

Biases in ocean color over a Secchi disk

JAIME PITARCH*

*NIOZ Royal Netherlands Institute for Sea Research, Department of Coastal Systems, and Utrecht University, PO Box 59, 1790AB, Den Burg, Texel, the Netherlands *jaime.pitarch@nioz.nl*

Abstract: The oldest record of ocean color measurements consists of visual comparisons to a standardized color scale, the Forel-Ule scale (FU). Analysis of FU archived data allows the construction of a century-long time series. In situ protocols of FU measurements require the perceived color to be estimated over the water column above a Secchi disk (SD) at half of the depth where it goes out of sight, whereas satellites retrieve FU over the water column alone. I show in this article that these two methodologies lead to different FU readings and thus, merging both kinds of data will create artificial trends. In case 1 waters, radiative transfer simulations show that measuring over a SD shifts FU between 0 and $+ 2$ in respect to no SD, and there exists no possibility to relate the two in a univocal fashion. A univocal relationship is found if color is expressed in terms of the hue angle, which can be calculated from light spectra or RGB images.

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1. Introduction

1.1 Measuring color in terms of the Forel-Ule scale and the hue angle

Satellite-borne ocean color sensors are providing valuable global data at short revisit times. Archived data since the launch of SeaWiFS go back to late 1997, thus starting to be significant to study long-term trends, which is a major interest of the scientific community. In this context, it is worth mentioning the effort of ESA-CCI in providing consistently reprocessed multi-sensor data. With the last reprocessing to date, that data set contains observations from 1997 to 2016 [1]. However, in order to derive climatic trends, longer time series are required. For this reason, the analysis of historic color data, namely Forel-Ule (FU) observations, has received attention in the last years [2–5]. To provide continuity to the FU time series, several initiatives have proposed the development of FU products derived from atmospherically-corrected reflectance measured by mediumresolution ocean color sensors [4, 6]. The FU index can also be retrieved from RGB images. A more detailed information can be provided by the Hue angle, which also synthetizes the color of the water on a single number but as a continuous variable. Notably, a plugin that calculates the Hue angle and FU from any atmosphericallycorrected SeaWiFS, MODIS, MERIS and OLCI image has been created for the Sentinels Application Platform (SNAP).

Some of the quantities used in this article belong to the field of colorimetry. Necessary concepts are well explained in the works by Wernand and collaborators [2, 4, 6]. Briefly, any light radiance or reflectance spectrum, and any RGB image can be converted to the XYZ space. Normalization to the image brightness leads to only two independent numbers: $x = X/(X + Y + Z)$, $y = Y/(X + Y + Z)$. All visible colors for an average person are represented on the CIE 1931 diagram, in Fig. 1. The point (x_w, y_w) = $(1/3,1/3)$ corresponds to the absence of color, a flat spectrum. Points on the boundary correspond to pure color, a spectral Dirac delta. All colors along a radius from (x_w, y_w) have the same dominant wavelength and differ only in their contrast. For this reason, color can be expressed in terms of the angle respect to the increasing abscissae, when the origin is set at (x_w, y_w) : H = arctan $[(y-y_w)/(x-x_w)]$, namely the Hue angle. The transmission spectra of the 21 FU standards can be measured and converted to (x,y) (Fig. 1(a)) [2]. Thus, every FU index is related to a Hue angle. Hue angle observations can then be converted to FU by storing in a table the Hue angle values of the 21 FU standards and looking for the nearest value for a given Hue angle observation. The contrary is not possible beyond the angular resolution of the FU scale.

1.2 Statement of the problem

In situ protocols of FU observations require that a Secchi disk is held at half of the Secchi disk depth, $z_{SD}/2$ [2, 7]. Then, the color of the water above the disk is compared to the FU scale and an index from this scale is chosen. On the other hand, satellite observations measure color over the full water column. The following paragraphs show evidence that a Secchi disk changes the color of the water above it. In situ and remotely derived FU measurements are thus intrinsically biased and merging both kinds of data into a single data set can introduce artificial trends if such bias is not removed.

