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Global distribution of Case-1 waters: An analysis from SeaWiFS measurements

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Abstract

"Case-1" has been a term frequently used to characterize water type since the seventies. However, the distribution of Case-1 waters in global scale has been vague, though open ocean waters are often referred to as Case-1 in the literature. In this study, based on recent bio-optical models for Case-1 waters, an inclusive and quantitative Case-1 criterion for remote sensing applications is developed. The criterion allows Case-1 waters to have about two-fold variations of non-pigment absorption and particle backscattering around their exact Case-1 values, allowing a large range of waters to be classified as Case-1. Even so, application of this criterion to ocean color data from the SeaWiFS satellite sensor suggests that Case-1 waters occupy only about 60% of the global ocean surface. Regionally, more Case-1 waters are found in the southern hemisphere than in the northern hemisphere, and most Indian Ocean waters are found to be Case-1. The Case-1 percentage and spatial distribution change with season, and with the boundaries chosen in the criterion. Nevertheless, this study for the first time provides a quantitative and geographical perspective of Case-1 waters in global scale, and further demonstrates that many open ocean waters are not necessarily Case-1.

Keywords: Case-1; Case-2; Ocean color; Remote sensing; Bio-optical model

1. Introduction

Studies of ocean optics in the past decades have found that there are three major water constituents in addition to water molecules that determine water's inherent optical properties (absorption and scattering): phytoplankton and its associates, colored dissolved organic matter (CDOM), and inorganic mineral particles (Carder et al., 1991; IOCCG, 2000; Sathyendranath et al., 1989). In modeling the optical properties and in particular to retrieve the phytoplankton pigment (chlorophyll-a) concentration from ocean color (i.e., water-leaving radiance or radiance of sea), a scheme to simplify the dependence of optical properties on water constituents was proposed: i.e., the Case-1 and Case-2 separation of natural waters (Morel, 1988; Morel & Prieur, 1977).

The concept of Case-1 and Case-2 waters, originally proposed by Morel and Prieur (1977), has evolved over the past decades (Gordon & Morel, 1983; IOCCG, 2000; Mobley et al., 2004; Morel, 1988; Prieur & Sathyendranath, 1981; also see Mobley et al., 2004 for review), and the definitions are not uniform. Commonly, Case-1 waters are those whose inherent optical properties (Preisendorfer, 1976) can be adequately described by phytoplankton (represented by chlorophyll concentration, or Chl) (Gordon & Morel, 1983; IOCCG, 2000; Morel, 1988), whereas Case-2 waters are otherwise. In other words, Case-1 waters, at least, require that the optical properties of other optically active constituents (CDOM and particles in particular) closely follow the optical properties of phytoplankton (Morel, 1988; Morel & Maritorena, 2001). Clearly, this definition of Case-1 water is *not* based on its geographical location, *nor* on the Chl value. In fact, coastal waters could be Case-1, whereas open ocean waters could be Case-2. However, the term "Case-1" is frequently used in the literature to characterize open ocean waters.

On the other hand, in the recent decades, many bio-optical models, remote-sensing algorithms for Chl retrievals, and applications in ocean-color remote sensing have been developed specifically for Case-1 waters e.g. (Gross et al., 2000; Haltrin, 1999; Morel, 1988; Morel & Maritorena, 2001; Ohlmann et al.,

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2000; O'Reilly et al., 1998; Stamnes et al., 2003). For instance, in the NASA software package SeaDAS, the default band-ratio algorithm used to estimate Chl requires water to be Case-1 (SeaWiFS, 2000). To use these Case-1 specific models and algorithms, knowledge of the distribution of Case-1 waters in global scale and its temporal variations is required.

Ideally, concurrent measurements of both optical properties (absorption and scattering) and Chl are required to map the global distribution of Case-1 waters. In practice, however, the only feasible means is to use ocean color data from satellite sensors. Therefore, based on the latest bio-optical models for Case-1 waters developed from extensive measurements (Morel & Maritorena, 2001), in this study we devised an inclusive remote-sensing criterion to map Case-1 waters using remote-sensing reflectance (a measure of ocean color). Further, we applied this criterion to the lately updated satellite data from the Sea-viewing Wide Field-of-view Sensor (SeaWiFS, "reprocessing 4") to provide a global perspective of Case-1 waters and its seasonal variations for the first time. Our goal is to obtain a quantitative understanding of the Case-1 water distribution on a global scale. In particular, we want to examine whether most open ocean waters (i.e., 90% or more) are Case-1.

