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Extending satellite ocean color remote sensing to the near-blue ultraviolet bands

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26 **Abstract:**

27 Ultraviolet (UV) radiation has a profound impact on marine life, but historically and
28 even currently, most ocean color satellites cannot provide radiance measurements in the UV,
29 and thus UV penetration, in the global ocean. We develop a system (termed as UVISR_{dl}) in
30 this study, based on deep learning, to estimate remote sensing reflectance (R_{rs}) at 360, 380,
31 and 400 nm (collectively termed as near-blue UV bands, nbUV) from R_{rs} in the visible bands
32 that are obtained by ocean color satellites. This system is tested using both synthetic and
33 field-measured data that cover a wide range and large number of values, with the resulted
34 coefficient of determination close to 1.0 and bias close to 0 between UVISR_{dl} estimated and
35 known $R_{rs}(\text{nbUV})$. These results indicate excellent predictability of $R_{rs}(\text{nbUV})$ from
36 $R_{rs}(\text{visible})$ via UVISR_{dl}. The system was further applied to VIIRS (the Visible Infrared
37 Imaging Radiometer Suite) data with the estimated $R_{rs}(\text{nbUV})$ evaluated using matchup field
38 measurements, and obtained a mean absolute relative difference (MARD) at 360 nm of ~14%
39 for oceanic waters and ~50% for coastal waters. These results are equivalent to those reported
40 in the literature for satellite $R_{rs}(\text{visible})$ in oceanic and coastal waters. Examples of the global
41 distribution of $R_{rs}(\text{nbUV})$, and subsequently the diffuse attenuation coefficient at the nbUV
42 bands ($K_d(\text{nbUV})$), are generated after applying UVISR_{dl} to $R_{rs}(\text{visible})$ from the VIIRS data.
43 The system lays the groundwork to generate decade-long $R_{rs}(\text{nbUV})$ and $K_d(\text{nbUV})$ from
44 satellite ocean color data, which will be useful and important for both ocean color remote
45 sensing and biogeochemical studies.

46

47

48 1. Introduction

49 Ultraviolet (UV) radiation is part of solar energy, which plays complex roles in
50 biogeochemical processes on land and in ocean (Cullen and Neale 1994; Smith et al. 1992;
51 Zepp et al. 2007). For instance, high doses of UV can inhibit the growth of plants and
52 phytoplankton, while low doses under some conditions can be a useful energy source for
53 phytoplankton photosynthesis (Gao et al. 2012). In addition, phytoplankton may develop
54 mycosporine-like amino acids (MAAs) in response to UV radiation; these MAAs are strongly
55 UV absorbing, functioning as a “shield” to protect photosynthesis pigments (Moisan and
56 Mitchell 2001; Morrison and Nelson 2004). Further, dissolved organic matter (DOM) has a
57 high absorption capacity for UV radiation and undergoes photochemical conversion under
58 sunlight, indicating that DOM is very sensitive to sunlight in the UV domain (Piccini et al.
59 2009; Zepp et al. 2007). UV radiation may also impact the diel vertical movement of
60 zooplankton (Rose et al. 2012). In the atmosphere, since the most absorbing aerosol species
61 contribute absorption in the shorter (UV-visible) wavelengths (Kahn et al. 2016), research on
62 UV radiation will also help improve atmospheric correction (Frouin et al. 2019). As indicated
63 in Werdell et al. (2018), the future use of hyperspectral spectrometer from UV (~350 nm) to
64 near-infrared (~900 nm) will improve the accuracy in ocean color remote sensing. All these
65 suggest the necessity to map UV penetration in the global ocean.

66 The distribution of underwater UV radiation depends on two factors: UV intensity at the
67 sea surface and the diffuse attenuation coefficients for downwelling irradiance (K_d ; m^{-1}) at
68 these UV wavelengths. The first factor is governed by ozone and atmospheric properties,
69 which can now be well estimated using satellite measurements (Herman and Celarier 1997;
70 Kuchinke et al. 2004; Smyth 2011b; Vasilkov et al. 2001). K_d is an apparent optical property
71 of the ocean; although there are many field measurements (Conde et al. 2000; Dupouy et al.
72 2018; Overmans and Agustí 2019; Tedetti and Sempéré 2006) and more than four decades of
73 $K_d(\text{visible})$ from ocean color satellites, there is no standard global $K_d(\text{UV})$ product distributed
74 by the remote sensing agencies. This is in part because the shortest wavelength of the past
75 and most of the present-day ocean color satellites is ~410 nm. Thus, there are no global
76 measurements of oceanic optical properties in the UV domain by satellites. Two decades ago,

77 Vasilkov et al. (2001) presented a preliminary oceanic distribution of UV radiation in the
78 280-320 nm range based on TOMS (the Total Ozone Mapping Spectrometer) and SeaWiFS
79 (the Sea-viewing Wide Field-of-view Sensor) products, but the empirical coefficients for the
80 $K_d(\text{UV})$ model were not derived from globally inclusive measurements. Thus its applicability
81 to the global ocean is unknown. In short, the penetration of UV radiation in the global ocean
82 is still far from known, nor the impact of UV radiation on marine life on a basin scale. Only
83 some recent ocean color satellite sensors and the planned PACE (Plankton, Aerosol, Cloud
84 and ocean Ecosystem, US) include bands in the UV domain. For instance, the OLCI (Ocean
85 and Land Colour Instrument, Europe) on Sentinel 3 has a band at 400 nm, SGLI (Second
86 Generation Global Imager, Japan) has one at 380 nm, HY1C (HaiYang-1C, China) has one at
87 355 nm, and PACE will have hyperspectral measurements starting from 350 nm.

88 The model to estimate $K_d(\text{UV})$ used in Vasilkov et al. (2001) is based on the “Case 1”
89 concept (Morel 1988). The authors evaluated K_d at 313, 320, 340, and 380 nm with 15
90 measurements from the CalCOFI cruises and obtained an uncertainty of ~20%. Similarly, to
91 fill the information gap of K_d in the UV domain, based on ~50-100 measurements made in the
92 Mediterranean Sea and Atlantic Ocean, Smyth et al. (2011b) proposed empirical relationships
93 to estimate K_d at 305, 325, 340, and 380 nm using the total absorption coefficient at 443 nm
94 ($a(443)$, m^{-1}). Because K_d is dominated by the absorption coefficient (Gordon 1989a), these
95 approaches require the absorption coefficient of colored dissolved organic matter (CDOM) to
96 co-vary with the concentration of chlorophyll (Chl), but such a correlation is not always
97 strong even for oceanic waters (Kahru and Mitchell 1998; Lee and Hu 2006). As pointed out
98 by Smyth et al. (2011b), the correlation is actually weak between $a(443)$ and $K_d(305)$. This
99 may not be a surprise, as very different relationships have been found between $K_d(310)$ and
100 $K_d(465)$ for different waters (Højerslev and Aas 1991), and significantly different $K_d(\text{UV})$
101 exists between waters of the Mediterranean Sea and South Pacific for the same Chl (Morel et
102 al. 2007). Thus, the applicability of such empirical schemes in the global ocean is limited,
103 although global Chl, $a(443)$, and $K_d(490)$ are adequately available from satellite ocean color
104 measurements.

105 In a separate empirical approach, Fichot et al. (2008) developed algorithms to estimate
106 K_d of 320, 340, and 380 nm based on the SeaWiFS bands after principal component analysis,

107 with the 335 data points used for the algorithm development covering waters from the Gulf of
108 Mexico to many other coastal regions around North America. This algorithm was later
109 refined to improve the estimates of inshore waters (Cao et al. 2014). While promising results
110 were reported (Cao et al. 2014; Fichot et al. 2008), basin-scale UV penetration, which is of
111 the most significance, remains unknown.

112 Another approach to obtain $K_d(\text{UV})$ is to extrapolate the inherent optical properties
113 (IOPs) obtained in the visible bands to UV and then estimate $K_d(\text{UV})$ through models
114 developed based on the radiative transfer equation (Lee et al. 2005). This approach requires *a*
115 *priori* information of the relationships of component IOPs in the UV to the visible domain,
116 which could be weak. For instance, the existence of MAAs may contribute significantly to
117 the phytoplankton absorption coefficient (a_{ph}) in the short UV wavelengths, while MAAs
118 may have very low or no absorption in the visible domain (Moisan and Mitchell 2001; Shick
119 and Dunlap 2002); thus, there is no clear indication of MAAs' existence from a_{ph} in the
120 visible. Also, the approach will require a robust estimate of the spectral shape parameter (S_g ;
121 nm^{-1}) of CDOM absorption coefficient (a_g) (Swan et al. 2013; Twardowski et al. 2004), as a_g
122 could be significantly higher in the UV domain (Mannino et al. 2008; Morel and Gentili 2009)
123 and S_g may also vary with spectral range (Twardowski et al. 2004). All estimates of these
124 components will bring various levels of uncertainty to $K_d(\text{UV})$.

125 Given the issues mentioned above, we present a scheme centered on deep learning to
126 estimate remote sensing reflectance (R_{rs} ; sr^{-1}) in the near-blue UV domain (nbUV hereafter)
127 from R_{rs} in the visible (~410-700 nm), with nbUV specifically for 360, 380, and 400 nm. The
128 reason for the shortest wavelength as 360 nm is in part because UV radiation for wavelengths
129 shorter than ~350 nm is extremely low (Vantrepotte and Mélin 2006); in part because there is
130 no clear relationship between $a_{ph}(\lambda < 350 \text{ nm})$ and $a_{ph}(\text{visible})$ (Dupouy et al. 1997; Morrison
131 and Nelson 2004; Sathyendranath et al. 1987), where the contribution from MAAs could play
132 a significant role for the short UV wavelengths (Moisan and Mitchell 2001; Shick and
133 Dunlap 2002); and because more advanced ocean color satellites start measurements around
134 350 nm. However, these factors do not forbid the development of systems from estimating R_{rs}
135 for wavelengths shorter than 360 nm after a better understanding of the relationships between
136 IOPs of wavelengths shorter than 360 nm and those in the visible bands.

137 It is certainly possible to develop a deep-learning-based system to estimate $K_d(\text{nbUV})$
138 from $K_d(\text{visible})$, as $K_d(\text{visible})$ can be adequately calculated from $R_{rs}(\text{visible})$ (Lee et al. 2013;
139 Lee et al. 2005). We decided not to take this approach here because R_{rs} is the core input to
140 estimate water properties and because $R_{rs}(\text{nbUV})$ can also be applied in some atmospheric
141 correction algorithms (He et al. 2012; Wang 2007). In addition, $R_{rs}(\text{nbUV})$ can be used to
142 improve the inversion of a_{ph} and a_g in ocean color remote sensing (Wei and Lee 2015; Wei et
143 al. 2016). Furthermore, as an additional option for cross-validation, $R_{rs}(\text{nbUV})$ in oceanic
144 waters obtained from MODIS (the Moderate Resolution Imaging Spectroradiometer) and/or
145 VIIRS (the Visible Infrared Imaging Radiometer Suite) can be used to compared with those
146 from OLCI, SGLI, and/or HY1C.