Fig. 1. Change in color over a Secchi disk (SD) at different depths. Panel a): CIE 1931 (x,y) coordinates of the remote-sensing reflectance for three different chlorophyll-a concentrations (see legend). Squares: infinite water column: Circles: SD at variable depths, until the surface. Diamonds: SD at $z_{SD}/2$. Overlapped, in grey dots, the coordinates of the 21 FU colors. Panel b): remote-sensing reflectance for the case $C = 0.2$ mg m⁻³ in panel a).

Table 1. Forel-Ule index and Hue angle of simulated remote sensing reflectance for the simulation detailed in Fig. 1.

C (mg m ^{-3})	0.2	0.8	2.0
$z_{SD}(m)$	31.45	14.97	8.44
$\rm H_{\rm \scriptscriptstyle \infty}$ (°	220.84	199.14	164.54
FU_{∞}			h
$H_{SD} (°)$	211.35	174.89	145.91
FU _{SD}			

To test the hypothesis of color change in the presence of a SD, I have performed a series of radiative transfer simulations using EcoLight [8], see the Methods section for details on the bio-optical models and simulation setup. For chlorophyll concentrations (C) of 0.2, 0.8 and 2.0 mg m⁻³, several runs are made for a range of SD positions, from a very large depth up to the surface. Secchi disk depth was estimated using Preisendorfer's model [9]. Simulated color (Fig. 1) without the SD and with the SD at $z_{SD}/2$ are highlighted. For a given chlorophyll concentration, the R_{rs}-derived color in the CIE 1931 coordinates (x,y) follows a trajectory that, starting from no SD, shifts towards higher contrast as the SD rises from a very large depth and becomes visible, but at some point between no SD and SD at $z_{SD}/2$, the trajectory bends towards the white point (x_w, y_w) = $(1/3,1/3)$, when the disk is right at the surface. If the trajectory was along a straight line, the perceived color would be the same for every SD position, with only variations in the contrast, but as there is a curvature, the perceived color changes. A look at the R_{rs} values in panel b) shows that not only the magnitude of R_{rs} changes as the SD approaches the surface, but also the shape: R_{rs} for the SD at $z_{SD}/2$ has the peak shifted towards greener wavelengths with respect to no SD. This phenomenon is present for different values of chlorophyll concentration, and seems higher for $C = 0.8$ mg m⁻³ than for the other two simulated values. FU and Hue angle for an infinite water column $(H_{\infty} FU_{\infty})$ and over a SD at $z_{SD}/2$ (H_{SD} FU_{SD}) are reported in Table 1 for these simulations, showing water looks greener above a SD.

Fig. 2. a) A digital picture taken from a ship in the Mediterranean Sea of a Secchi disk in the water at $z_{SD}/2$. b) Hue angle of the image, in degrees.

Experimental evidence of the color change over a SD can be obtained from digital pictures. Figure 2(a) shows a picture of seawater and a SD which was held at $z_{\text{SD}}/2$. Corresponding panel b) shows the Hue angle calculated for each pixel. A sharp drop in the Hue angle over the surface of the disk is clearly noted: whereas the Hue angle over the full water column is $\sim 221^\circ$ (FU = 2), it is $\sim 209^\circ$ (FU = 3) over the disk.

An algebraic R_{rs} model for shallow waters (Eq. 18 in [10]), was used to model a SD at different depths (Fig. 4 in [10]), showing a similar result as Fig. 1 here. Application of that model can provide a physical explanation for the color shift: a SD adds a term to the reflectance that has a peak at the window of maximum transparency (at green wavelengths for blue waters) and dominates over the reflectance of the infinite water column when the SD is at $z_{SD}/2$. In another study, measurements showed that visuallyderived FU over a SD were higher than relative FU matchups derived from radiometry (Fig. 10a in [4]). Thus, from a practical perspective, it would be desirable to derive relationships between FU measured with and without SD for a range of optical properties, to be applied as correction factors prior to future data merging. I restrict the problem to open oceanic case 1 waters, that is, those where IOPs covary as a function of chlorophyll [11].

