$, but is derived from Eq. (7) which only makes sense if it operates on $L_{u1}(\lambda, 0^-)$. This expression is subsequently used in [1] to demonstrate apparent significant impact on derived water leaving radiances compared to use of the standard expression (Eq. (6)). Our concerns are as follows:

- 1. The logical implication of Eq. (7) is that it should operate on $L_{u1}(\lambda, 0^-)$ and not on $L_u(\lambda, 0^-)$ as suggested by Eq. (9). We believe that Eq. (9) is incorrect and that $L_u(\lambda, 0^-)$ should be replaced with $L_{u1}(\lambda, 0^-)$.
- 2. Equation (7) is theoretically derived but is not proven. This could be done using appropriately analysed Monte Carlo simulations. We currently have no opinion on this, but suggest whilst theoretically interesting, its value is diminished if it does indeed only apply for use with $L_{u1}(\lambda,0^-)$ which is not a measureable quantity. We would have to make major modifications to our code to support testing of this feature and do not believe that the potential value merits the effort involved.
- 3. The apparent 'improvements' in predictions of water leaving radiance given in [1] are not well validated with experimental data, and are invalid if point 1 is true. There are plenty of other possible sources of error e.g. in measurements of inherent optical properties that could explain the noted deviations between measured and modelled radiometry.
- 4. The original premise of [1] that multiple interactions at the sea surface has previously been overlooked is not true. This feature is well understood, has been incorporated into multiple radiative transfer modelling approaches and is consistent with the explanation leading to Eq. (6).

We will show that point 4 is true using our own Monte Carlo code and with the commercially available Hydrolight radiative transfer model, both of which we know resolve multiple interactions at the water-air interface. It will be proven that Eq. (6) holds for a theoretical scenario of 100% reflectance, using a simpler case than [2], and for a series of real water simulations covering a wide range of values of ω . Once these facts are demonstrated, it is a logical conclusion that since Eq. (6) holds, Equation (9) cannot simultaneously be correct and must therefore fall.

3. Methods

3.1. Monte Carlo simulations

The Monte Carlo code used in this study is a 3D forward tracing code for both ocean and atmosphere applications with multiple layers, with any combination of absorption, scattering and phase function optical parameters as well as an ocean surface abiding to Fresnel and Snell laws. It also has the possibility of placing photon counters at arbitrary depths above and below the simulated sea surface, counting photons directed at user-defined upwelling and downwelling angular sectors. The code has been used previously in multiple studies of in-water light fields [5,6], optical measurement artefacts [7,8] and fundamental theory of marine optics [9,10].

3.2. HydroLight simulations

A series of single wavelength (550 nm) simulations were performed using HydroLight 5.2 (Sequoia Scientific) with the sun placed in a black sky at 30° from vertical and the sea surface kept flat by assuming zero wind speed. A series of combinations of absorption and scattering coefficients were selected to cover a wide range of optical turbidity conditions, with the Petzold 'average particle' phase function used to determine the angular distribution of scattering [4,11 - Table 3.10].

4. Results

The first case considered here is a hypothetical scenario where a submerged laser beam is directed vertically upwards to the underside of the sea surface (see Fig. 1(a) for a schematic representation). In this case the sea retains the real refractive index of water $(n_w = 1.34)$ but is non-absorbing. The sky is completely black and any light exiting through the water-air interface is lost from the system. Light reflected downwards at the water-air interface is transmitted downwards until it hits a 100% reflecting mirror which redirects it back towards the surface. As the water is lossless, the initial radiance reaching the underside of the water-air interface, $L_{u1}(\lambda, 0^-)$, is simply the original output of the laser. In all cases we use a virtual radiance meter with a half-width collection angle of 7° to generate radiance signals in the simulated environment. To maximize computational efficiency, the input beam from the laser is set to have a 7° beam half-width to match the virtual sensor. Because the beam half-width in water was identical to the radiance collection angle (7°), the total subsurface radiance signal, $L_u(\lambda, 0^-)$, is the sum of photons reaching the interface during the initial and subsequent interactions at the sea surface, $L_{ux}(\lambda, 0^-)$. At each surface interaction a fraction of radiance is transmitted into the air using Eq. (2) to determine the probability of a transmission or reflectance event, with the total water leaving radiance, $L_w(\lambda, 0^+)$, being the sum of components transmitted at each interaction within the 7° collection angle of the simulated detector, $L_{wx}(\lambda, 0^+)$. This scenario is run within a Monte Carlo simulation environment that follows each photon until it exits the system. Using 10^9 input photons, the total number of photons reaching the underside of the surface layer was 102158181, giving an amplification factor of 1.0215 which is very close to the figure expected from Fresnel's Law and the n^2 law for radiances. As expected, all photons eventually exited the water, with 55629185 photons collected by the above surface radiance detector. The remainder of photons exited the system at angles outside the collection angle of the detector. Dividing the above surface photon count by the amplified below surface photon count gives a transmission factor of 0.5445, consistent with value of 0.5452 produced by Eq. (3) for this scenario. The small residual discrepancy in these values is potentially a consequence of having to use a finite collection angle for the virtual radiance sensor in order to collect adequate numbers of photons, while in theory the spread angle for radiance is infinitesimally small. Nonetheless, this result demonstrates that the fundamental basis of Eq. (5) is correct in describing a situation involving multiple surface interactions and that Eq. (6) naturally follows.