147 The paper is organized as follows. In Section 2, we describe the overall deep-learning
148 architecture for estimating $R_{rs}(\text{nbUV})$, and the data used to train and evaluate the system. In
149 Section 3, results and evaluations are presented. In Section 4, we show applications of this
150 system in the global ocean. In Section 5, we summarize our main findings and present future
151 perspectives.

152

153 **2. Data and methods**

154 **2.1 A deep-learning system for $R_{rs}(\text{nbUV})$: UVISR_{dl}**

155 For easy data processing, especially because of nonlinear relationships of R_{rs} between
156 different wavelengths, we take an approach centered on deep learning for estimating
157 $R_{rs}(\text{nbUV})$ from $R_{rs}(\text{visible})$. Figure 1 presents a schematic concept of this system, termed
158 UVISR_{dl}.

159 Like all deep-learning systems, UVISR_{dl} is composed of one input layer, various hidden
160 layers associated with many numbers of neurons, and one output layer. A key component of
161 any deep-learning system is the neural network model, and such models have been developed
162 in the past decade (Abadi et al. 2016; Géron 2019; Ketkar 2017; Steiner et al. 2019; Swami
163 and Jain 2011). Here, based on data characteristics, we selected the Keras model (Chollet) for
164 UVISR_{dl}. Keras is a deep-learning Application Programming Interface written in Python; it is

165 publicly available and running on top of the machine-learning platform TensorFlow (Chollet ;
166 Ketkar 2017). The number of hidden layers and the number of neurons of each layer were
167 determined following the concept of minimum loss (Géron 2019), a common approach for
168 developing a deep-learning system. Eventually, a system of four hidden layers, with 300
169 neurons for Layer-1, 75 for Layer-2, 38 for Layer-3, and 18 for Layer-4, is found to provide
170 the best performance for UVISR_{dl}.

171 For the training of UVISR_{dl}, we employed the Rectified Linear Unit (ReLU) function for
172 the activation function of each layer (Krizhevsky et al. 2012), which can largely avoid
173 gradient explosion and gradient disappearance (He et al. 2015). The optimization function of
174 the training used is the Adam algorithm (Kingma and Ba 2014). The setting of the learning
175 rate usually involves an adjustment process, in which the highest possible learning rate is
176 manually selected (Zeiler 2012). As a result, a learning rate of 2×10^{-5} is used in this study.
177 Training of UVISR_{dl} was eventually achieved when the loss function converges and the
178 iteration stops.

179 To avoid any interference between the nbUV wavelengths, a separate UVISR_{dl} was
180 trained specifically for each of the three nbUV bands in this effort. Further, given different
181 spectral band settings of satellite ocean color sensors, separate UVISR_{dl} was developed for
182 each specific satellite of interest.

183

184 **2.2 Data**

185 For all neural networks or deep-learning schemes, a large and inclusive dataset is crucial
186 for its training. Here, we use numerically synthesized data to develop UVISR_{dl}, which is
187 further evaluated using both synthesized and field-measured data.

188 **2.2.1 Training data**

189 Following IOCCG Report #5 (IOCCG-OCAG 2003; IOCCG 2006), we synthesized a
190 large (200,000 sets) dataset containing a wide range of IOPs in the 350-800 nm range (5-nm
191 resolution), which were then fed into a model for R_{rs} (Lee et al. 2004) to generate 200,000 R_{rs}
192 spectra. As most of the specifics for this synthesizing method are available in the literature

193 (IOCCG-OCAG 2003; IOCCG 2006), we provide only some of the components and
194 synthesizing steps in Appendix A for reference. A few key features are summarized below:

195 (1) For the IOPs spectra, while the contributions of pure seawater (Lee et al. 2015a;
196 Mason et al. 2016; Zhang and Hu 2009a) are considered constants, the absorption and
197 backscattering contributions from phytoplankton pigments, CDOM, and detrital-sediments
198 are considered variables. These component IOPs, except for the spectrum of a_{ph} , can be
199 expressed as a simple function (exponential or power-law) of wavelength (Bricaud et al. 1981;
200 Gordon and Morel 1983). Therefore, to best maintain the natural variation of bulk IOPs, a_{ph}
201 spectra were not modeled mathematically; instead, they were selected from >4,000 a_{ph}
202 spectra stored in the SeaBASS (the Sea-viewing Wide Field-of-view Sensor Bio-Optical
203 Archive and Storage System) and our own collections. To ensure coverage from oligotrophic
204 oceanic waters to coastal/inland eutrophic waters, we set $a_{ph}(440)$ to a range of 0.001-20.0
205 m^{-1} . Therefore, a wide range of $a_{ph}(\lambda)$, in both magnitude and spectral shapes, were utilized in
206 data synthesizing.

207 (2) As described in Appendix A and IOCCG Report #5 (IOCCG-OCAG 2003; IOCCG
208 2006), for each $a_{ph}(440)$ value, constrained random parameters were used to model the
209 contributions of other component IOPs. In this way, it better mimics the variabilities of these
210 components in natural environments while reducing likely unrealistic combinations, such as
211 very low $a_{ph}(440)$ with an extremely high absorption by CDOM.

212 Figure 2a shows examples of the synthesized R_{rs} spectra. The dataset of 200,000
213 IOPs- R_{rs} is divided randomly by an 8:2 ratio, with 160,000 for the training of UVISR_{dl} and
214 40,000 for the evaluation of UVISR_{dl}. Table 1 provides an overall picture of the data range
215 used for the evaluation. Visible bands used are 410, 440, 490, 550, and 670 nm for VIIRS,
216 410, 440, 490, 510, 555, and 670 nm for SeaWiFS, and 410, 440, 490, 530, 550, and 670 nm
217 for MODIS. The spectral bands of these satellite sensors have a bandwidth of 10-20 nm, and
218 the band centers are not exactly those specified here. Thus, to apply the trained UVISR_{dl} for
219 R_{rs} products from satellites, R_{rs} of the satellite bands were calculated for the 200,000 sets of
220 hyperspectral R_{rs} after applying each satellite sensor's band-specific response functions.
221 Subsequently, for example, nonlinear empirical conversions were developed to transfer
222 VIIRS R_{rs} of band 411 nm to $R_{rs}(410)$, which was also done for the other bands. Therefore,

223 for each satellite, the same UVISR_{dl} can be applied to both field and satellite R_{rs} .

224 2.2.2 Validation data

225 In addition to the above-mentioned synthesized data for the validation of UVISR_{dl}, a
226 wide range of field-measured R_{rs} are also used to test the performance of UVISR_{dl}. Figure 2b
227 shows examples of measured R_{rs} spectra (from a total of 202), which cover waters from
228 oceanic to turbid coastal regions. Details of the method for these measurements can be found
229 in Wei et al. (2015), where the skylight-blocked approach (SBA) (Lee et al. 2013; Tanaka et
230 al. 2006) was followed to obtain field R_{rs} . The uncertainty of SBA-measured R_{rs} is generally
231 <5% in oceanic waters, and ~10% in turbid, highly productive waters at the blue bands (Lin
232 et al. 2020). While the SBA measurements mostly cover coastal waters, the hyperspectral
233 (344-749 nm, ~0.5-nm resolution) R_{rs} data measured at the Marine Optical Buoy (MOBY)
234 (Clark et al. 1997), a typical oligotrophic site, were also accessed (from the NOAA
235 CoastalWatch, https://www.star.nesdis.noaa.gov/socd/moby/filtered_spec/) to evaluate
236 UVISR_{dl}. The quality of the MOBY data is classified into four classes: bad and cloudy,
237 suspicious, bad, and good. In this study, we used 6,184 R_{rs} spectra with the highest quality.

238

239 2.3 Accuracy Assessment

240 In addition to the coefficient of determination (R^2) in linear regression analysis, the
241 accuracy of the resulted $R_{rs}(\text{nbUV})$ is assessed with the following statistical measures:
242 root-mean-square difference (RMSD), mean absolute relative difference (MARD), and bias.
243 They are defined as follows:

$$\text{RMSD} = \sqrt{\frac{\sum_{i=1}^N (X_{\text{est},i} - X_{\text{mea},i})^2}{N}}, \quad (1)$$

$$\text{MARD} = \frac{1}{N} \sum_{i=1}^N \frac{|X_{\text{est},i} - X_{\text{mea},i}|}{X_{\text{mea},i}}, \quad (2)$$

$$\text{bias} = \frac{1}{N} \sum_{i=1}^N (X_{\text{est},i} - X_{\text{mea},i}), \quad (3)$$

244 where $X_{\text{est},i}$ and $X_{\text{mea},i}$ are predicted and known (synthesis, or *in situ*) values of $R_{rs}(\text{nbUV})$,
245 respectively, and N is the number of sample pairs.

247 **3. Results of $R_{rs}(\text{nbUV})$ from UVISR_{dl}**

248 **3.1 Synthetic data**

249 $R_{rs}(\text{nbUV})$ from UVISR_{dl} is first evaluated using the 40,000 synthetic data, with results
 250 for VIIRS spectral settings showing in Figure 3 (a-c) as examples. Similar results were
 251 obtained for SeaWiFS and MODIS, with statistical measures given in Table 2. Generally, for
 252 these synthesized data, the values of R^2 for the three wavelengths and three satellites are all
 253 close to 1.0, with values of RMSD and bias close to 0 and values of MARD under ~0.3%.
 254 These results indicate extremely high accuracy in predicting $R_{rs}(\text{nbUV})$ from R_{rs} data in five
 255 or six visible bands. This is due to the fact that R_{rs} is determined by the total absorption and
 256 backscattering coefficients. Because the spectral variations of CDOM absorption and particle
 257 backscattering are highly spectrally related, and because the spectral shapes of phytoplankton
 258 absorption show general patterns at least in the 350-700 nm domain, thus $R_{rs}(\text{visible})$ has
 259 some spectral “messages” or connections with R_{rs} at 360, 380, and 400 nm, although such
 260 spectral connections are likely more complex than that can be explained by simple nonlinear
 261 functions. This spectral interconnection was demonstrated in Lee et al. (2014) and Sun et al.
 262 (2015), where R_{rs} spectrum in the 400-800 nm with a resolution of 5 nm could be well
 263 constructed from R_{rs} measured at 15 bands in this spectral domain. Also, decades ago Austin
 264 and Petzold (1990) showed $K_d(\text{visible})$ could be estimated to some degree from using $K_d(490)$
 265 alone.

