A model for the assessment of UV penetration into ocean waters from space-based measurements and full radiative transfer calculations

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ABSTRACT

Increased levels of biologically harmful UV radiation have been shown to affect aquatic ecosystems, marine photochemistry, and their impact on carbon cycling. A quantitative assessment of UV effects requires an estimate of the in-water radiation field. An estimate of underwater UV radiation is proposed based on satellite measurements from the TOMS and SeaWiFS and models of radiative transfer (RT). The Hydrolight code, modified to extend it to the 290-400 nm wavelength range, is used for RT calculations in the ocean. Solar direct and diffuse radiances at the ocean surface are calculated using a full RT code for clear-sky conditions, which are then modified for clouds and aerosols. The TOMS total column ozone and reflectivity products are inputs for RT calculations in the atmosphere. An essential component of the in-water RT model is a model of seawater inherent optical properties (IOP). The IOP model is an extension of the Case-1 water model to the UV spectral region. Pure water absorption is interpolated between experimental datasets available in the literature. A new element of the IOP model is parameterization of particulate matter absorption in the UV based on recent *in situ* data. The SeaWiFS chlorophyll product is input for the IOP model. The in-water computational scheme is verified by comparing the calculated diffuse attenuation coefficient, K_d, with one measured for a variety of seawater IOP. The calculated K_d is in a good agreement with the measured K_d. The relative RMS error for all of the cruise stations is about 20%. The error may be partially attributed to variability of solar illumination conditions not accounted for in calculations. The conclusion is that we are now able to model ocean UV irradiances and IOP properties with accuracies approaching those visible region, and in agreement with experimental *in situ* data.

Keywords: UV radiation, radiative transfer models, seawater inherent optical properties

1. INTRODUCTION

Increased levels of biologically harmful UV radiation resulting from the depletion of Earth's ozone layer have been shown to affect aquatic ecosystems. One of the important effects of enhanced levels of UVB radiation is a reduction in the productivity of phytoplankton caused by inhibition of photosynthesis due to damage to the photosynthetic apparatus. Enhanced UVB radiation could also affect the photochemical production of carbonyl sulfide in seawater, thereby augmenting the greenhouse effect and affecting other long-term global biogeochemical cycles. Photochemical degradation of oceanic dissolved organic matter associated with changes in UV radiation flux may affect carbon cycling. A detailed overview of the effects of UV radiation on marine ecosystems has been published recently[1].

The quantitative assessment of UV effects on aquatic organisms requires an estimate of the in-water radiation field. The estimate of underwater irradiance on a global scale has been made using satellite measurements from the TOMS

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and SeaWiFS instruments and approximate models of radiative transfer (RT) in the atmosphere-ocean system[2]. RT calculations in the ocean were carried out with the Quasi-Single Scattering Approximation (QSSA). The QSSA is a computationally rapid model allowing the estimate of UV penetration into ocean waters on the global scale. However, the QSSA model accuracy is not sufficient for all cases. To improve in-water calculation accuracy and still keep the high calculation speeds, we propose use of a lookup table for downward irradiance pre-computed with a full RT model such as Hydrolight[3] with our extensions for UV ocean optical properties into the 290-400 nm wavelength range.

Solar direct and diffuse radiances at the ocean surface are calculated using a Gauss-Seidel vector RT code for clear-sky conditions, which are then modified for clouds and aerosols. The aerosol/cloud correction is based on TOMS measurements of the Lambertian Equivalent Reflectivity (LER) and applied to the downward irradiance calculated for clear-sky conditions. The TOMS total column ozone product is input for RT calculations in the atmosphere. An essential component of the in-water RT model is a model of seawater inherent optical properties (IOP) in the UV spectral region. Unlike models of IOP in the visible, models of IOP in the UV are still evolving. We are proposing an IOP model that is an extension of the Case-1 water model to the UV spectral region. Pure water absorption is interpolated between experimental datasets available in the literature. A new element of the IOP model is parameterization of particulate matter absorption in the UV based on recent *in situ* data. The IOP model is verified by comparing the measured and computed values of the diffuse attenuation coefficient.

2. MODEL OF SEAWATER INHERENT OPTICAL PROPERTIES (IOP)

The UV-IOP model used here is similar to one proposed in a previous paper[2], and is an extension of the Case-1 water model to the UV spectral region (290 – 400 nm). The model was updated by specifying chlorophyll-specific absorption coefficients as a function of chlorophyll concentration.