2. Remote-sensing criterion for Case-1 waters

After atmospheric correction, spectral water-leaving radiance is derived from the radiance data collected by an ocean color satellite sensor (Gordon, 1997). This radiance can be easily converted to spectral remote-sensing reflectance ($R_{rs}(\lambda)$), defined as a ratio of water-leaving radiance to downwelling irradiance just above the surface. The latter can be adequately modeled with information derived from the process of atmospheric correction, for example, aerosol type and optical thickness (Gordon, 1997).

Absorption, backscattering, and diffuse attenuation coefficients as well as Chl could be further derived from $R_{rs}(\lambda)$ with a bio-optical algorithm (e.g., Carder et al., 1999; Hoge & Lyon, 1996; Lee et al., 2002; Maritorena et al., 2000; Mueller & Trees, 1997; Roesler & Perry, 1995). However, such derived parameters are associated with various uncertainties, especially for Chl, due to the assumptions used in the algorithms, such as the spectral shapes of chlorophyll and CDOM absorption (Nelson & Robertson, 1993; Wang et al., 2005), the specific-absorption coefficient of Chl (Bricaud et al., 1995, 1981), and so on. Different algorithms may yield different Chl estimates (O'Reilly et al., 1998). These characteristics make it difficult to use the derived parameters to map Case-1 waters. Causing further uncertainty is that sometimes the water type (Case-1 or Case-2) needs to be known *before* an algorithm is used to derive these parameters (O'Reilly et al., 1998). Hence, it is highly desirable to use $R_{rs}(\lambda)$ directly to separate water types such as Case-1 and Case-2.

As previously noted, Case-1 definitions are not uniform in the literature (Mobley et al., 2004). However, here we concur with the generally accepted concept that Case-1 waters are those whose inherent optical properties can be determined solely by Chl (Gordon & Morel, 1983; Loisel & Morel, 1998; Morel, 1988). Therefore, for optically deep waters, a unique relationship exists between Chl and Case-1 $R_{rs}(\lambda)$ (Haltrin, 1999; Morel, 1988; Morel & Maritorena, 2001). And, based on the Case-1 bio-optical models developed from extensive measurements of Chl and optical properties, the spectral remote-sensing reflectance ($R_{rs}(\lambda)$) of Case-1 waters can be calculated when Chl is known (Maritorena & Siegel, 2005; Morel & Maritorena, 2001). Specifically, spectral models have been developed to calculate Case-1 water diffuse attenuation (K_d) and backscattering (b_b) coefficients for a given chlorophyll value (Loisel & Morel, 1998; Morel, 1988; Morel & Maritorena, 2001). In the initial steps of calculating absorption coefficient (a) and irradiance reflectance (R) (Morel & Maritorena, 2001), K_d is converted to absorption coefficient with an average cosine (Kirk, 1994) value of 0.75, and R is $\sim 0.33 b_b/a$. This R value is then combined with K_d to calculate another set of a following the Gershun's equation (Morel & Maritorena, 2001). After three iterations (Morel & Maritorena, 2001), stable $a(\lambda)$ and $R(\lambda)$ values are obtained. Because R_{rs} is also a function of b_b/a for Case-1 waters (Morel & Gentili, 1993), $R_{rs}(\lambda)$ is obtained for the given Chl. Following this approach, Case-1 $R_{rs}(\lambda)$ were calculated for Chl values ranging between 0.02 and 30.0 mg m^{-3} (500 points with a step of $\sim$0.01 in log scale). Further, the following spectral ratios were derived:

$$\mathrm{RR}_{12} = \frac{R_{rs}(412)}{R_{rs}(443)}, \quad \mathrm{RR}_{53} = \frac{R_{rs}(555)}{R_{rs}(490)}. \tag{1}$$

Here 412, 443, 490, and 555 are the center wavelengths (in nm) of SeaWiFS bands 1, 2, 3, and 5, respectively. RR_{12} represents the relative abundance of CDOM per Chl (Carder et al., 1999), RR_{53} is viewed as a measure of Chl (e.g., Aiken et al., 1995; O'Reilly et al., 1998) and $R_{rs}(555)$ as a measure of particle backscattering (Carder et al., 1999).