266 We would like to emphasize that the relationships between $R_{rs}(\text{nbUV})$ and $R_{rs}(\text{visible})$ of
 267 the synthesized dataset are complex and nonlinear, as presented in Figure 4. As a validation
 268 of the synthesized data, Figure 4 also includes R_{rs} from field measurements (both SBA and
 269 MOBY), which shows that field data are well within the envelope of the synthesized R_{rs} . This
 270 comparison suggests that the synthesized dataset is inclusive, although some combinations of
 271 IOPs potentially may not exist or are extremely rare in natural aquatic environments. The two
 272 clusters between $R_{rs}(\text{nbUV})$ and $R_{rs}(440)$ represent the impact of the two driving component
 273 IOPs on R_{rs} spectral shapes in the nbUV: a_{ph} and a_g . Specifically, for the ~350-440 nm range,

274 a_g increases exponentially with the decrease of wavelength, but a_{ph} generally decreases with
275 the decrease of wavelength. Thus, for waters having higher contributions from a_g than from
276 a_{ph} , $a(360)$ will be significantly higher for the same $a(440)$. Consequently, $R_{rs}(360)$ will be
277 lower for the same $R_{rs}(440)$. This contrast represents a common situation in coastal waters
278 (depth < 1,000 m), which will be shown later.

279 Because $R_{rs}(360)$ does not co-vary with $R_{rs}(440)$, these patterns show that uncertainty
280 will be large if $R_{rs}(440)$ alone is used to predict $R_{rs}(nbUV)$; and this uncertainty would
281 increase if the gap between the target and reference wavelengths becomes wider. However, as
282 shown earlier, the R^2 values are close to 1.0 when $R_{rs}(\text{visible})$ was fed into a deep-learning
283 system to obtain $R_{rs}(nbUV)$, indicating that nonlinear connections exist between $R_{rs}(nbUV)$
284 and $R_{rs}(\text{visible})$ and that deep learning has the capability to capture such relationships,
285 although not in an explicit way.

286 It is also interesting that although VIIRS has no band around 510-530 nm compared to
287 SeaWiFS and MODIS, the statistical measures for the predicted $R_{rs}(nbUV)$ from VIIRS
288 $R_{rs}(\text{visible})$ are similar to that of the two earlier sensors. This result suggests that the band
289 around 510-530 nm is not critical for estimating $R_{rs}(nbUV)$ from $R_{rs}(\text{visible})$, at least for the
290 data tested here.

291

292 **3.2 Field-measured data**

293 We further evaluated $UVISR_{dl}$ using field-measured data, with Figure 5 (a-c) showing
294 the results for SBA measurements and Figure 6 (a-c) for MOBY measurements, with the
295 VIIRS spectral bands as examples. Performances of the two datasets for MODIS and
296 SeaWiFS bands are included in Table 2. Similar to the performance of the synthetic dataset,
297 for SBA measurements, the R^2 values for the three $R_{rs}(nbUV)$ and three satellites are ~ 0.99 ,
298 with RMSD and bias close to 0. The MARD values are $\sim 2\%$, $\sim 4\%$, and $\sim 10\%$ for 400, 380,
299 and 360 nm, respectively, much higher than those of the synthesized data. The higher MARD
300 values are not surprising for the following reasons: 1) the measured R_{rs} is never error-free; 2)
301 the uncertainty in field measured R_{rs} is always around a few percent even under the best
302 arrangement with SBA (Lin et al. 2020) and can be around 10% in the blue for highly

303 absorbing waters (Lin et al. 2020); and 3) likely insufficient representation of natural R_{rs} in
304 the synthesized data for the training of UVISR_{dl}, which could be refined in the future after
305 obtaining more high-quality measurements of R_{rs} (UV-visible) in broad aquatic environments.
306 The less than 10% MARD and close to 0 bias indicate highly reliable R_{rs} (nbUV) predicted by
307 UVISR_{dl} from R_{rs} (visible).

308 Excellent results are also found with MOBY-measured R_{rs} (see Figures 6a-6c), where
309 the RMSD and bias are close to 0, and the MARD values are less than ~9% for the estimated
310 R_{rs} (nbUV) by UVISR_{dl}. The R^2 value (0.88) for R_{rs} (360) is slightly lower than that of the
311 SBA dataset, which is in part due to the much narrower range (~0.005-0.020 sr⁻¹) of R_{rs} (360)
312 from a single site. On the other hand, it also indicates potentially larger uncertainties for
313 wavelengths deeper in the UV domain, especially, as shown below, if MAAs are present.
314 Note that a result of ~9% MARD for R_{rs} (360) is close to the highest accuracy that can be
315 achieved in field measurements (Lin et al. 2020; Zibordi and Talone 2020).

316

317 **3.3 Potential impact of absorption by MAAs**

318 As we stated earlier, we set the shortest wavelength for R_{rs} (nbUV) at 360 nm, in part
319 because that the absorption coefficient of MAAs in the 300-350 nm range can be significantly
320 higher (for instance, up to a factor of ~4) than that at 440 nm (see Figure 1B in Moisan and
321 Mitchell 2001). In particular, because MAAs have no or low contributions to a_{ph} in the visible,
322 there is no clear relationship between a_{ph} (visible) and a_{ph} (300-350). On the other hand,
323 MAAs may exist in many phytoplankton groups, particularly in dinoflagellates *L. polyedra*
324 and *Phaeocystis Antarctica* (Moisan and Mitchell 2001; Vernet and Whitehead 1996). Thus,
325 the spectral information of a_{ph} in the visible is insufficient to accurately predict a_{ph} in the
326 300-350 nm domain due to the potentially existence of MAAs. Consequently, errors in the
327 estimated a_{ph} (300-350) will be propagated to the estimated total absorption and then
328 R_{rs} (300-350). The empirical algorithms to estimate K_d in the wavelengths of ~320 nm using
329 R_{rs} in the visible bands developed earlier (Fichot et al. 2008; Smyth 2011a; Vasilkov et al.
330 2001) likely did not encounter waters having strong MAAs, or the data used were dominated
331 by strong absorption due to CDOM. Because K_d is primarily determined by the absorption

332 coefficient, such empirical algorithms for the estimate of $K_d(300-350)$ could result in larger
333 uncertainties than those for wavelengths in the nbUV when MAAs are present.

334 For the a_{ph} spectra used in our data synthesizing, very few spectra show contributions of
335 MAAs at 360 nm, where the $a_{ph}(360)/a_{ph}(440)$ ratio is 0.66 ± 0.35 , although it is in a range of
336 0.15-3.82. On the other hand, the ratio of $a_g(360)/a_g(440)$ is ~ 3.3 for an a_g slope of 0.015
337 nm^{-1} . That means for a situation $a_{ph}(440) = a_g(440)$, MAAs contribute to the most $\sim 50\%$ to
338 $a(360)$ when $a_{ph}(360)/a_{ph}(440)$ is also around 3.0. For most situations where $a_{ph}(360)/a_{ph}(440)$
339 is less than 1.0, the value of $a(360)$ is dominated by that from $a_g(360)$; thus, it is feasible to
340 reasonably predict $a(360)$ from $a(\text{visible})$, and then $R_{rs}(360)$ from $R_{rs}(\text{visible})$. As would be
341 expected, there could be larger uncertainties in the estimated $R_{rs}(360)$ if there are strong
342 contributions from MAAs while the contribution of a_g is secondary.

343 **4. Application to ocean color satellites**

344 **4.1 Global $R_{rs}(\text{nbUV})$ from VIIRS**

345 With the developed and validated UVISR_{dl}, it is possible to generate global $R_{rs}(\text{nbUV})$
346 from past and current ocean color satellite measurements. For example, Figure 7 shows
347 global distributions of $R_{rs}(\text{nbUV})$ predicted from VIIRS. Note that both NOAA CoastWatch
348 (<https://coastwatch.noaa.gov/cw/index.html>) and NASA OBPG
349 (<https://oceancolor.gsfc.nasa.gov/>) can provide consistent VIIRS ocean color products, but
350 for easier spatial matchup with the products from SeaWiFS and MODIS, seasonal composites
351 of $R_{rs}(\text{visible})$ from NASA OBPG were acquired and utilized here.

352 Not surprisingly, $R_{rs}(\text{nbUV})$ is very high in the open ocean, especially in the ocean gyres,
353 a result of significantly low CDOM and phytoplankton in the oligotrophic ocean (Hu et al.
354 2012; Siegel et al. 2005). The predicted $R_{rs}(\text{nbUV})$ in the South Pacific Gyre (the star in
355 Figure 7b) is $\sim 0.022 \text{ sr}^{-1}$, which is consistent with that reported in Tedetti et al. (2010),
356 although the years of measurements are different.

357 Expectedly, $R_{rs}(\text{nbUV})$ is significantly lower in coastal waters, but even for $R_{rs}(360)$, it
358 is higher than zero in many coastal regions (see Figure 8 for example). Such distributions
359 suggest caution in assuming $R_{rs}(\text{nbUV})$ as zero in the process of atmospheric correction (He

360 et al. 2012), where other approaches (Wang and Jiang 2018; Wei et al. 2020) could be used
361 for the estimation of R_{rs} in the blue bands.

362

363 **4.2 Evaluation of VIIRS $R_{rs}(\text{nbUV})$ with *in situ* measurements**

364 We further compared $R_{rs}(\text{nbUV})$ from VIIRS with matchup *in situ* measurements (82
365 matchups for SBA, and 730 for MOBY) to assess the quality of $R_{rs}(\text{nbUV})$ estimated from
366 satellite data. The SBA measurements were obtained mainly in coastal regions (see Figure 9
367 for locations of measurements) in the period of 2012-2019, with matchup limited to within ± 5
368 hours and 3x3 VIIRS pixels between satellite and *in situ* measurements (Werdell and Bailey
369 2005). Figures 10 and 11(a-f) present scatterplots between predicted and measured $R_{rs}(\text{nbUV})$
370 for visual comparison, with statistical measures presented in Table 3. In view that neither *in*
371 *situ* nor satellite $R_{rs}(\text{nbUV})$ can be considered as “truth,” the mean absolute unbiased relative
372 difference (MAURD) is calculated to check consistency between the two determinations.

$$373 \quad \text{MAURD} = \frac{1}{N} \sum_1^N \left| \frac{\text{Data}_1 - \text{Data}_2}{\text{Data}_1 + \text{Data}_2} \right| \times 2 \quad (4)$$

374 where Data_1 and Data_2 represent data from two independent determinations, respectively.