2. Radiative transfer simulations setup

A synthetic data set was created using EcoLight [8]. Raman scattering and fluorescence by chlorophyll and colored dissolved organic matter (CDOM) were included in the simulations. The sky was set cloud free and the atmosphere was set of a typical marine case 1 waters. Chlorophyll concentration (C) was varied in a logarithmically uniform interval. For each value, the bio-optical model "new case 1" was applied to obtain the related IOPs. Particle absorption (phytoplankton plus non-algal) was modelled according to $a_p(\lambda) = A(\lambda)C^{E(\lambda)}$. Wavelength-dependent $A(\lambda)$ and $E(\lambda)$ coefficient are provided with EcoLight. A(λ) is the particle absorption at C = 1 mg m⁻³. E(λ) accounts for the packaging effect, i.e., the loss of absorption efficiency for increasing chlorophyll. These coefficients are the merged result from various sources, but in the range 400-1000 nm, they are the provided by Bricaud et al. [12]. They calibrated the coefficients for the chlorophyll range 0.02 to 25 mg m⁻³. For this reason, I restrict the presentation of results to this range as well.

Absorption by CDOM was modeled by making it proportional to the respective particle absorption at 440 nm, $a_g(440) = f_{ya_p}(440)$. This value is projected to the full spectral range by applying $a_g(\lambda) = a_y(440)e^{-5(\lambda^2+40)}$, with S = 0.014 nm⁻¹. The actual value of the coefficient f_v is a matter of discussion in the Results section.

Detailed description of modeling of scattering in the "new case 1" model are provided in the technical documentation of Hydrolight/EcoLight. Briefly, non-water attenuation was modeled as a chlorophyll-dependent power law, and total scattering was obtained by subtraction. Particle phase function was modeled a linear combination of one phase function for small and one for large particles, with the relative weight shifting from the first to the second as chlorophyll concentration increases [8].

This article does not intend to be a study on Secchi disk models. Readers interested in the matter may refer to Preisendorfer's treatise on Secchi disk science [9] and the new theory proposed by Lee et al. [10]. The greatest practical advantage of Lee's model comparing to Preisendorfer's lays on the fact that the former can be estimated from R_{rs} whereas Preisendorfer's cannot. However, this advantage is not relevant here as the radiances at depth are available from Ecolight's output. From a theoretical perspective, Lee et al. challenged several characteristics of Preisendorfer's classical theory as (1) color contrast definition, (2) assumption of equal radiance distributions over the Secchi disk and over the surrounding water in the equation that propagates the contrast to the surface, and (3) usage of photometric broad band quantities instead of narrow spectral windows for transparency estimation. Despite all these considerations, a performance comparison between both z_{SD} models is still lacking and so to date there is yet no a definite answer regarding which theory is the most accurate for each water type. Thus for the remaining of this article, both z_{SD} models are applied.

Secchi disk depth was estimated with a newly developed Fortran routine for HydroLight/EcoLight that implements both Preisendorfer's [9] and Lee's [10] models. Both models need an estimate of the vertically averaged diffuse attenuation coefficient (K_d) . This quantity is directly computed by applying its definition, between the surface and a guess of z_{SD} . This procedure is repeated iteratively until convergence to the final z_{SD} estimate is reached. Thus the implementation of Lee's model is different here to the implementation in a remote sensing context, where K_d is estimated from R_{rs} .

The color over a SD at a given depth was modeled by setting a Lambertian bottom of the same diffuse reflectance as that of the SD. The reader may keep in mind that a horizontally infinite bottom is visually detectable at much greater depths than a SD of a finite size, but this approach is used only for color estimation purposes.

The spectral range was set from 350 nm to 720 nm, to cover the full visible, and in 5 nm intervals, enough to resolve the spectral features in case 1 waters. Except when explicitly noted, the sun was placed at the zenith. From each EcoLight run, the CIE 1931 coordinates (x,y) of the nadir-viewing R_{rs} were stored, from which the Hue angle and the Forel-Ule index were derived. The diffuse reflectance of the SD in water was set at ρ = 0.85 [9]. A sensitivity analysis (not shown) revealed negligible influence on the FU and Hue calculations at $z_{SD}/2$ for the *ρ* range 0.75-0.95.