A monotonic line exists between the calculated RR_{12} and RR_{53} values (the blue line in Fig. 1a), because by definition optical properties of Case-1 waters are determined by Chl alone. This monotonic line can be represented accurately (less than 1% error) by the following empirical polynomial function (RR_{53} in a range of $\sim$0.2 to $\sim$2.0):

$$\mathrm{RR}_{12}^{[\mathrm{CS1}]} = 0.9351 + 0.113/\mathrm{RR}_{53} - 0.0217/(\mathrm{RR}_{53})^2 + 0.003/(\mathrm{RR}_{53})^3. \tag{2a}$$

The superscript [CS1] represents Case-1. Similarly, a monotonic line exists between $R_{rs}(555)$ and RR_{53} for Case-1 waters (blue line in Fig. 1b):

$$R_{rs}(555)^{[\mathrm{CS1}]} = 0.0006 + 0.0027\,\mathrm{RR}_{53} - 0.0004(\mathrm{RR}_{53})^2 - 0.0002(\mathrm{RR}_{53})^3. \tag{2b}$$

Included in Fig. 1a and b are the dependences of RR_{12} and $R_{rs}(555)$ on RR_{53} (discrete points), calculated from field-measured R_{rs} data extracted from the SeaWiFS Bio-optical Archive and Storage System (SeaBASS, Werdell & Bailey, in press). Apparently, for both RR_{12} and $R_{rs}(555)$, the above Case-1 relationships represent the average trends contained in measurements.

Eqs. (2a) and (2b) provide guidance on the CDOM absorption (RR_{12}) and particle backscattering ($R_{rs}(555)$) per Chl (RR_{53}) for Case-1 waters. For natural waters, however, because CDOM and particles do not necessarily co-vary with Chl, the optical properties (absorption and backscattering coefficients, in particular) will show deviations around their exact Case-1 values, as shown in Fig. 1a and b. To map the global distribution of Case-1 waters using $R_{rs}(\lambda)$ values, the rigorous Case-1 relationships represented by Eqs. (2a) and (2b) need to be relaxed, and a quantitative boundary needs to be defined. A water pixel is considered as Case-1 if the following two conditions are met simultaneously:

$$(1-\gamma)RR_{12}^{[CS1]} \le RR_{12} \le (1+\gamma)RR_{12}^{[CS1]}, \tag{3a}$$

and

$$(1-v)R_{rs}(555)^{[CS1]} \le R_{rs}(555) \le (1+v)R_{rs}(555)^{[CS1]}. \tag{3b}$$

The inclusiveness of Case-1 water then relies on the selection of the values of γ and v. For the exact Case-1 water defined by Eqs. (2a) and (2b) (blue lines in Figs. 1 and 2), $\gamma=0$ and $v=0$. Practically, non-zero values have to be used to account for imperfections and approximations of models and measurements. To be inclusive (though arbitrary), we chose $\gamma=0.1$ and $v=0.5$ (i.e., we allowed a ±10% deviation of RR_{12} and at the same time a ±50% deviation of $R_{rs}(555)$ around their exact Case-1 values: $RR_{12}^{[CS1]}$ and $R_{rs}(555)^{[CS1]}$). The cyan and green lines in Fig. 1a and b represent the upper and lower boundaries, respectively. For each RR_{53}, the selected deviation range for $R_{rs}(555)$ is more than a factor of two, which is consistent with the range of scattering coefficients of Case-1 waters for a given Chl (Gordon & Morel, 1983). The ±10% deviation of RR_{12} implies an error of about −40% (when $\gamma=10\%$) to 100% (when $\gamma=-10\%$) in the ratio of $a_{CDOM}(443)/a_{Chl}(443)$ for the same Chl value, when a three-component bio-optical model is used (Sathyendranath et al., 2001, 1989). Here $a_{CDOM}(443)$ and $a_{Chl}(443)$ are the absorption coefficients of CDOM and chlorophyll at 443 nm, respectively. The deviation ranges in RR_{12} and $R_{rs}(555)$ thus indicate a loosely defined co-variation between absorption (and backscattering) coefficients and Chl (i.e., an inclusive remote-sensing criterion to classify Case-1 waters).