375 Overall, for these $R_{rs}(\text{nbUV})$ the MAURD values are between 0.31 (at 400 nm) and 0.40
376 (at 360 nm) for the SBA matchups, with biases of ~ 0.0002 - 0.0005 sr^{-1} . For the MOBY
377 matchups, the MAURD values are around 0.12, with biases of ~ 0.00023 - 0.0012 sr^{-1} .
378 Unsurprisingly, these measures are worse than those when evaluating $R_{rs}(\text{nbUV})$ using
379 field-measured data, as there are other uncertainties and/or errors contributing to these
380 differences, which include not-exact spatial-temporal matchup and uncertainties in
381 atmospheric correction, especially in coastal waters (IOCCG 2010; Wang 2007). For these
382 likely error sources related to satellite data, Figures 10 and 11 (d-f) include comparisons of
383 the blue bands (410, 440, and 490 nm), where the MAURD values are ~ 0.21 - 0.29 and RMSD
384 is $\sim 0.0012 \text{ sr}^{-1}$ for the SBA matchups, which are just slightly better than those of $R_{rs}(\text{nbUV})$.
385 Note that there are a few stations where VIIRS $R_{rs}(410, 440, 490)$ are much lower than the *in*
386 *situ* R_{rs} measured by the SBA. As $R_{rs}(\text{nbUV})$ is estimated based on the values in the visible
387 bands, such lower values from VIIRS will lead to lower values of $R_{rs}(\text{nbUV})$, which then
388 contributes to higher MAURD at the nbUV bands, especially in the coastal waters. For the

389 MOBY matchups, a fixed location of oceanic waters, the MAURD values at the blue bands
390 (410-490 nm) are just slightly better than those at the nbUV bands (360-400 nm), with the
391 RMSD values around 0.0022 sr^{-1} for the wavelengths of 360-410 nm. The low R^2 value for
392 these matchups results from the narrow dynamic range of the R_{rs} values, where the water
393 properties of such a system do not vary significantly. Overall, because of the difficulties and
394 uncertainties in spatial-temporal matching as well as atmospheric correction and these
395 performance measures being similar to those reported in the literature when evaluating R_{rs}
396 from ocean color satellites (Antoine et al. 2008; Mélin et al. 2016; Zibordi et al. 2009), these
397 results indicate satisfactory $R_{rs}(\text{nbUV})$ from VIIRS, although it is certainly necessary to carry
398 out more evaluations in the future.

399

400 **4.3 $K_d(\text{nbUV})$ from ocean color satellites**

401 After obtaining $R_{rs}(\text{nbUV})$ from VIIRS, it is then possible to estimate $K_d(\text{nbUV})$
402 semi-analytically following Lee et al. (2005). The total absorption (a) and backscattering (b_b)
403 coefficients at the nbUV-visible bands will be derived first from $R_{rs}(\text{nbUV-Visible})$ using a
404 semi-analytical algorithm (Lee et al. 2002; Wang et al. 2009; Werdell et al. 2013). Since K_d is
405 a function of a and b_b (Gordon 1989b; Lee et al. 2005; Lee et al. 2013), it is then
406 straightforward to calculate $K_d(\text{nbUV})$ when $a(\text{nbUV})$ and $b_b(\text{nbUV})$ are known. As an
407 example, Figure 12 shows global distributions of $K_d(360)$ and $K_d(380)$ (with the Sun at zenith)
408 derived from VIIRS for seasonal composite of October to December 2012. At the center of
409 the South Pacific Gyre, $K_d(360)$ is $\sim 0.031 \text{ m}^{-1}$, and $K_d(380)$ is around $\sim 0.025 \text{ m}^{-1}$ during this
410 period, which show general consistency with those reported previously (Morel et al., 2007),
411 although the field measurements were taken in Nov. 2004. As stated earlier, there are other
412 algorithms developed to estimate K_d in the UV domain using R_{rs} in the visible (Fichot et al.
413 2008; Smyth 2011a; Vasilkov et al. 2001). It is thus important to evaluate the performances of
414 these algorithms for the global ocean, which is out of the scope of this effort.

415

416 **4.4 Further implications for the “Case 1” approach in oceanic waters**

417 As aforementioned in the introduction, the earlier approaches (Højerslev and Aas 1991;
418 Smyth 2011b; Tedetti et al. 2010; Vasilkov et al. 2005) estimated $K_d(\text{nbUV})$ using Chl or K_d
419 (or a) at one visible band as the input, which is based on the “Case 1” concept proposed by
420 Morel and Prieur (1977) decades ago, where the inherent (sometime even the apparent)
421 optical properties could be estimated using Chl alone (Morel 1988; Morel and Maritorea
422 2001). However, as shown in Højerslev et al. (1991) and Morel et al. (2007) for various
423 oceanic waters, significantly different relationships between $K_d(\text{UV})$ and $K_d(\text{visible})$ or
424 between $K_d(\text{UV})$ and Chl exist; thus, such a scheme to predict $K_d(\text{UV})$ from one variable runs
425 into difficulties for the global ocean. To highlight this difficulty, Figure 13 shows scatterplots
426 between $K_d(360)$, $K_d(380)$ and $K_d(490)$, respectively, where the R^2 values are ~ 0.8 even for
427 the waters with bottom depth deeper than 1,000 m. For R_{rs} of global oceans, the R^2 values are
428 ~ 0.89 between $R_{rs}(360)$, $R_{rs}(380)$ and $R_{rs}(440)$ obtained from the VIIRS (see Figure 14).
429 These patterns clearly indicate that not all $R_{rs}(\text{nbUV})$ or $K_d(\text{nbUV})$ of oceanic waters can be
430 accurately predicted from $R_{rs}(440)$ or $K_d(490)$, respectively. This further echoes that oceanic
431 waters are not necessarily “Case 1” (IOCCG 2000; Lee and Hu 2006); thus, a scheme to
432 estimate R_{rs} or K_d in the UV domain based on the “Case 1” assumption may result in large
433 uncertainties.

434

435 **4.5 Consistency of $R_{rs}(\text{UV})$ among SeaWiFS, MODIS, and VIIRS**

436 Following the same deep-learning approach, UVISR_{dl} systems were developed for the
437 spectral bands of SeaWiFS and MODIS (which is certainly also possible for other satellites
438 after adjusting UVISR_{dl} accordingly). It is then interesting to see if the $R_{rs}(\text{nbUV})$ products
439 from these satellites are consistent. Observations by SeaWiFS and MODIS (Aqua) are
440 overlapped between 2002 and 2010; observations by MODIS (Aqua) and VIIRS (SNPP) are
441 overlapped from 2012 onward. We thus picked October to December in 2005 to compare
442 SeaWiFS and MODIS and used October to December in 2012 to compare MODIS and
443 VIIRS. The unbiased relative difference (URD) of $R_{rs}(\text{nbUV})$ between two satellite sensors is
444 calculated to evaluate the consistency, with URD defined as:

$$\text{URD} = \frac{\text{Sensor}_2 - \text{MODIS}}{\text{Sensor}_2 + \text{MODIS}} \times 2, \quad (5)$$

445 where Sensor_2 is either for SeaWiFS or VIIRS.

446 Figure 15 (*a, c, e*) shows the global distributions of URD calculated between MODIS
 447 and VIIRS $R_{rs}(\text{nbUV})$; Figure 15 (*b, d, f*) shows the histograms of URD at each nbUV band;
 448 and Figure 16a presents scatterplots of $R_{rs}(\text{nbUV})$ between VIIRS and MODIS at 360 nm. We
 449 can see that $R_{rs}(\text{nbUV})$ from the two pairs of sensors agree with each other very well, where
 450 the URD values are generally around 0 in the tropical and subtropical regions, but higher near
 451 the polar regions and many coastal areas (e.g., west coast of India). This higher value reflects
 452 the strong spatial variation of coastal water properties and different spatial and temporal
 453 coverages of these satellite sensors. The average URD(360) is -0.017, with R^2 value as 0.95,
 454 and the slope is close to 1.0 in the linear regression (see Figure 16a). These measures are
 455 similar to those at 440 nm (see Figure 16b), both being independent measurements.
 456 Furthermore, Figures 16c and 16d compare the $R_{rs}(360)$ and $R_{rs}(440)$ between SeaWiFS and
 457 MODIS, demonstrating similar statistical measures at 360 nm and 440 nm, which is parallel
 458 to the comparison between MODIS and VIIRS. These evaluations indicate highly consistent
 459 $R_{rs}(\text{nbUV})$ among these satellite ocean color measurements, as long as $R_{rs}(\text{visible})$ is
 460 consistent among them.

461

462 **5. Summary and future perspectives**

463 To fill the data gap of UV penetration in the global ocean, especially for measurements
 464 after the launch and operation of modern ocean color satellites, a deep-learning-based system
 465 (UVISR_{dl}) is developed to estimate R_{rs} at the near-blue UV bands (specifically at 360, 380,
 466 and 400 nm in this study) with R_{rs} in the visible (410-670 nm) as the input. We show that
 467 UVISR_{dl}-estimated $R_{rs}(\text{nbUV})$ agree very well (<10% difference) with those from
 468 radiometric measurements, although larger differences are found between VIIRS $R_{rs}(\text{nbUV})$
 469 and matchup *in situ* data when measurements were taken in coastal regions. With estimated
 470 $R_{rs}(\text{nbUV})$ and known $R_{rs}(\text{visible})$ of the global oceans from ocean color satellites,
 471 $K_d(\text{nbUV-visible})$ of the global oceans can then be calculated semi-analytically; thus,

472 penetration of radiation in the nbUV domain in the global oceans can be clearly characterized
473 through the combination of UV radiation products at the ocean surface. Such information will
474 be useful for a broad range of biogeochemical studies. In addition, the availability of
475 $R_{rs}(\text{nbUV})$ can help both atmospheric correction and decomposition of the total absorption
476 coefficient into its components.