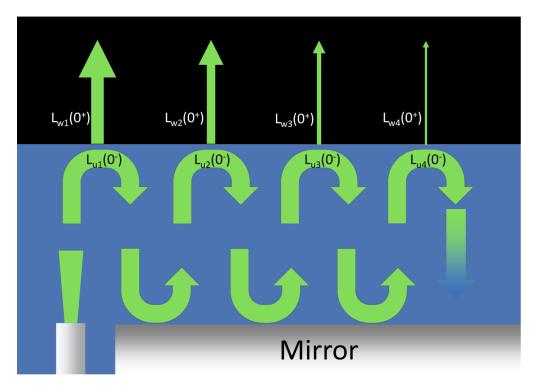


Fig. 1. Schematic representation of scenario 1 where an underwater laser points vertically upwards towards the underside of the sea surface. The medium retains the real refractive index of water but does not absorb or scatter light. Light reflected downwards from the underside of the sea surface is reflected upwards from a 100% reflective mirror. The fate of photons are followed through multiple interactions with the sea surface until they finally exit into the atmosphere.

The second scenario more closely resembles real world conditions where an above surface light beam is incident on the sea surface from above at an angle of 30° to the vertical (see Fig. 2 for a schematic representation). The light source is the sun in a black sky with no diffuse component of downwards irradiance. The sea has a real refractive index of 1.34 and a range of optical conditions are simulated with the absorption coefficient, *a*, set to 0.1 m⁻¹ and the scattering coefficient, *b*, iterating through values of 0.1, 0.2, 0.3, 0.4, 0.5, 0.75 and 1 m⁻¹. The angular distribution of scattered photons was determined using the average Petzold phase function. The simulation is carried out in a Monte Carlo environment where photons are lost if they are absorbed or exit through the sea surface. Within the water column, photons which are redirected towards and interact with the sea surface are dealt with using Eq. (2) to determine the probability of being transmitted or reflected. Photons returned back into the water column are allowed to progress through multiple surface interactions until they are either absorbed or transmitted into the atmosphere. The total below and above surface upwards radiances are given by the sums of all photons reaching and being transmitted through the water-air interface respectively. All radiance counters have a half-width angle of 7°.

A total of N = 10^9 photons were propagated through each simulated set of inherent optical properties. Fig. 3(a) shows the resulting estimates of $\tau_{\rm w.a.}$, obtained by dividing $L_{\rm w}(\lambda,0^+)$ / $L_{\rm u}(\lambda,0^-)$, consistent with Eq. (6), as a function of the single scattering albedo, $\omega = b/(a+b)$. Vertical error bars show standard deviations of the number of photons caught in the receiver n calculated using the formula for binomial experiments $\sigma = sqrt(N^*p^*(1-p))$, where p = n/N

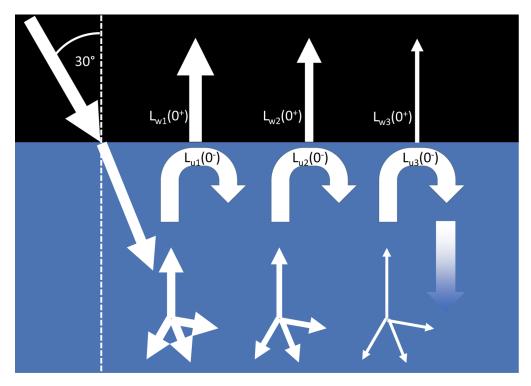


Fig. 2. Schematic representation of the radiative transfer processes involved in both Monte Carlo and HydroLight simulations for scenario 2. Light entering the water is both absorbed and scattered. The fate of photons are followed through multiple interactions with the sea surface until they are absorbed or finally exit into the atmosphere.