3. Global distribution of Case-1 waters

The above criterion was then applied to SeaWiFS 9-km data ("reprocessing 4") to map the global distribution of Case-1 waters. Seasonally averaged normalized water-leaving radiance ($[L_w(\lambda)]_N$) for the first five bands (412, 443, 490, 510, and 555 nm) between 23 March 2003 and 23 March 2004 were acquired from the Goddard Space Flight Center (http://oceans.gsfc.nasa.gov/SeaWiFS/Binned/). $R_{rs}(\lambda)$ (and then RR_{12} and RR_{53}) were calculated as $[L_w(\lambda)]_N/F_0(\lambda)$ (Morel & Gentili, 1996), where F_0 is the solar constant.

As an example, RR_{12}, RR_{53}, and $R_{rs}(555)$ values for Autumn 2003 (21 September–20 December) of the global ocean are presented in Fig. 2a and b. Clearly, when RR_{53} is perceived as a measure of Chl (the numbers in the parenthesis), even for waters with Chl less than 1.0 mg/m^3 (a range for most open ocean waters, Antoine et al., 1996), there are wide variations in both RR_{12} and $R_{rs}(555)$ for each RR_{53} value, suggesting significantly varying combinations of CDOM and suspended particles for the same Chl value. When compared with the relationships of RR_{12} and $R_{rs}(555)$ obtained from in situ measurements (Fig. 1), they are generally consistent with each other, respectively. For SeaWiFS data, however, there are more points whose RR_{12} values are less than 0.75 for RR_{53} ranging between 0.3 and 1.4. These points are located in coastal areas where SeaWiFS data may be erroneous (in the