477 This study is an initial step to estimate $R_{rs}(\text{nbUV})$, using a deep-learning scheme, from
478 R_{rs} at the available visible bands of ocean color satellites, where its evaluation is still limited.
479 It is important and necessary to evaluate $R_{rs}(\text{nbUV})$ obtained by UVISR_{dl}, and subsequently
480 $K_d(\text{nbUV})$ with more inclusive global measurements to obtain a comprehensive
481 characterization and understanding of UVISR_{dl} for ocean color satellites. Some current ocean
482 color satellites, e.g., the OLCI, SGLI, and HY1C, and other planned future ocean color
483 satellites, e.g., the PACE, cover a few bands in the 350-400 nm range. It will thus be valuable
484 to evaluate $R_{rs}(\text{nbUV})$ obtained from UVISR_{dl} by comparing to $R_{rs}(\text{nbUV})$ measured directly
485 by satellites, although both determination has its own uncertainties. While $R_{rs}(\text{nbUV})$ from
486 UVISR_{dl} should not be considered as a means to replace $R_{rs}(\text{nbUV})$ from satellite
487 measurements at the nbUV bands, it nevertheless can be an important data source to fill the
488 data gaps in the past and present and a data source when atmospheric correction runs into
489 difficulties in the nbUV bands.

490

491

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505

506

507 **References**

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759

760 **Appendix A:**

761 To train UVISR_{dl}, we created a large synthetic dataset covering wide ranges of inherent
762 optical parameters (IOPs) and remote sensing reflectance (R_{rs}). The generation of this dataset
763 generally follows the IOCCG Report 5 (IOCCG-OCAG 2003; IOCCG 2006) for synthesizing
764 wide ranges of IOPs spectra, but an analytical model (Lee et al., 2004) was used to calculate
765 R_{rs} from these IOPs, as generating such a large dataset with the Hydrolight software will take
766 too long. However, this R_{rs} model was developed based on Hydrolight simulations where the
767 accuracy is within ~1% on average, so the error of using an analytical formula for R_{rs} on the
768 deep-learning system of this study is negligible.

769 Following the description in IOCCG-OCAG (2003), the absorption (a) and
770 backscattering (b_b) coefficients, the two key component IOPs for R_{rs} , are modeled as

$$a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_{dm}(\lambda) + a_g(\lambda). \quad (\text{A1a})$$

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bph}(\lambda) + b_{bdm}(\lambda). \quad (\text{A1b})$$

771 Here subscripts “ w , ph , dm , g ” represent pure seawater, phytoplankton pigments, detritus and
772 minerals, and gelbstoff (e.g., CDOM), respectively.

773 Values of $a_w(\lambda)$ were taken from combinations of the literature. Specifically, a_w values of
774 350-550 nm are from Lee et al. (2015b), 551-725 nm from Pope and Fry (1997), 726-800 nm
775 from Smith and Baker (1981). From more than 4,000 measured $a_{ph}(\lambda)$ spectra (350-800 nm, 5
776 nm step), 720 $a_{ph}(\lambda)$ spectra were selected with $a_{ph}(440)$ in a range of ~0.001-39.0 m^{-1} , thus
777 covering oceanic waters to waters with phytoplankton blooms.

778 Following the practice taken by the IOCCG-OCAG (2003), a_{dm} and a_g were modeled as

$$a_{dm}(\lambda) = a_{dm}(440)e^{-S_{dm}(\lambda-440)}, \quad (\text{A2a})$$

$$a_g(\lambda) = a_g(440)e^{-S_g(\lambda-440)}, \quad (\text{A2b})$$

779 where the slope parameters S_{dm} (~0.007-0.015 nm^{-1}) and S_g (~0.01 - 0.02 nm^{-1}) were taken as
780 random values as in IOCCG-OCAG (2003), and $a_{dm}(440)$ and $a_g(440)$ were modeled as

$$a_{dm}(440) = p_1 \times a_{ph}(440), \quad (\text{A3a})$$

$$a_g(440) = p_2 \times a_{ph}(440). \quad (\text{A3b})$$

781 Parameters p_1 and p_2 were controlled random values, generating reasonable $a_{dm}(440)$ and
782 $a_g(440)$ values for a given $a_{ph}(440)$ (IOCCG-OCAG 2003).

783 Values of $b_{bw}(\lambda)$ were taken from the literature (Zhang and Hu 2009b). Spectra of b_{bph}
 784 were also modeled as in IOCCG-OCAG (2003), where b_{bph} is aa

$$b_{bph}(\lambda) = B_{ph}(c_{ph}(\lambda) - a_{ph}(\lambda)), \quad (A4a)$$

$$c_{ph}(\lambda) = p_3 \times c_{ph}(550) \left(\frac{550}{\lambda}\right)^{p_4}, \quad (A4b)$$

785 and B_{ph} is the backscattering ratio of phytoplankton and a value of 1% was taken. Parameters
 786 p_3 and p_4 were random values within given ranges as in IOCCG-OCAG (2003). Similarly,
 787 spectra of b_{bdm} were modeled as

$$b_{bdm}(\lambda) = 0.0183 p_5 \times b_{dm}(550) \left(\frac{550}{\lambda}\right)^{p_6}, \quad (A5)$$

788 with p_5 and p_6 also random values within given ranges.

789 The relationship between r_{rs} and IOPs from Lee et al. (2004) was employed:

$$r_{rs}(\lambda) = g_w \frac{b_{bw}(\lambda)}{a(\lambda) + b_b(\lambda)} + g_p \frac{b_{bp}(\lambda)}{a(\lambda) + b_b(\lambda)}, \quad (A6a)$$

$$g_p(\lambda) = G_0 \left[1 - G_1 \exp\left(-G_2 \frac{b_{bp}(\lambda)}{a(\lambda) + b_b(\lambda)}\right) \right], \quad (A6b)$$

790 Here g_w is the model parameter related to molecular scattering, and g_p is the model parameter
 791 related to particle-scattering phase function, and values of G_{0-2} are constants for a given light
 792 geometry and particle phase function. $R_{rs}(\lambda)$ can be computed from $r_{rs}(\lambda)$ (Gordon et al. 1988)
 793 with a relationship as

$$R_{rs}(\lambda) = \frac{0.52 r_{rs}(\lambda)}{1 - 1.7 r_{rs}(\lambda)}. \quad (A7)$$

794 In the above system for the calculation of R_{rs} , a_{ph} is a free variable, while parameters p_1-p_6 are
 795 determined randomly in constrained ranges for each a_{ph} . The generation of these constrained
 796 random values followed that in IOCCG-OCAG (2003), and described in Craig et al. (2020).

797 The 720 $a_{ph}(\lambda)$ spectra were divided into 12 groups, with each group having its own $a_{ph}(440)$
 798 range. These $a_{ph}(\lambda)$ spectra were normalized to its $a_{ph}(440)$ to obtain a_{ph} spectral shapes. Total

799 of 200,000 $a_{ph}(\lambda)$ were then generated by multiplying $a_{ph}(440)$ to these spectral shapes, with

800 $a_{ph}(440)$ randomly varying in a range of 0.001-20.0 m^{-1} , while the spectral shapes were

801 selected based on the $a_{ph}(440)$ value. Subsequently 200,000 groups of hyperspectral

802 $a(\lambda)$ & $b_b(\lambda)$ were generated following Eqs. A1-A5, and then 200,000 hyperspectral R_{rs} spectra

803 were generated with Eqs. A6-A7, where the resulted $R_{rs}(550)$ is in a range of ~0.0008-0.090

804 sr^{-1} .

805 **Table Captions:**

806

807 Table 1. Range of remote sensing reflectance (taking $R_{rs}(555)$ as an example) used for
808 evaluation of UVISR_{dl}. CV is the ratio of standard deviation to the mean.

809

810 Table 2. Statistical measures of UVISR_{dl} after being applied to both synthetic and field
811 measured datasets.

812

813 Table 3. Statistical measures between matchup VIIRS and measured R_{rs} . N is the number of
814 matchup measurements.

815 **Figure Captions:**

816

817 Fig. 1. Schematic chart of the deep-learning-based system for estimating $R_{rs}(\text{nbUV})$ using
818 $R_{rs}(\text{visible})$: UVISR_{dl}.

819

820 Fig. 2. Examples of R_{rs} spectra used in this study: (a) synthesized R_{rs} spectra for the
821 development and validation of UVISR_{dl}, and (b) measured R_{rs} spectra to evaluate UVISR_{dl}.

822

823 Fig. 3. Comparison between $R_{rs}(\text{nbUV})$ and UVISR_{dl}-predicted $R_{rs}(\text{nbUV})$ of the synthetic
824 dataset: (a) $R_{rs}(360)$, (b) $R_{rs}(380)$, and (c) $R_{rs}(400)$.

825

826 Fig. 4. Relationship between $R_{rs}(\text{nbUV})$ and $R_{rs}(440)$ of both synthetic and measured (SBA
827 and MOBY) datasets: (a) $R_{rs}(360)$ vs $R_{rs}(440)$, (b) $R_{rs}(380)$ vs $R_{rs}(440)$, and (c) $R_{rs}(400)$ vs
828 $R_{rs}(440)$.

829

830 Fig. 5. Comparison between $R_{rs}(\text{nbUV})$ and UVISR_{dl}-predicted $R_{rs}(\text{nbUV})$ of the measured
831 SBA dataset: (a) $R_{rs}(360)$, (b) $R_{rs}(380)$, and (c) $R_{rs}(400)$.

832

833 Fig. 6. Comparison between $R_{rs}(\text{nbUV})$ and UVISR_{dl}-predicted $R_{rs}(\text{nbUV})$ of the measured
834 MOBY dataset: (a) $R_{rs}(360)$, (b) $R_{rs}(380)$, and (c) $R_{rs}(400)$.

835

836 Fig. 7. Global distribution of seasonal composite $R_{rs}(\text{nbUV})$ for the period of October to
837 December 2012 obtained from VIIRS: (a) $R_{rs}(360)$, (b) $R_{rs}(380)$ (white star showing
838 measurements during November 2004), (c) $R_{rs}(400)$, and (d) $R_{rs}(410)$.

839

840 Fig. 8. Same as Fig. 7, except for showing $R_{rs}(360)$ of three coastal regions.

841

842 Fig. 9. Locations of matchup field measurements (SBA and MOBY) to evaluate $R_{rs}(\text{nbUV})$
843 from VIIRS.

844

845 Fig. 10. Comparison between VIIRS and field measurements SBA R_{rs} : (a) $R_{rs}(360)$, (b)

846 $R_{rs}(380)$, (c) $R_{rs}(400)$, (d) $R_{rs}(410)$, (e) $R_{rs}(440)$, and (f) $R_{rs}(490)$.

847 Fig. 11. Comparison between VIIRS and field measurements MOBY R_{rs} : (a) $R_{rs}(360)$, (b)
848 $R_{rs}(380)$, (c) $R_{rs}(400)$, (d) $R_{rs}(410)$, (e) $R_{rs}(440)$, and (f) $R_{rs}(490)$.