is the probability of photons being caught by the receiver. Values derived from simulations are very close to the value of 0.5452 expected for a refractive index of 1.34. There is a small variation in $\tau_{w,a}$ with increasing single scattering albedo, but this is attributable to the angular distribution of photons in the 7 deg cone which is used to generate the radiance signal in these simulations and there may be an element of noise associated with the stochastic nature of Monte Carlo simulations. Again, there is a distinction between theoretical radiances with infinitesimally small spread angles and practical measurements or even, in this case, simulations with finite collection angles. Irrespective of this, there is no general increase in $\tau_{w,a}$ with increasing ω as predicted in [1]. This result strongly contradicts the assertion that the effect of multiple surface interactions in turbid waters significantly influences the resultant $\tau_{w,a}$.

Figure 3(b) shows the results of HydroLight simulations for the same range of conditions used in the Monte Carlo runs. Values of $\tau_{w,a}$ derived from HydroLight simulations show less overall variability with ω , possibly reflecting greater accuracy in the determination of radiance signals as a function of collection angle. Nonetheless, close inspection reveals small scale structure that is rather similar to the minor fluctuations observed in Figure 3(a). Again, however, there is no evidence to suggest a general increase in $\tau_{w,a}$ with increasing turbidity as predicted in [1].

Application of Eq. (9) from the revised D&S model [3] generates values of $\tau_{w,a}$ ranging from 0.66 for $\omega = 0.5$ and upwards mean cosine $\mu_u = 0.5$ and steadily increasing as the input parameters increase. Use of this model would overestimate $\tau_{w,a}$ by amounts that increase linearly with increasing albedo, and reach $\sim 40\%$ for a scenario such as $\omega = 0.75$ and $\mu_u = 0.65$. This is a major divergence that is not supported by either the Monte Carlo or Hydrolight simulations presented here.

 $\omega = b/(a+b)$

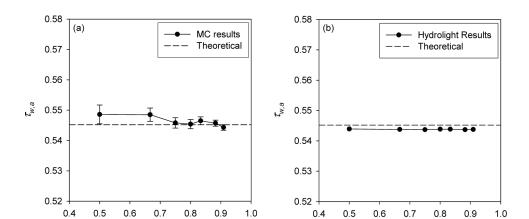


Fig. 3. Estimates of $\tau_{w,a}$ with increasing single scattering albedo, ω , for (a) Monte Carlo and (b) HydroLight simulations correspond well with theoretical values (dashed lines) and show no increase with increasing turbidity.

 $\omega = b/(a+b)$

5. Discussion

The original premise of the D&S approach was based on an assertion that multiple interactions at the sea surface were previously ignored [1]. This is a misrepresentation of previous efforts in the field. Any competent simulation of underwater light fields would necessarily include the possibility of multiple surface interactions. Taking Monte Carlo simulations as an example, it has been obvious since inception that photons would need to be followed to the point of annihilation through absorption or exit from the system at a specified boundary. The Monte Carlo code used in this study was not developed specifically for this paper. It is broadly typical of many such others used across the field and it specifically deals with multiple interactions at the sea surface.

Of course, one might note that the Monte Carlo code has the Fresnel formula built in so perhaps it is no surprise that these simulations return results consistent with its use? What has been proven here? D&S do not dispute the use of Eq. (2) for pure water [1]. This means that we are in agreement with D&S when Eq. (2) is used to describe any single surface interaction in our Monte Carlo simulations. They claim, however, that it needs to be augmented to account for multiple interactions using an approach based on conservation of energy (their Eq. (4)). If this was correct we would expect to see a corresponding effect emerge from Monte Carlo simulations that include multiple interactions. This is what has been tested here and found to be erroneous. There is no evidence in our Monte Carlo simulations to support the D&S formulation of multiple surface interactions encapsulated in their Eq. (4) [1]. Instead we have shown that there is no significant change in $\tau_{w.a}$ with increasing turbidity. This is consistent with the existing theoretical understanding of the system expressed as Eq. (6) in this document.