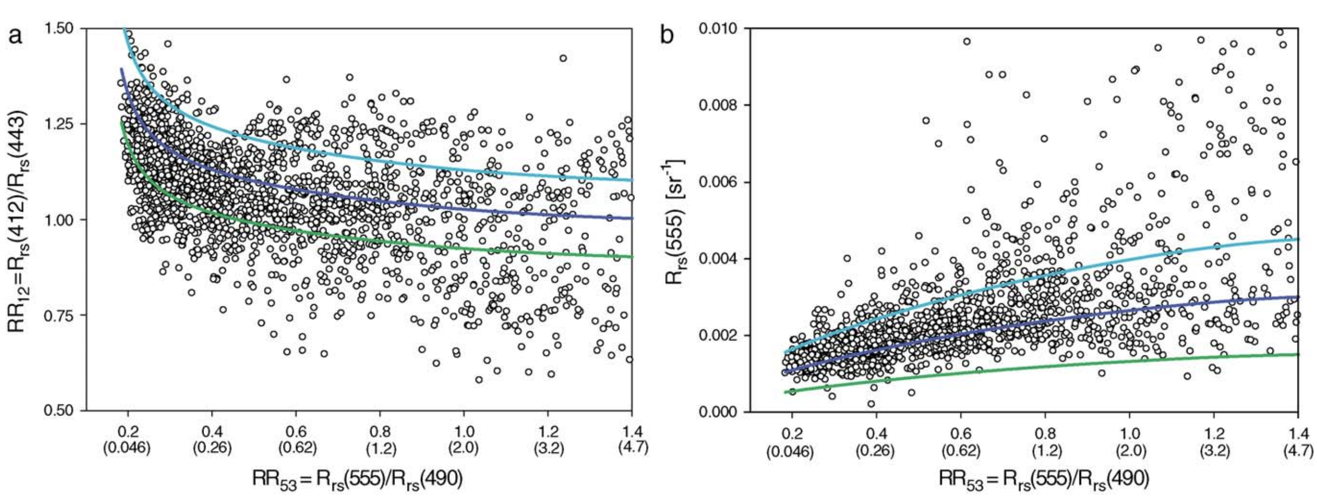

Fig. 1. RR_{12} (a) and $R_{rs}(555)$ (b) predicted by the Case-1 bio-optical model (blue lines), as well as the corresponding data (discrete points) extracted from the SeaBASS data set. RR_{12} values greater than 1.50 and $R_{rs}(555)$ values greater than 0.01 sr^{-1} are not shown. Blue lines indicate "exact" Case-1 waters. Cyan and green lines indicate ±10% deviation of RR_{12} (a) and ±50% deviation of $R_{rs}(555)$ (b), respectively. Case-1 water in this study is defined as those points that fall between the cyan and green lines on both graphs (i.e., both Eqs. (3a) and (3b) are met simultaneously). Numbers in parenthesis (X-axis) are the corresponding Chl values (in mg m^{-3}) derived from the OC2 algorithm.

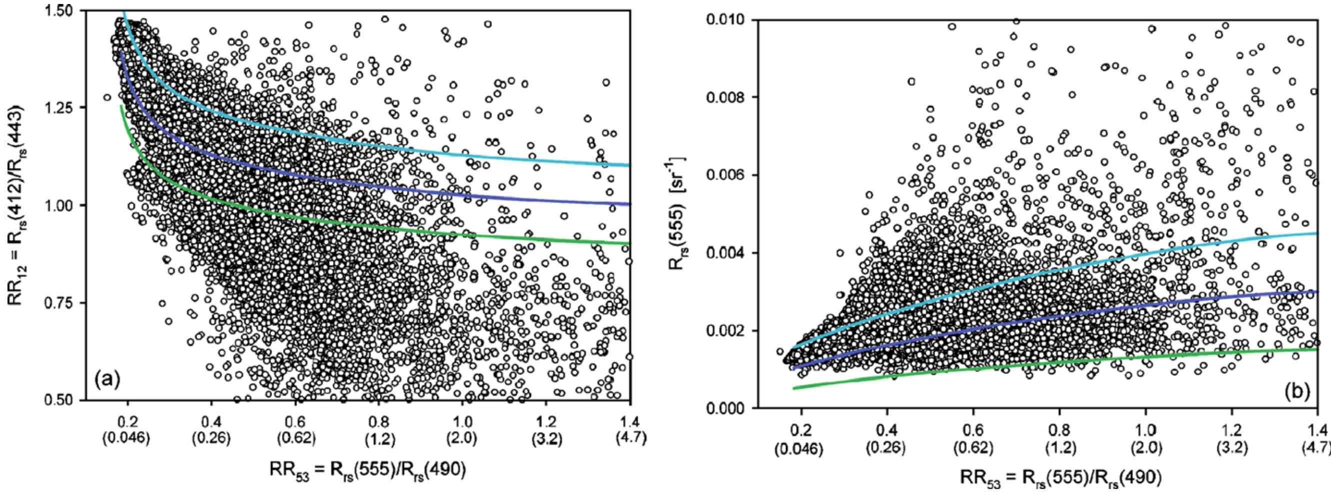

Fig. 2. Similar to Fig. 1, but the discrete data points represent those extracted from the SeaWiFS global data for Autumn 2003 (21 Sept.–20 Dec. 2003). RR_{12} values less than 0.50 and $R_{rs}(555)$ values greater than 0.01 sr^{-1} are not shown.

blue bands, in particular) due to the imperfect atmospheric correction (e.g., Hu et al., 2000). Another possible reason is that the field data from SeaBASS did not cover the global ocean evenly. Nevertheless, these points contribute about 5% of the SeaWiFS observed sea surface, therefore have limited effects to the analyses of global distribution of Case-1 waters.

Fig. 3 shows the global distribution of Case-1 and non-Case-1 waters based on the inclusive remote-sensing criterion (Eqs. (3a) and (3b)). Approximately 60% of the global surface water is found to belong to the Case-1 category. Regionally, most of the Case-1 waters are in the tropical and subtropical areas, along with waters in the Indian Ocean. About half of the non-Case-1 waters are found in high latitudes (especially in the northern hemisphere), and many of them are open ocean waters. In the mid Pacific, a lot of surface waters (these waters do not necessarily overlap with the equatorial upwelling regions) do not meet the Case-1 criterion, possibly due to lower CDOM per Chl (see below, and Siegel et al., 2005) than those predicted by the Case-1 bio-optical model (Morel & Maritorena, 2001). Seasonally, there is no substantial change in the total percentage of Case-1 waters from Spring to Autumn, but the percentage drops significantly in Winter, a result from a significant increase of non-Case-1 waters in the southern high latitudes. The spatial distribution of Case-1 waters also varies seasonally.