849
850 Fig. 12. Global distribution of seasonal composite $K_d(\text{nbUV})$ for the period of October to
851 December 2012 obtained from VIIRS: (a) $K_d(360)$, and (b) $K_d(380)$.

852
853 Fig. 13. Relationships between $K_d(\text{nbUV})$ and $K_d(490)$ of global waters obtained from VIIRS:
854 (a) $K_d(360)$ vs $K_d(490)$, and (b) $K_d(380)$ vs $K_d(490)$. Color dots are for bottom depth > 1,000
855 m, and gray dots, for bottom depth < 1,000 m. The R^2 values are for the data with depth >
856 1,000 m.

857
858 Fig. 14. Same as Fig. 13, except between $R_{rs}(\text{nbUV})$ and $R_{rs}(440)$: (a) $R_{rs}(360)$ vs $R_{rs}(440)$,
859 and (b) $R_{rs}(380)$ vs $R_{rs}(440)$. Color dots are for data with bottom depth > 1,000 m, and gray
860 points for data with bottom depth < 1,000 m.

861
862 Fig. 15. Global distribution (left) and histogram (right) of URD(nbUV) between MODIS and
863 VIIRS for seasonal data of October–December 2012: (a) 360 nm, (b) 380 nm, and (c) 400
864 nm.

865
866 Fig. 16. Comparison of R_{rs} between MODIS and VIIRS (a, b), and between MODIS and
867 SeaWiFS (c, d).

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871

872 **Table 1. Range of remote sensing reflectance (taking $R_{rs}(555)$ as an example) used for**
 873 **evaluation of UVISR_{dl}. CV is the ratio of standard deviation to the mean.**

874

Data	Data Sources (Data Number)	Band	Min (sr⁻¹)	Max (sr⁻¹)	Mean (sr⁻¹)	CV
Training data	Synthetic data (160,000)		7.7×10^{-4}	0.091	0.016	0.85
	Synthetic data (40,000)		7.8×10^{-4}	0.089	0.019	0.84
Validation data	SBA data (202)	$R_{rs}(555)$	1.1×10^{-3}	0.020	0.0048	0.84
	MOBY (6,184)		8.1×10^{-4}	3.3×10^{-3}	0.0013	0.086

875

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877

878 **Table 2. Statistical measures of UVISR_{AI} after being applied to both synthetic and field**
 879 **measured datasets.**

880

881 **(a): Synthetic dataset**

882

Data (Data Number)	Sensor	Band	RMSD (sr⁻¹)	MARD	bias (sr⁻¹)	MAURD	R²
Synthetic data (40,000)	SeaWiFS	360	1.1×10 ⁻⁴	2.3×10 ⁻³	2.3×10 ⁻⁶	0.023	>0.99
		380	5.7×10 ⁻⁵	1.7×10 ⁻³	3.8×10 ⁻⁷	0.015	>0.99
		400	1.2×10 ⁻⁵	7.6×10 ⁻⁴	1.2×10 ⁻⁶	0.0075	>0.99
	MODIS	360	1.1×10 ⁻⁴	2.6×10 ⁻³	-2.2×10 ⁻⁷	0.026	>0.99
		380	5.3×10 ⁻⁵	1.4×10 ⁻³	-3.8×10 ⁻⁷	0.015	>0.99
		400	1.2×10 ⁻⁵	3.7×10 ⁻⁴	4.0×10 ⁻⁷	0.0038	>0.99
	VIIRS	360	1.0*10 ⁻⁴	2.5×10 ⁻³	5.0×10 ⁻⁶	0.024	>0.99
		380	5.9×10 ⁻⁵	1.5×10 ⁻³	-1.3×10 ⁻⁶	0.015	>0.99
		400	1.4×10 ⁻⁵	6.2×10 ⁻⁴	1.4×10 ⁻⁶	0.006	>0.99

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887 **(b): Field dataset**

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889

Data (Data Number)	Sensor	Band	RMSD (sr⁻¹)	MARD	bias (sr⁻¹)	MAURD	R²
SBA data (202)	SeaWiFS	360	3.4×10^{-4}	0.098	1.1×10^{-4}	0.094	>0.98
		380	2.2×10^{-4}	0.041	-1.8×10^{-5}	0.041	>0.99
		400	8.6×10^{-5}	0.015	2.8×10^{-5}	0.015	>0.99
	MODIS	360	3.3×10^{-4}	0.085	7.7×10^{-5}	0.082	>0.98
		380	2.1×10^{-4}	0.045	-8.7×10^{-6}	0.045	>0.99
		400	8.8×10^{-5}	0.020	-5.8×10^{-5}	0.020	>0.99
	VIIRS	360	3.5×10^{-4}	0.095	1.2×10^{-5}	0.091	>0.98
		380	2.1×10^{-4}	0.041	-1.5×10^{-5}	0.042	>0.99
		400	8.3×10^{-5}	0.015	-4.7×10^{-5}	0.015	>0.99
MOBY data (6184)	SeaWiFS	360	1.1×10^{-3}	0.076	9.0×10^{-4}	0.072	>0.88
		380	6.1×10^{-4}	0.038	4.6×10^{-4}	0.037	>0.96
		400	1.8×10^{-4}	0.011	5.7×10^{-5}	0.011	>0.99
	MODIS	360	1.2×10^{-3}	0.083	9.9×10^{-4}	0.078	>0.87
		380	5.6×10^{-4}	0.035	4.1×10^{-4}	0.034	>0.95
		400	1.9×10^{-4}	0.012	9.4×10^{-5}	0.012	>0.99
	VIIRS	360	1.2×10^{-3}	0.085	1.0×10^{-3}	0.081	>0.87
		380	6.0×10^{-4}	0.038	4.3×10^{-4}	0.037	>0.95
		400	1.9×10^{-4}	0.011	7.8×10^{-5}	0.011	>0.99

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891

892 **Table 3. Statistical measures between matchup VIIRS and measured R_{rs} . N is the**
 893 **number of matchup measurements.**

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895

Field data	Band	N	RMSD (sr ⁻¹)	MARD	bias (sr ⁻¹)	MAURD	R ²
SBA	360	82	0.0016	0.48	0.0005	0.40	0.74
	380		0.0015	0.39	0.0004	0.34	0.77
	400		0.0013	0.33	0.0002	0.31	0.80
	410		0.0012	0.30	0.0002	0.29	0.82
	440		0.0011	0.23	-0.00008	0.25	0.82
	490		0.0013	0.18	-0.0004	0.21	0.80
MOBY	360	730	0.0023	0.14	1.2×10 ⁻³	0.13	0.25
	380		0.0022	0.13	9.2×10 ⁻⁴	0.12	0.26
	400		0.0019	0.12	2.3×10 ⁻⁴	0.12	0.23
	410		0.0017	0.11	-3.2×10 ⁻⁵	0.11	0.22
	440		0.0013	0.11	-4.2×10 ⁻⁴	0.11	0.17
	490		0.00082	0.11	-3.9×10 ⁻⁴	0.12	0.06

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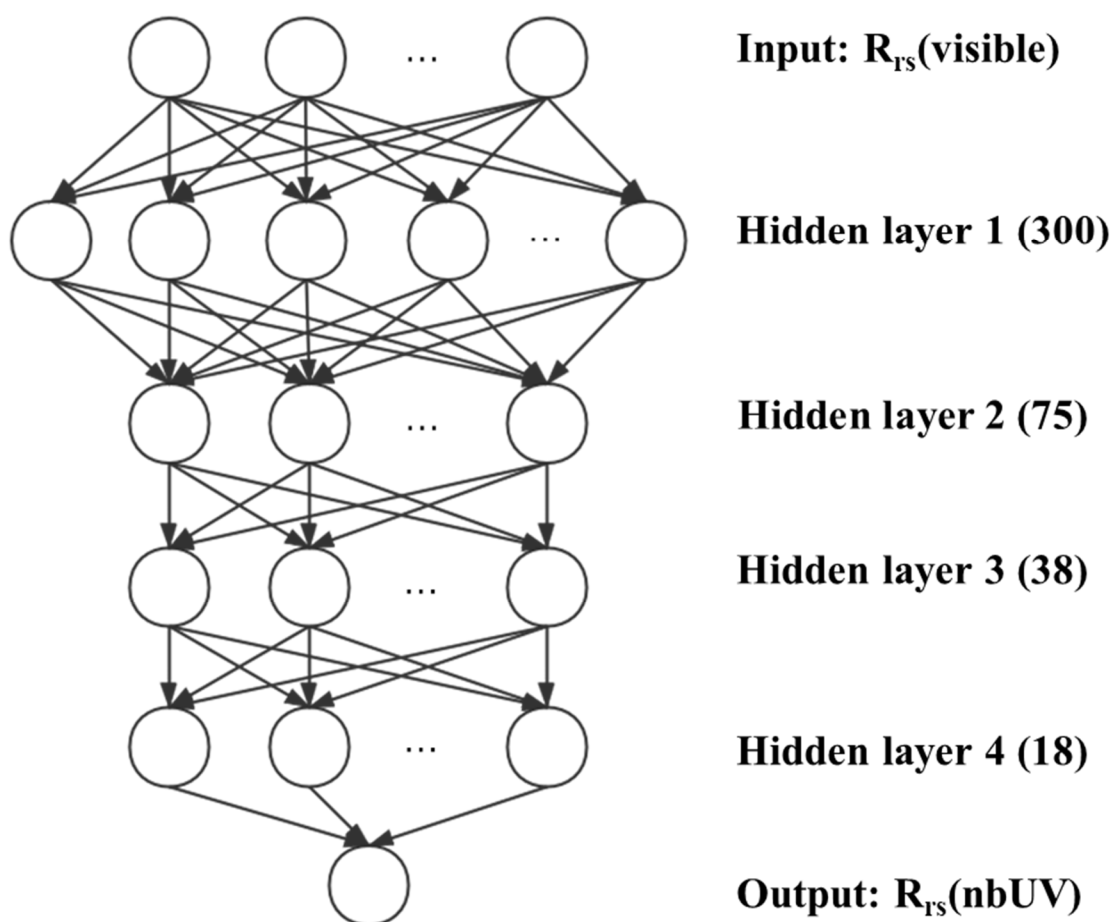
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898 **Figures:**

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Keras Model



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903 Fig. 1. Schematic chart of the deep-learning-based system for estimating $R_{rs}(\text{nbUV})$ using

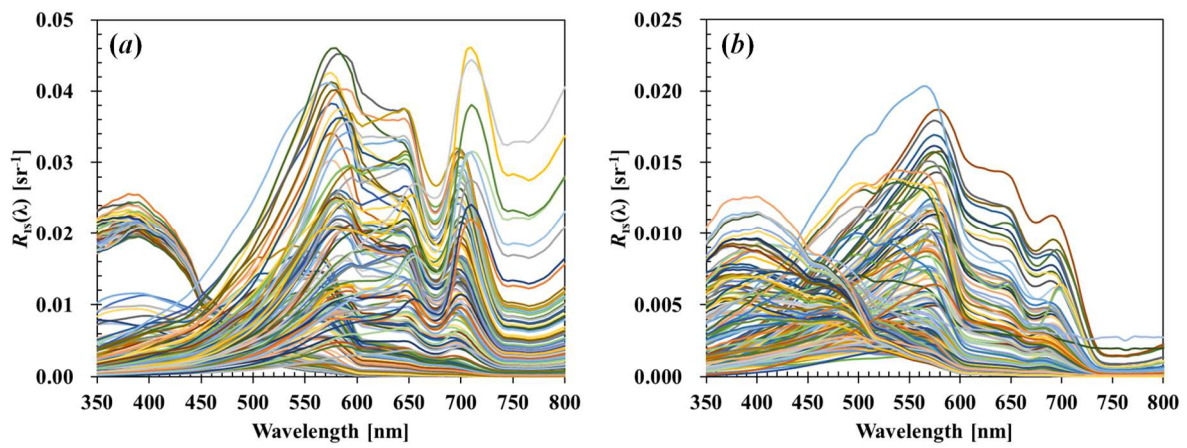
904 $R_{rs}(\text{visible})$: UVISR_{d1}.