3. Results and discussion

3.1 Color-to-chlorophyll relationships

The main goal of this article is to quantify changes in the FU index and the Hue angle when a SD is introduced, for fixed optical properties of the water. Nevertheless, it is desirable to have a bio-optical model with a reasonable accuracy for the global ocean, as trends of color and transparency are normally translated to chlorophyll units [3, 5]. As a first requisite, simulated reflectances for a given chlorophyll must agree with observations. A means to evaluate this goodness is to compare the simulated Rrschlorophyll matchups with the OC4v6 curve. This curve is the relationship between the chlorophyll concentration and a blue-to-green ratio called the maximum band ratio MBR $max[R_{rs}(443),R_{rs}(490),R_{rs}(510)]/R_{rs}(555)$, whose variability with chlorophyll concentration [13] was derived from measurements gathered in the NOMAD data set [14]. This curve is plotted in Fig. 3. Posteriorly, the MBR is calculated for the Ecolightderived R_{rs} using the "new case 1" model with the default $f_v = 0.2$. The plot highlights that, for a given chlorophyll concentration, simulated R_{rs} are "less green" than what predicted by the OC4v6 curve. A means to compensate this bias is increasing the weight of CDOM in the absorption budget. For global case 1 waters, Morel [15] reported $a_{\alpha}(440)$ $= 0.032C^{0.63}$, that leads to $f_v = 0.6154$. After updating this coefficient in the "new case 1" model, the simulated R_{rs} follow much more closely the OC4v6 curve.

Fig. 3. Maximum band ratio calculated from the EcoLight output R_{rs} using the "new case 1" model respect to the related chlorophyll concentration. Blue dots: using $f_y = 0.2$, the default value in the model. Red dots: using $f_v = 0.6154$, after *Morel* [15]. The OC4v6 curve [13] is added for comparison.

Fig. 4. Brown line: fit by *Wernand et al.* [3] after EcoLight simulations with the "new case 1" model. Black line: fit by *Boyce et al.* [5] from matched in situ FU and chlorophyll data, for an infinite water column. Red squares: simulated FU values for the simulation setup described in the Methods section, for $f_y = 0.2$ (default). Blue squares: same as the res squares, but using $f_y = 0.6154$, after *Morel* [15], for an infinite water column. Green squares: same as the blue squares, but placing a Secchi disk at $z_{SD}/2$ for each run, with z_{SD} calculated according to Preisendorfer's model [9]. Brown-green squares: same as the green squares, but with z_{SD} calculated according to Lee's model [10].

This low CDOM content in the absorption budget in the "new case 1" model can explain part of the large discrepancies between the FU-to-chlorophyll relationships reported in Boyce et al. [5] and Wernand et al. [3]. These are plotted together in Fig. 4. Wernands's curve $(C = 0.061e^{0.666FU})$ was derived from EcoLight simulations for an infinite water column using the "new case 1" model with $f_y = 0.2$, whereas Boyce's curve $(C = 0.016 \text{FU}^{2.44})$ was derived using in situ FU and chlorophyll matchups.

The sun zenith angle is set here at 40°. The "new case 1" model with $f_v = 0.2$ (red squares) essentially reproduces Wernand's curve. If the updated value $f_y = 0.6154$ is used (blue squares), FU is augmented in 0 or 1 units for the same chlorophyll, due to increased CDOM. Then, if color is measured over a Secchi disk at $z_{SD}/2$ (green squares), FU increases further 0 to 2 units for both models, with Lee's model predicting sometimes one FU unit more than Preisendorfer's. These last two simulation follow Boyce's curve very well until $FU = 6$. For higher values, simulations underestimate Boyce's curve. It is likely that the case 1 assumption in the simulations does not hold for high chlorophyll in Boyce's data set, and non-chlorophyll covarying substances increase the FU index further. On the other hand, at the lower edge, FU saturates at 1 for chlorophyll less than 0.05 mg m⁻³. Thus, chlorophyll variability in the oligotrophic oceans [16] appears not resolvable with FU readings.

3.2 Bias quantification

Once confidence on the chosen bio-optical model has been gained, the main issue of the article is tackled: to quantify differences between the color of an infinite water column (H_∞FU_∞) and the color of the water column above a Secchi disk at $z_{SD}/2$ (H_{SD},FU_{SD}), simulations are directly compared in Fig. 5 using both Preisendorfer's and Lee's models. Panel a) shows that a SD increases FU between 0 and 2 units, with stronger effect for FU between 3 and 5. This graph compares well to results by Wernand et al. [4]. Due to the discrete nature and the small value of the changes, the relationship between both FU is ambiguous. For example, if a $FU_{SD} = 3$, the respective FU_{∞} can be 2 or 3. This ambiguity can be resolved if color is compared in the continuous range of the Hue angle, in panel b).