To examine the individual effects of the two conditions set by Eqs. (3a) and (3b), Fig. 4a and b exemplify Case-1 water distribution when only one of the conditions is applied, respectively. In Fig. 4a, where Eq. (3a) alone was applied,

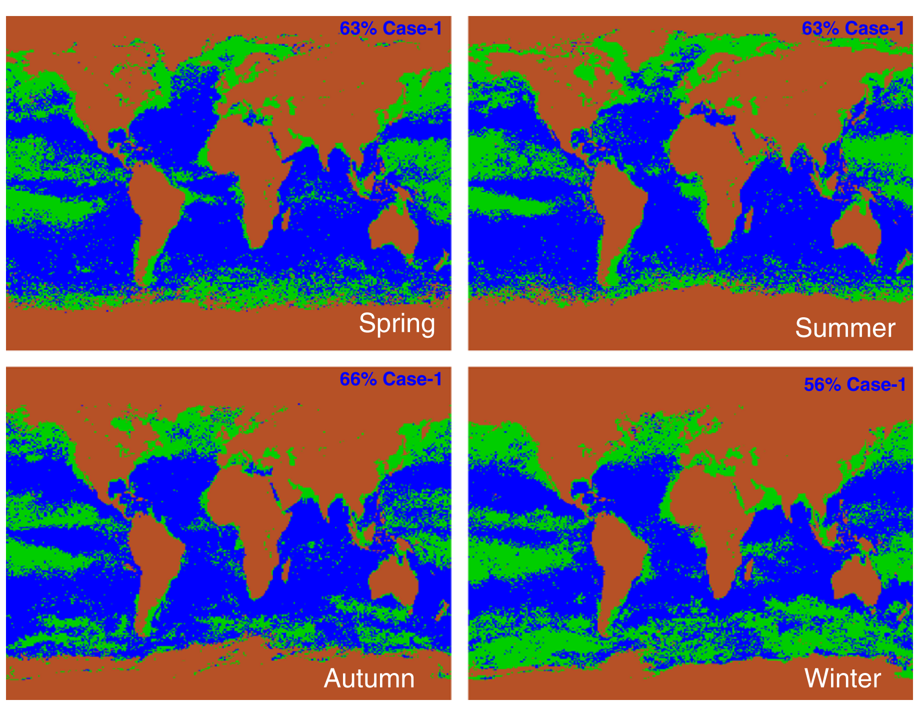

Fig. 3. Global distribution of Case-1 waters (blue color) and its seasonal variations as derived from SeaWiFS measurements. See text for Case-1 definition.

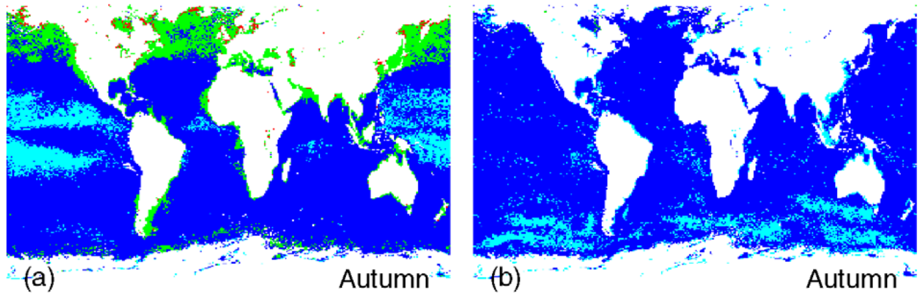

Fig. 4. SeaWiFS-derived Case-1 waters (blue color) for Autumn 2003 defined by Eq. (3a) with $\gamma=0.1$ (a) and by Eq. (3b) with $v=0.5$ (b), respectively. In (a), cyan color represents $RR_{12}>1.1RR_{12}^{[CS1]}$; green color represents RR_{12} between 0.5 and $0.9RR_{12}^{[CS1]}$; and red color for $RR_{12}<0.5$. In (b), cyan color represents $R_{rs}(555)>1.5R_{rs}(555)^{[CS1]}$; and green color for $R_{rs}(555)<0.5R_{rs}(555)^{[CS1]}$.