The total IOP are the sums of the IOP of pure seawater and scattering and absorbing water constituents:

$$a(\lambda) = a_w(\lambda) + a_p(\lambda) + a_{DOM}(\lambda); \quad b(\lambda) = b_w(\lambda) + b_p(\lambda)$$

where subscripts *w, p,* and *DOM* denote the pure seawater, the particulate matter, and colored dissolved organic mater (CDOM), respectively. At present, there are no consensus values for the pure water absorption coefficient in the UV. According to the recent findings[4,5] the pure water absorption coefficient is significantly lower than previous values[6]. A comparison of available datasets on the pure water absorbance in the UV is given in the paper[7]. In this study we use interpolation between data given in the papers[4,8] as recommended in the paper[9]. The pure seawater scattering coefficient is accepted from the paper[6].

The CDOM absorption coefficient and the particulate matter scattering coefficient are parameterized in the conventional form:

$$a_{DOM}(\lambda) = a_0 \exp[-S(\lambda - \lambda_0)]; \quad b_p(\lambda) = b_0(\lambda / \lambda_0)^{-m}$$

We adopt an average value of the DOM spectral slope for the UV spectral region S=0.017 nm^{-1} as recommended in the paper[10] and an average estimate of the parameter m=1 as recommended in the paper[11]. The particulate matter absorption is expressed through chlorophyll concentration, C, and the chlorophyll-specific absorption coefficient: $a_p(\lambda) = Ca^*_p(C,\lambda)$. Parameterization of the chlorophyll-specific absorption coefficient in the UV is similar to the one developed in the visible[12]: $a^*_p(C,\lambda) = A(\lambda)C^{-B(\lambda)}$. The coefficients $A(\lambda)$ and $B(\lambda)$ were determined from CalCOFI data sets[7,13].

The IOP model contains three input quantities: a_0, b_0, and C. To reduce the number of the input parameters, the Case-1 water model[11] is assumed. According to the model, the DOM absorption at 440 nm is 20% of the total absorption of pure seawater and particulate matter pigments[14]. This assumption determines the important parameter a_0. According to the Case-1 water model, the particulate total scattering coefficient is a function of chlorophyll concentration. A value of the particulate total scattering coefficient at 550 nm is approximated as $b_0 = 0.416C^{0.766}$ (see papers[14,15]. Thus, all the input parameters are functions of only one physical input quantity – the chlorophyll concentration that comes from satellite ocean color measurements.

3. COMPUTATIONAL SCHEME

Our method to compute UV irradiance in the ocean is based on using three sets of lookup-tables. Two of these tables were used to compute irradiance on the ocean surfaces: one for cloud-free condition and the other for cloudy conditions. Once the downward irradiance on the ocean surface was determined, the third table was used to compute irradiances at different ocean depths. The calculation of the UV irradiance at the ocean surface for cloud-free conditions was carried out with a Gauss-Seidel vector RT code (MODRAD[16]) for the ocean atmosphere system. For cloudy cases, we used the DISORT code[17] that is much faster than MODRAD, particularly for thick clouds, because it is a scalar code and neglects polarization. The RT simulations in the atmosphere were carried out in the UV region of 290-400 nm and for solar zenith angles ranging 0.5 to 84 degrees. A lookup table of solar direct and diffuse radiances at the ocean surface was generated in these simulations. The paper by *Z. Ahmad et al.* (present Proceedings) provides more details of the codes and the simulations done with the codes.

The aerosol/cloud correction is based on daily TOMS measurements of scene reflectivity at 360 nm. The reflectivity data are on a 1^o by 1^o grid. If the reflectivity value is less than 0.10 for a given grid cell, then we assume the scene to be cloud-free and use the MODRAD generated tables. For grids with scene reflectivity greater than 0.10, we assume the presence of clouds and used both MODRAD and DISORT generated tables. For cloud-free grids, we first compute an effective aerosol optical thickness and then interpolated the look-up table for the appropriate solar zenith angle and ozone amount to get the direct and diffuse irradiances on the ocean surface. Reduction of surface irradiance by clouds is calculated using the well-known approach for satellite estimations of surface irradiance[18]. According to the approach, the cloud transmittance can be approximated with high accuracy by a simple expression, $T \approx 1-R$, where R is the TOMS measured scene Lambert Equivalent Reflectivity (LER) at 360 nm.

The surface irradiance lookup tables are used as input to in-water RT simulations. Our UV-extended model of seawater IOP was implemented in the version 4.06 of Hydrolight[2]. The backscattering coefficient, which is normally much less than the absorption coefficient in the UV, is determined by the choice of the phase scattering function while running Hydrolight. The Petzold phase scattering function was assumed[2]. Hydrolight simulations were conducted for vertically homogeneous waters. Based on these assumptions, a lookup table for in-water irradiances in the UV was generated for chlorophyll concentrations that varied from 0.01 to 5 mg/m^3.