Fig. 5. Differences in water color (FU in panel a) and Hue angle in Panel b)) derived from Ecolight simulations, using the "new case 1" bio-optical model with $f_y = 0.6154$, after Morel [15], with and without a Secchi disk. In panel a), square size corresponds to the relative number of occurrences.

Fig. 6. Difference in the calculated Hue angle the Remote sensing reflectance over a Secchi disk at $z_{SD}/2$ respect to the Hue angle over an infinite water column. The least squares 9th degree polynomials fit are plotted as well.

When the Hue angle error ($\Delta H = H_{SD} - H_{\infty}$) is plotted against H_∞ (Fig. 6), differences are more evident. Results show that estimating z_{SD} with Lee's model predicts a more pronounced negative shift in ΔH than using Preisendorfer's model, except for the lower edge of H∞. At the higher end, for the bluest oceanic waters, surprisingly Preisendorfer's model predicts a slight blueing when a SD is introduced. Instead, Lee's model predicts a slight greening.

To provide a correction formula for both approaches, 9th degree polynomials have been tried as fitting functions, $\Delta H = \sum_{n=1}^{\infty}$ $\Delta H = \sum_{i=0}^{9} x^i$, where *x* is H_∞ normalized to its standard

deviation after mean subtraction, $x = (H_w - \mu)/\sigma$, with $\mu = 179.5^\circ$ and $\sigma = 56.18^\circ$. Coefficients were found by robust non-linear regressions with bisquare weights. Table 2

	p_0	p_1	p ₂	p ₃	p_4	p ₅
Preisendorfer	-23.16 $(-23.37,$ -22.94	-12.41 $(-13.33,$ -11.49	18.37 (16.47, 20.27)	24.63 (19.73, 29.52)	17.55 (12.75, 22.35)	7.137 $(-0.8082,$ 15.08)
Lee	-23.27 $(-23.52,$ -23.03	-9.132 $(-10.19,$ -8.073	15.06 (12.87, 17.25)	17.96 (12.3, 23.62)	10.36 (4.812, 15.91)	-1.657 $(-10.84,$ 7.527
	p ₆	p_7	p_8	p ₉	r^2	RSME
Preisendorfer	-9.037 $(-15.21,$ -2.869	-13.99 $(-17.57,$ -10.41	-6.683 $(-10.33,$ -3.034	-1.106 $(-1.956,$ -0.2552	0.9994	0.2181°
Lee	-6.505 $(-13.63,$ 0.6248	-1.726 $(-5.862,$ 2.41)	0.9892 $(-3.229,$ 5.208)	0.3713 $(-0.6117,$ 1.354)	0.9991	0.2521 °

Table 2. Coefficients (with 95% confidence bounds) and statistics of the best fit 9th degree polynomial over the data points in Fig. 6.

provides coefficients and related statistics of both fits.

4. Conclusions

Visual color estimations have historically used a Secchi disk due to the need of enhanced brightness, as the reflectance of the water is low. A side effect of this protocol is that the color is altered. To my understanding, this issue has remained unnoticed so far because this change is small and is masked by high brightness differences.

Differences in published FU-to-chlorophyll relationships [3,5] are affected by the biooptical model used in the simulations and the FU estimation (with or without a SD). The simulations also have revealed that the FU scale saturates at 1 below $C \sim 0.05$ mg m⁻³, which impedes ability to track variations in color of the ultra-oligotrophic zones [16].

After choice of a suitable bio-optical model for the global ocean, a formula that links the Hue angle of an infinite ocean to that in the presence of a Secchi disk at z_{SD} , has been obtained. An analog formula for FU measurements is not possible due to the excessive discretization of this scale. Therefore, I suggest that modern color measurements using spectral radiometers or digital cameras are always expressed in Hue units if possible. Measurements carried out by volunteers in the framework of citizen science initiatives do not use a Secchi disk in most cases, but this possibility should be considered and a flag should be enabled to differentiate between both methodologies. Integration of modern Hue angle data with historic FU measurements becomes possible by (1) converting all Hue data without a SD to Hue with a SD and convert to FU index. In this case, FU data series will be extended until modern times for climate studies.

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