~76% of the global surface ocean (blue color) belongs to this further relaxed Case-1 category. For a large portion of waters in the mid Pacific (cyan color), their RR_{12} values are greater than $1.1RR_{12}^{[CS1]}$, indicating relatively lower CDOM per Chl (Siegel et al., 2005). In the high latitude northern hemisphere (green color), RR_{12} value are smaller than $0.9RR_{12}^{[CS1]}$ and indicate relatively higher CDOM per Chl. This is because R_{rs} is inversely proportional to absorption coefficient (Morel & Gentili, 1993), smaller RR_{12} values indicate higher absorption by CDOM at 412 nm (and then relatively more CDOM) (Carder et al., 1999; Sathyendranath et al., 2001; Siegel et al., 2005). Note that CDOM absorption also affects the spectral ratio of $R_{rs}(\lambda)$ (Carder et al., 1989; Sathyendranath et al., 2001). Therefore, if the same empirical band-ratio Chl algorithm (e.g., OC2 or OC4 algorithm, O'Reilly et al., 1998) is applied to the global ocean, Chl may be overestimated in the green colored waters while underestimated in the cyan colored waters, even without considering the phytoplankton "packaging effect" (Bricaud et al., 1995; Bricaud & Morel, 1986).

Fig. 4b shows the distribution of Case-1 waters during Autumn 2003 when Eq. (3b) alone was applied ($v=0.5$). The percentage of such Case-1 waters in the global ocean is ~88%, a result of the relatively large v value. Most (~90%) of the cyan colored waters, representing higher backscattering per Chl, are in the high latitude southern hemisphere, with the rest spread around many coastal regions (especially river plumes). Clearly, the effects of the two criteria do not completely overlap, suggesting independent variations of absorption and scattering coefficients, which might be the results of different biogeochemical processes (e.g., Balch et al., 2005; Behrenfeld et al., 2005; Boss & Zaneveld, 2003).

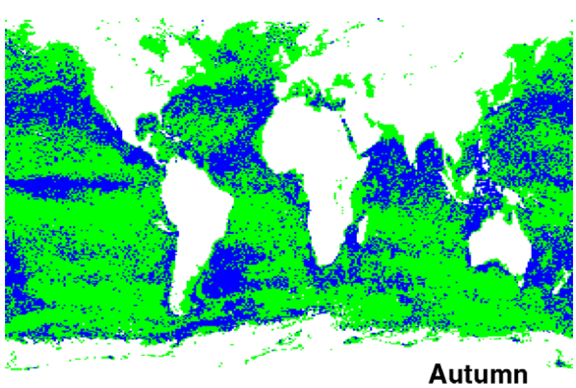

Fig. 5. Global distribution of Case-1 waters (blue color) for Autumn 2003 when the criterion for Case-1 definition is slightly tightened, i.e., v in Eq. (3b) is changed from 0.5 to 0.3 while γ in Eq. (3a) remains as 0.1.

The percentage of Case-1 waters depends on the quantitative boundaries (γ and v values). For example in Fig. 5, where we keep $\gamma=0.1$ but change v from 0.5 to 0.3 (which still represents a factor of 1.8 deviation range in $R_{rs}(555)$), we see the effects of more tightly defined Case-1 waters for Autumn 2003, where the percentage of Case-1 waters (blue color) drops to 32%. Even so, using this slightly tightened standard, some coastal waters may still belong to Case-1, while many open ocean waters fall out of the Case-1 category. Indeed, the optical properties of many open ocean waters do not co-vary with Chl (Siegel & Michaels, 1996), if the quantitative standard for "co-vary" is a ±30% deviation range from its expected value.