4. VERIFICATION OF THE IOP MODEL

We verified the IOP model by a comparison of the calculated and measured diffuse attenuation coefficients, K_d. In general, K_d depends on the angular structure of the light field and, thus, on depth (even in a homogeneous ocean). However, K_d mainly depends on seawater IOP[19]. The diffuse attenuation coefficient does not depend on absolute values of surface irradiance. Therefore, the comparison of the calculated and measured K_d is suitable for verification of the IOP model. To simplify the comparison we computed the diffuse attenuation coefficient for clear-sky conditions only, even though some measurements were done for partial-cloud conditions. A single low-latitude vertical profile of ozone with the total column amount of 325 DU was assumed in the computations.

In situ data used in the comparisons are from measurements taken in the framework of the ACE-ASIA experiment in the Pacific Ocean. The measurements cover the time period from April 16, 2001 to March 17, 2001, while the spatial coverage of the data is from 25^oN to 39^oN and 177^oW to 178^oE. The underwater measurements were performed using the MER PRR-800 high resolution, underwater profiling reflectance radiometer. The data set includes profile measurements of downward irradiance, E_d, upward irradiance, E_u, and upward radiance, L_u, at 17 wavelengths ranging from 313 nm to 710 nm (the UV wavelengths are 313, 320, 340, 380, and 395 nm). The diffuse attenuation coefficient, K_d, was calculated from the downward irradiance. Measurements of surface chlorophyll concentrations were also available for the same cruise.

Figure 1 shows a comparison of the measured and computed diffuse attenuation coefficients averaged over a layer of 6-16 m. The comparison is done for the cruise station with chlorophyll concentrations less than 0.7 mg/m^3 to ensure the validity of assumptions of the Case-1 water model. Data from station 9 were excluded from the comparison because of excessively large differences between the measured and calculated vertical profiles of K_d. The correlation coefficient is equal to 0.89 for wavelengths 313, 320, and 340 nm. Its value of 0.87 is slightly lower for wavelength 380 nm. The relative RMS error for all of the cruise stations is about 20%. The computations were conducted for clear-sky conditions. The presence of aerosols and/or clouds changes the angular distribution of incident radiation and slightly changes the estimated value of K_d. The scatter of the calculated K_d around the 1:1 line in Figure 3 may be partially attributed to changes in the ratio of direct to diffuse radiation caused by aerosols and cloudiness. It is important to note that there is no obvious bias between the measured and calculated $K_{d,}$ suggesting that the IOP model reasonably reflects the observed absorption and scattering in the ocean.

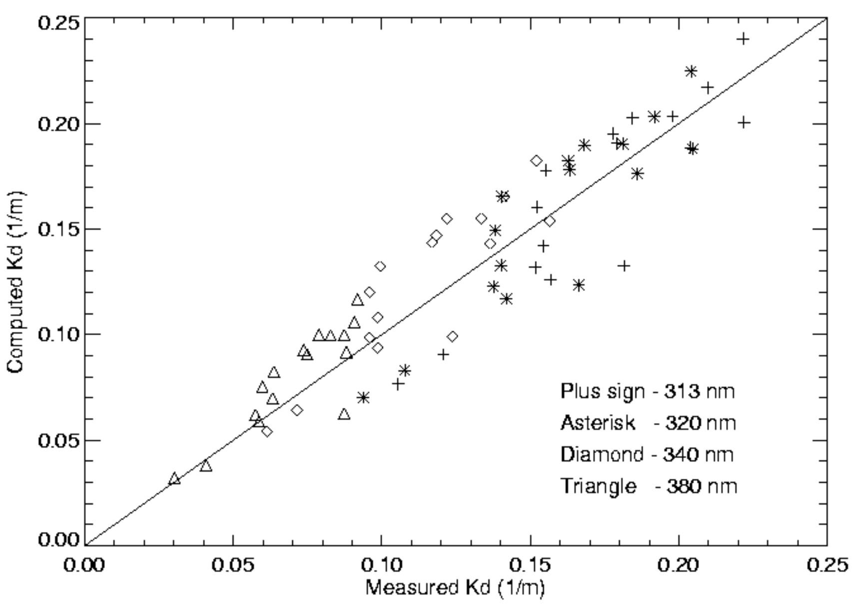

Fig. 1. Comparison of the measured and calculated K_d averaged over a 10 m layer.