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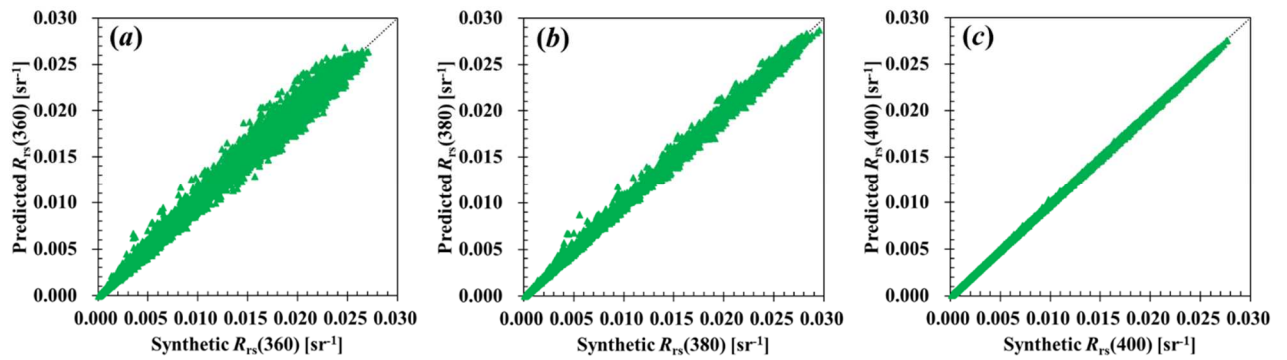
911 Fig. 2. Examples of R_{rs} spectra used in this study: (a) synthesized R_{rs} spectra for the
912 development and validation of UVISR_{dl}, and (b) measured R_{rs} spectra to evaluate UVISR_{dl}.

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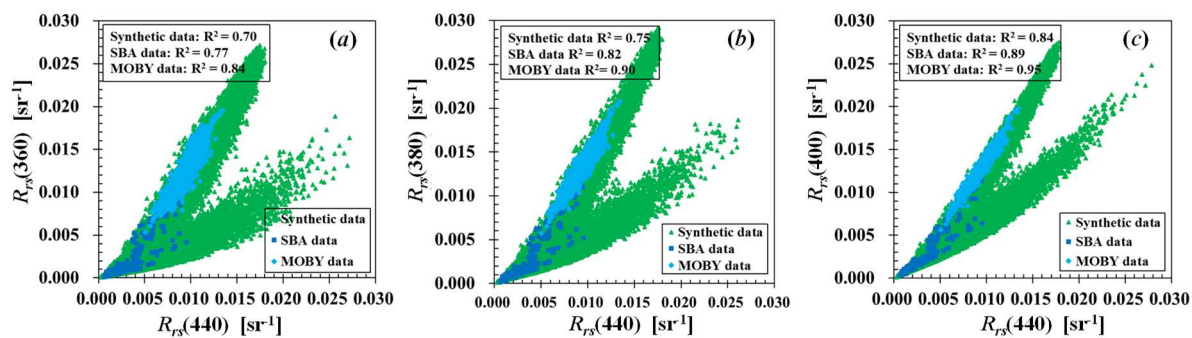


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Fig. 3. Comparison between $R_{rs}(\text{nbUV})$ and UVISR_{dl}-predicted $R_{rs}(\text{nbUV})$ of the synthetic dataset: (a) $R_{rs}(360)$, (b) $R_{rs}(380)$, and (c) $R_{rs}(400)$.

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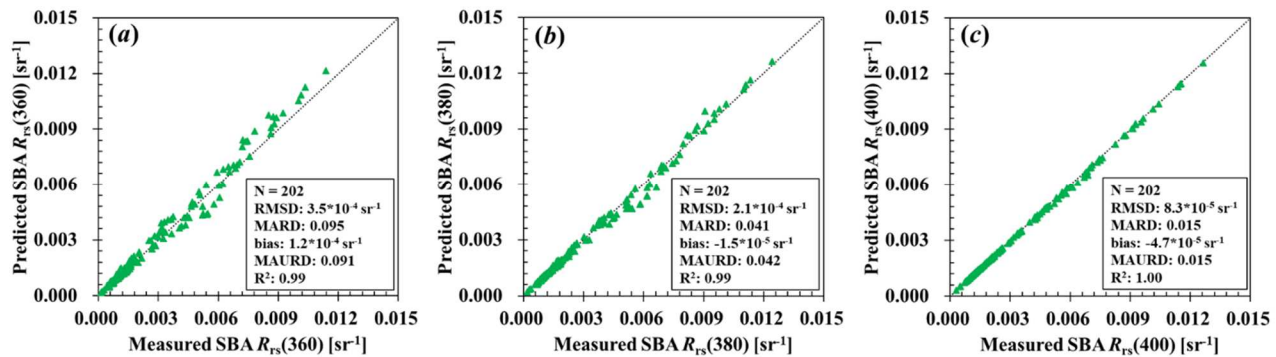
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930 Fig. 4. Relationship between $R_{rs}(nbUV)$ and $R_{rs}(440)$ of both synthetic and measured (SBA
931 and MOBY) datasets: (a) $R_{rs}(360)$ vs $R_{rs}(440)$, (b) $R_{rs}(380)$ vs $R_{rs}(440)$, and (c) $R_{rs}(400)$ vs
932 $R_{rs}(440)$.

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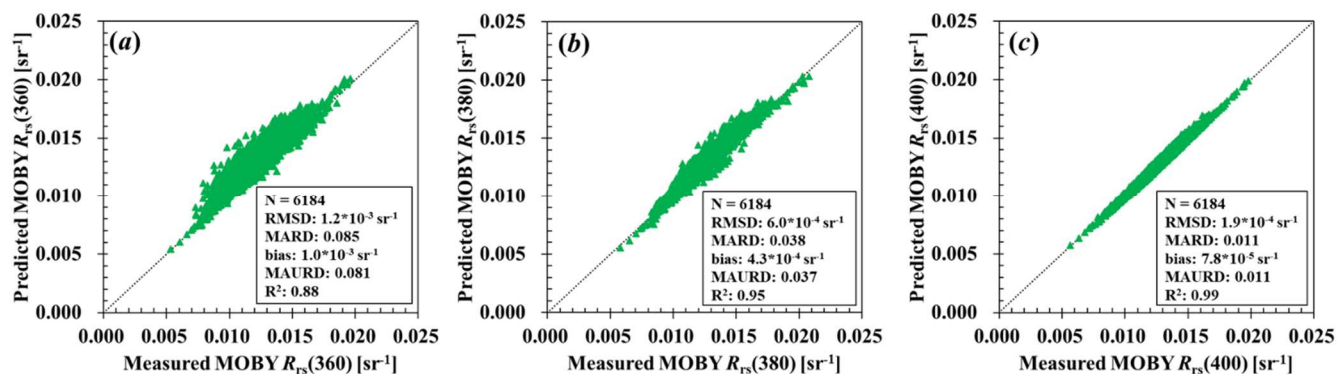
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Fig. 5. Comparison between $R_{rs}(\text{nbUV})$ and UVISR_{dl} -predicted $R_{rs}(\text{nbUV})$ of the measured SBA dataset: (a) $R_{rs}(360)$, (b) $R_{rs}(380)$, and (c) $R_{rs}(400)$.

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946 Fig. 6. Comparison between $R_{rs}(\text{nbUV})$ and UVISR_{dl} -predicted $R_{rs}(\text{nbUV})$ of the measured

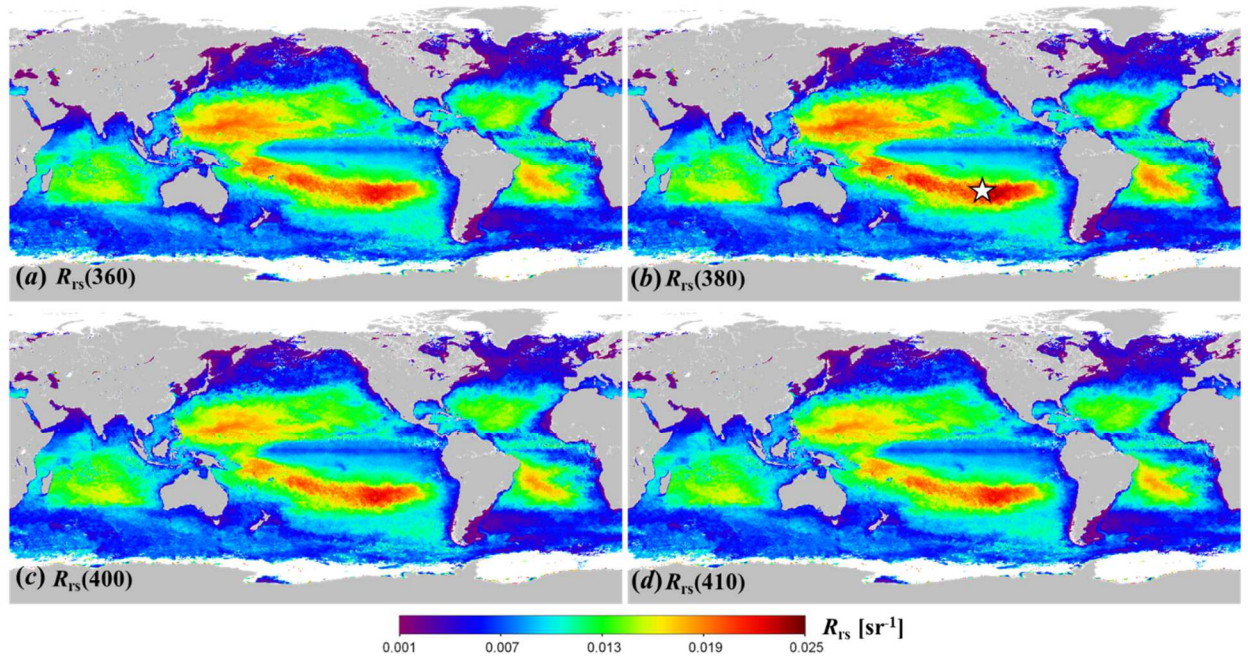
947 MOBY dataset: (a) $R_{rs}(360)$, (b) $R_{rs}(380)$, and (c) $R_{rs}(400)$.