So where does the divergence between our approach and that taken by D&S arise? In [1] D&S developed an expression (their Eq. (4) and subsequent derivations) that purports to describe the evolution of light propagation from the first surface interaction onwards. The logical conclusion is that this expression must be operating on the initial upwards radiance immediately beneath the sea surface before any subsequent interactions have taken place, i.e. $L_{u1}(\lambda, 0^-)$. However D&S suggest that it is operating on the total subsurface upwards radiance signal, $L_u(\lambda, 0^-)$. We agree with G&V that this is the most likely source of error in this aspect of the D&S approach. The net effect of this suggested error is a form of double accounting where the additional terms in

their Eq. (11) further amplify an upwards radiance signal that has already had contributions from multiple interactions included.

It is possible that in their Eq. (4) D&S have found a new relationship between the total upwards radiance and the initial upwards radiance before multiple interactions are considered. Unfortunately our existing code is not set up to test this and would require substantial modification to do so. Given the overall outcome of our study which confirms the veracity of the standard theory, this does not seem like a sensible use of time. It may be the case that others can confirm or deny this aspect of the story using other versions of Monte Carlo code.

At its core, the D&S approach is based on a misunderstanding of the underlying physics of refraction at the sea surface. Whilst we have demonstrated the original formulation works using an approach based on tracking photons, the physics is better understood by considering electromagnetic theory. Refraction of light at the interface is a consequence of the wave nature of light and is required in order to conserve energy. There is no distinction between photons that have previously struck the sea surface and been reflected back into the water and those reaching the interface for the first time. All of them contribute to the incident electromagnetic field at that point, and the total field is subject to the laws of refraction and reflection at that point. This is the physical basis that leads to Eq. (6).

Conclusions

Monte Carlo simulations that explicitly include the effects of multiple interactions at the sea surface have demonstrated that the standard approach to simulating light transmission through the sea surface are valid. These results were further confirmed using the HydroLight simulation software package which also resolves multiple interactions. We reiterate the conclusion of G&V [2] that Eq. (6) is correct. Investigators measuring or modelling $L_u(\lambda, 0^-)$ can be confident in predicting $L_w(\lambda, 0^+)$ using Eq. (6).

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References

- 1. P. J. Dev and P. Shanmugam, "New theoretical formulation for the determination of radiance transmittance at the water-air interface," Opt. Express 25(22), 27086-27103 (2017).
- 2. H. R. Gordon and K. J. Voss, "New theoretical formulation for the determination of radiance transmittance at the water-air interface: comment," Opt. Express 26(15), 19137-19139 (2018).
- P. J. Dev and P. Shanmugam, "New theoretical formulation for the determination of radiance transmittance at the water-air interface: reply," Opt. Express 26(15), 19140–19143 (2018).
- 4. C. D. Mobley, Light and Water: Radiative Transfer in the Natural Waters (Academic, 1994).
- 5. P. J. Flatau, J. Piskozub, and J. R. V. Zaneveld, "Asymptotic light field in the presence of a bubble-layer," Opt. Express 5(5), 120-123 (1999).
- 6. J. Piskozub, T. Neumann, and L. Wozniak, "Ocean color remote sensing: choosing the correct depth weighting function," Opt. Express 16(19), 14683-14688 (2008).
- 7. J. Piskozub, P. J. Flatau, and J. R. V. Zaneveld, "Monte Carlo study of the scattering error of a quartz reflective absorption tube," J. Atmos. Oceanic Technol. 18(3), 438-445 (2001).
- D. McKee, J. Piskozub, R. Röttgers, and R. A. Reynolds, "Evaluation and Improvement of an Iterative Scattering Correction Scheme for in situ Absorption and Attenuation Measurements," J. Atmos. Oceanic Technol. 30(7), 1527-1541 (2013).
- 9. D. J. Bogucki, J. Piskozub, M.-E. Carr, and G. D. Spiers, "Monte Carlo simulation of propagation of a short light beam through turbulent oceanic flow," Opt. Express 15(21), 13988–13996 (2007).
- 10. J. Piskozub and D. McKee, "Effective scattering phase functions for the multiple scattering regime," Opt. Express **19**(5), 4786–4794 (2011).
- 11. T. J. Petzold, "Volume scattering functions for selected ocean waters," in Light in the Sea, J. E. Tyler, ed. (Dowden Hutchinson & Ross, 1977).