It should be noted that excluding absorption by CDOM in the IOP model results in a substantial reduction of K_d, suggesting that the CDOM absorption is an essential factor affecting the UV penetration into the ocean[20]. CDOM absorption in the UV is not negligible even for the clearest waters with chlorophyll concentrations lower than 0.1 mg/m^3. The Case-1 water model of CDOM absorption assumes that there are both background absorption by CDOM that is independent of chlorophyll and absorption entirely correlated with chlorophyll. However, *in-situ* data collected in the CALCOFI cruises show that correlation between CDOM absorption in the UV and chlorophyll concentration may not be high even in Case-1 waters[13]. This fact shows a need for further improvements to the IOP model in the UV.

5. EXAMPLE OF MODEL APPLICATION

The entire computational scheme was applied for mapping in-water irradiances and penetration depths. The penetration depth, *Z*10, is defined as a depth at which total downward irradiance is reduced to 10% of its surface value. If downward irradiance is reduced to less than 10% at the maximum depth of lookup tables of 20 m, the penetration depth is calculated by using the diffuse attenuation coefficient averaged over the upper level of 20 m.

Figure 2 shows a map of the penetration depth computed by using SeaWiFS monthly chlorophyll concentrations and TOMS reflectivity for July 1998 as inputs for the model. The main features of the penetration depth map are determined by spatial distribution of chlorophyll concentration (see SeaWiFS monthly maps at http:://daac.gsfc.nasa.gov). The effects of other environment factors: cloudiness structure and total ozone distribution cannot be distinguished clearly. This fact additionally proves that the diffuse attenuation coefficient can be used for verification of the IOP model.

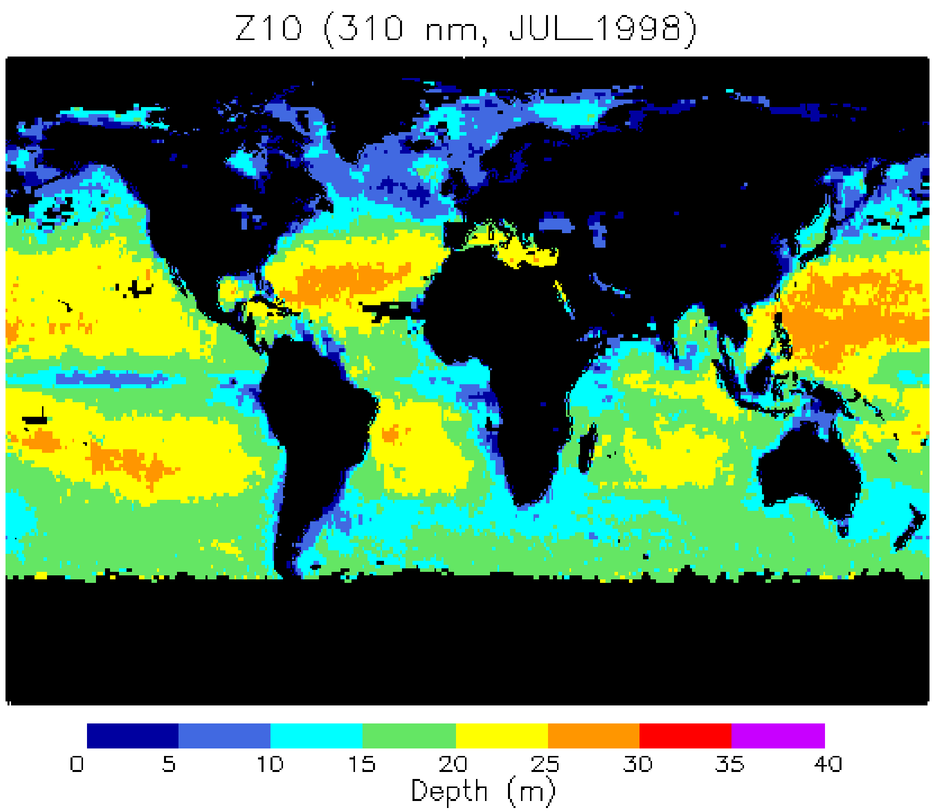

Fig. 2. Map of the penetration depth computed for SeaWiFS monthly chlorophyll for July 1998.

The 10% penetration depths for UVB and DNA dose were mapped in the paper[2]. The penetration depths in this paper were calculated by using the computationally efficient but not exact QSSA model. The QSSA accuracy is estimated by a comparison of K_d calculated by the QSSA model with K_d exactly calculated with the UV-extended Hydrolight. The above-described IOP model was used in both RT models. The calculations were done for a variety of environment and geometrical conditions of *in situ* measurements in the ACE-ASIA experiment. Figure 3 shows the comparison of K_d. According to the data in Figure 3 the QSSA model underestimates K_d by 20% on average.