4. Summary

In this study, an inclusive Case-1 remote-sensing criterion was developed from the widely accepted Case-1 bio-optical models (Morel & Maritorena, 2001). This criterion compares the relationships between $R_{rs}(412)/R_{rs}(443)$ and $R_{rs}(555)/R_{rs}(490)$, and between $R_{rs}(555)$ and $R_{rs}(555)/R_{rs}(490)$, to their expected Case-1 values from the bio-optical models. Because only limited natural waters follow the quantitative relationships for Case-1 waters exactly, some boundaries were selected to include more waters as Case-1 (Gordon & Morel, 1983). The boundaries include a ±10% deviation in $R_{rs}(412)/R_{rs}(443)$ and a ±50% deviation in $R_{rs}(555)$ from their exact Case-1 values. Such boundaries are corresponding to about two-fold variations in the $a_{CDOM}(443)/a_{Chl}(443)$ ratio and in the backscattering coefficient at 555 nm for the same Chl value, respectively.

Application of this inclusive Case-1 remote-sensing criterion to the lately updated ("reprocessing 4"), seasonally averaged (less random errors than daily collections), SeaWiFS data yielded global distribution of Case-1 waters. Only about 60% of global surface waters could be considered as Case-1 by this criterion. A substantial portion of the open ocean is non-Case-1. The spatial distribution of Case-1 waters changes with season. Further, Case-1 distribution patterns obtained from the two individual conditions (absorption component and scattering component) do not always overlap, suggesting independently varying water constituents. The spatial resolution of the SeaWiFS data used in this study is 9 km, as used in other global studies (e.g., Siegel et al., 2005). Because oceanic waters are relatively uniform over large distances, we would not expect our results to change significantly if higher spatial resolution data were used.

The Case-1 coverage, as shown above, strongly depends on the deviation boundaries chosen in the criterion. For example, if the ±50% deviation for $R_{rs}(555)$ is tightened to ±30%, the global Case-1 percentage drops to ∼32% for measurements made in Autumn 2003. The Case-1 distribution also depends on the quality of the R_{rs} data from the satellite sensor. Though R_{rs} of open ocean is believed to be accurately retrieved from the SeaWiFS sensor (Gordon & Wang, 1994), it is well known that it is troublesome to accurately remove the atmospheric effects in coastal regions. However, because coastal waters only occupy a small portion of the global ocean surface (e.g., only ∼5% of the water pixels are associated with RR_{12} values less than 0.75), the effects of erroneous coastal R_{rs} on the global Case-1 water distribution are expected to be small.

From the results presented here and from earlier discrete measurements (Bricaud et al., 1981), it is clear that many open ocean waters are not necessarily Case-1, while coastal and highly productive waters can be Case-1. Indeed, even in the clearest open ocean waters, the Sargasso Sea, water constituents have been found to not co-vary (Siegel & Michaels, 1996) or co-vary but with a time lag or phase shift (Hu et al., in press).

There is no doubt that the Case-1 bio-optical models (Morel, 1988; Morel & Maritorena, 2001) provide us an easy and useful tool to quickly estimate water's optical properties simply by concentrations of chlorophyll. It is necessary to keep in mind, however, that there are large deviations around the statistically averaged values even for open ocean waters. As pointed out by Morel and Prieur (1977) in their seminal paper, there is often no clear optical or geographical boundary between Case-1 and Case-2 waters. Hence, the Case-1 percentage as well as its spatial coverage presented in this study should not be treated in an absolute sense. Rather, they serve synoptically as a cautious note to algorithm developers and oceanographers when the term "Case-1" is used. For more reliable applications of remote sensing algorithms, it is better to take approaches or algorithms that do not need a Case-1 clause, as suggested by Mobley et al. (2004). Further, now with the improved ability to derive global distributions of a_{Chl}, a_{CDOM}, and particle backscattering from satellite data (Carder et al., 1999; Doerffer & Schiller, 2006; Hoge & Lyon, 1996; Lee et al., 2002; Loisel & Stramski, 2000; Maritorena et al., 2000), it would be much more useful to define and map water masses based explicitly on these optical properties (Behrenfeld et al., 2005; Gould & Arnone, 2003; Prieur & Sathyendranath, 1981) that directly control the radiance of sea.

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