Underestimation of K_d by the QSSA model could lead to the approximately 20% overestimation of the penetration depths mapped in the paper[2]. However, computation of the penetration depth in that paper was done with using the pure water absorption coefficient adopted from the paper[6]. These values of the pure water absorption coefficient in the UV were significantly larger than the values accepted in the present paper. The resulting overestimation of the penetration depth due to the QSSA model was, to some extent, cancelled out by using the larger values of the pure water absorption coefficient.

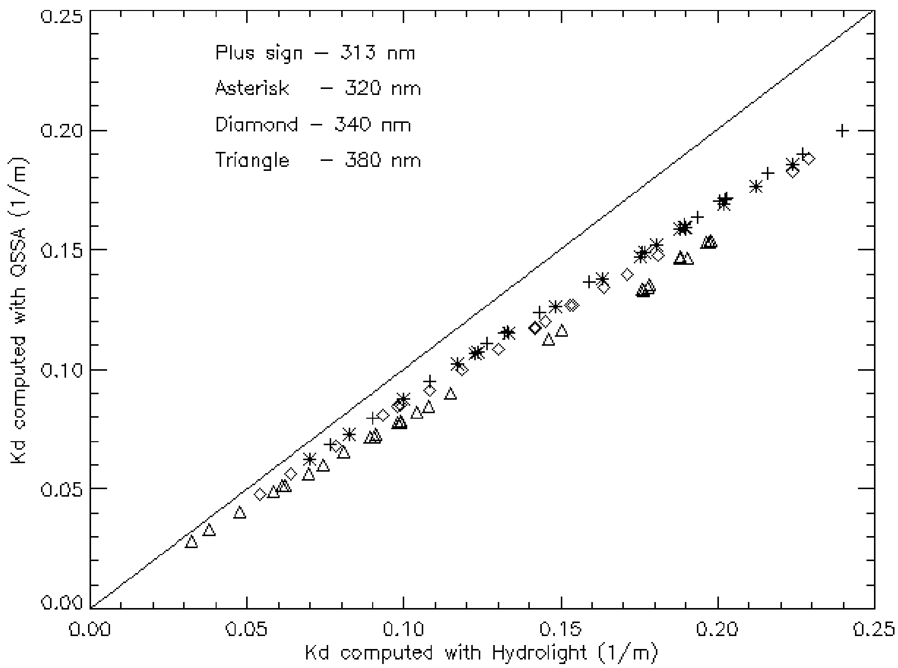

Fig. 3. Comparison of K_d calculated with Hydrolight and QSSA for geometrical and environment conditions of *in situ* measurements.

6. CONCLUSIONS

A model for assessment of UV penetration into the ocean on the global scale has been developed. The estimates of underwater UV radiation are performed on a basis of satellite measurements from the TOMS and SeaWiFS and accurate models of radiative transfer. The computational scheme is based on a lookup table approach. The lookup tables for downward irradiance were generated using the MODRAD/DISORT codes for RT calculations in the atmosphere and the UV-extended Hydrolight code for RT calculations in the ocean for the 290-400 nm wavelength range. Solar direct and diffuse radiances at the ocean surface are calculated using the MODRAD code for clear-sky conditions, which are then modified for clouds and aerosols. The TOMS total column ozone and LER products are inputs for RT calculations in the atmosphere. An essential component of the in-water RT model is a model of seawater inherent optical properties. The IOP model is an extension of the Case-1 water model to the UV spectral region. Pure water absorption is interpolated between experimental datasets available in the literature. A new element of the IOP model is parameterization of particulate matter absorption in the UV based on recent *in situ* data. The comparison between the measured and computed K_d proves the IOP model is reasonably adequate in the UV. K_d calculated with the UV-extended Hydrolight is in a rather good agreement with the measured K_d. The relative RMS error for all of the cruise stations is about 20%. The error may be partially attributed to changes in the angular distribution of surface radiation caused by aerosols and cloudiness. Excluding absorption by colored dissolved organic matter in the IOP model results in a substantial reduction of K_d thus suggesting that the CDOM absorption is an essential factor affecting the UV penetration into the ocean. It is shown that the QSSA model underestimates K_d by 20% on average. An important result is that we are now able to model ocean UV irradiances and IOP properties with accuracies approaching those visible region, and in agreement with experimental *in situ* data.

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