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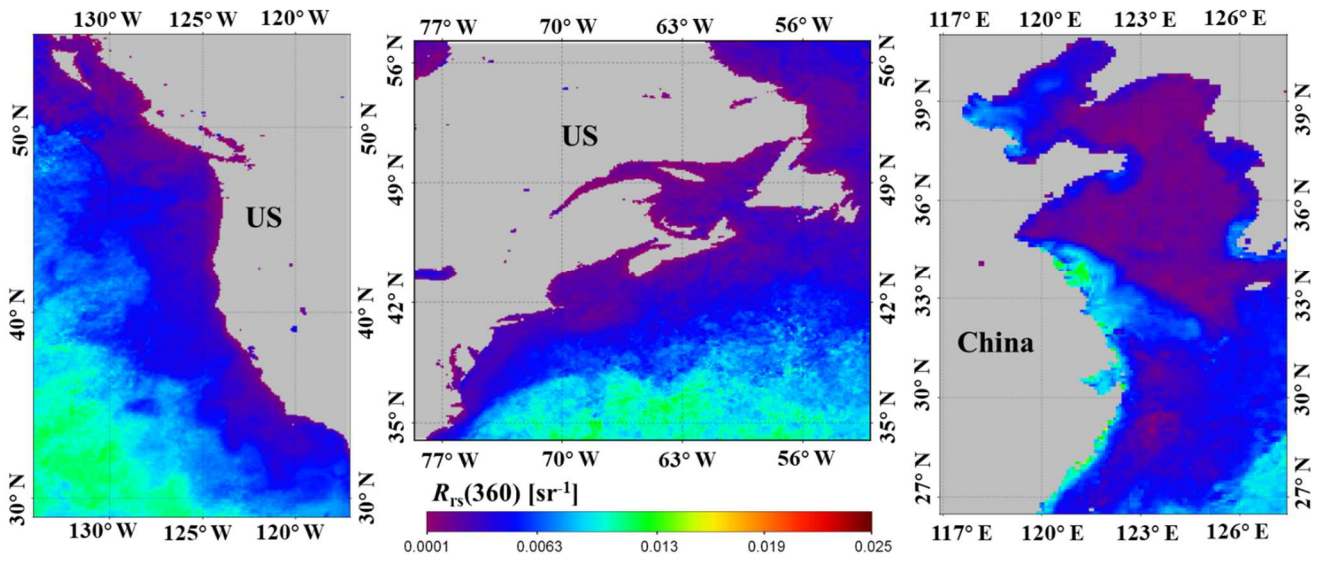
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954 Fig. 7. Global distribution of seasonal composite $R_{rs}(\text{nbUV})$ for the period of October to
955 December 2012 obtained from VIIRS: (a) $R_{rs}(360)$, (b) $R_{rs}(380)$ (white star showing
956 measurements during November 2004), (c) $R_{rs}(400)$, and (d) $R_{rs}(410)$.

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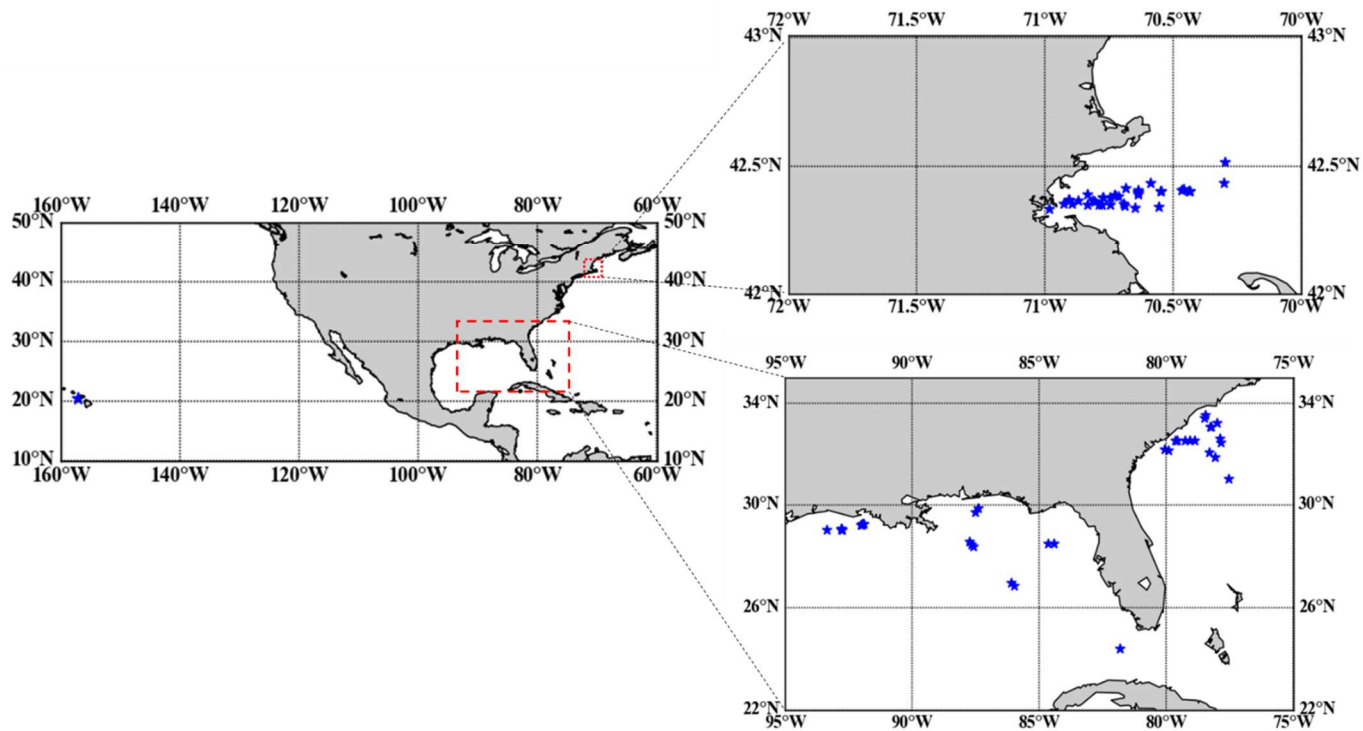
960 Fig. 8. Same as Fig. 7, except for showing $R_{rs}(360)$ of three coastal regions.

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967 Fig. 9. Locations of matchup field measurements (SBA and MOBY) to evaluate $R_{rs}(nbUV)$

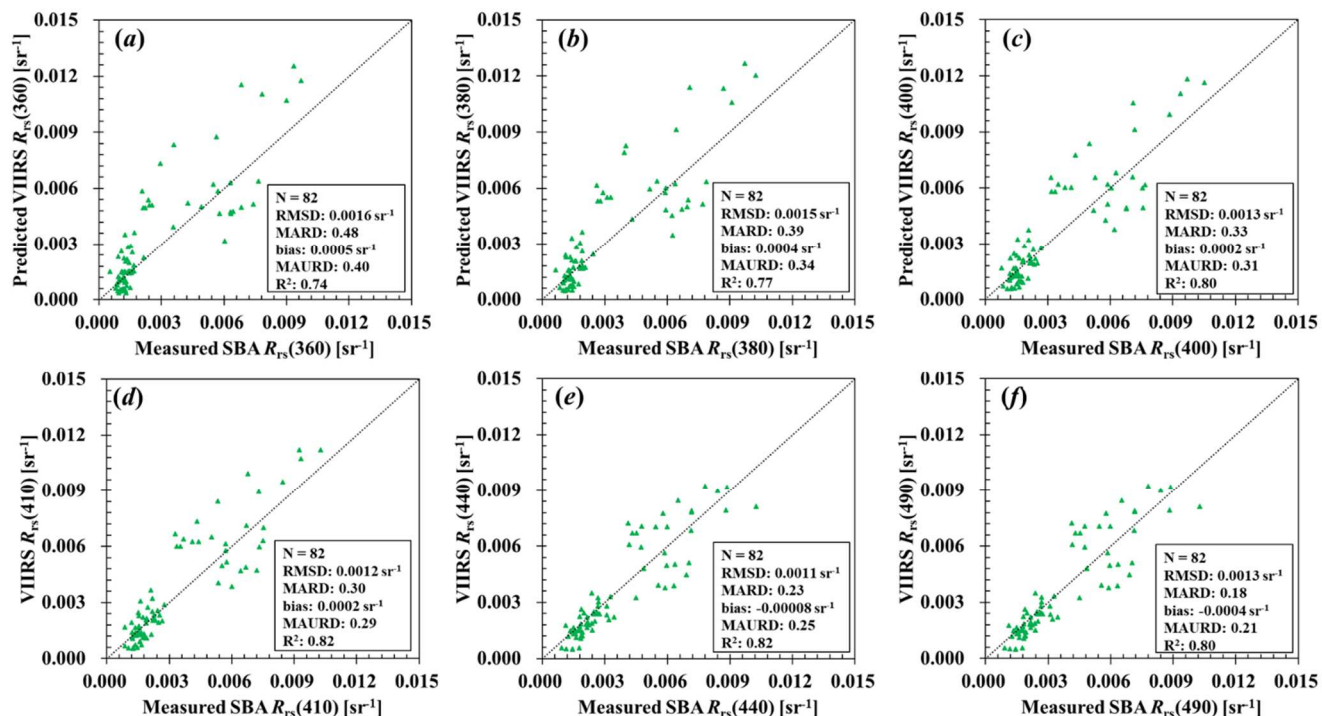
968 from VIIRS.

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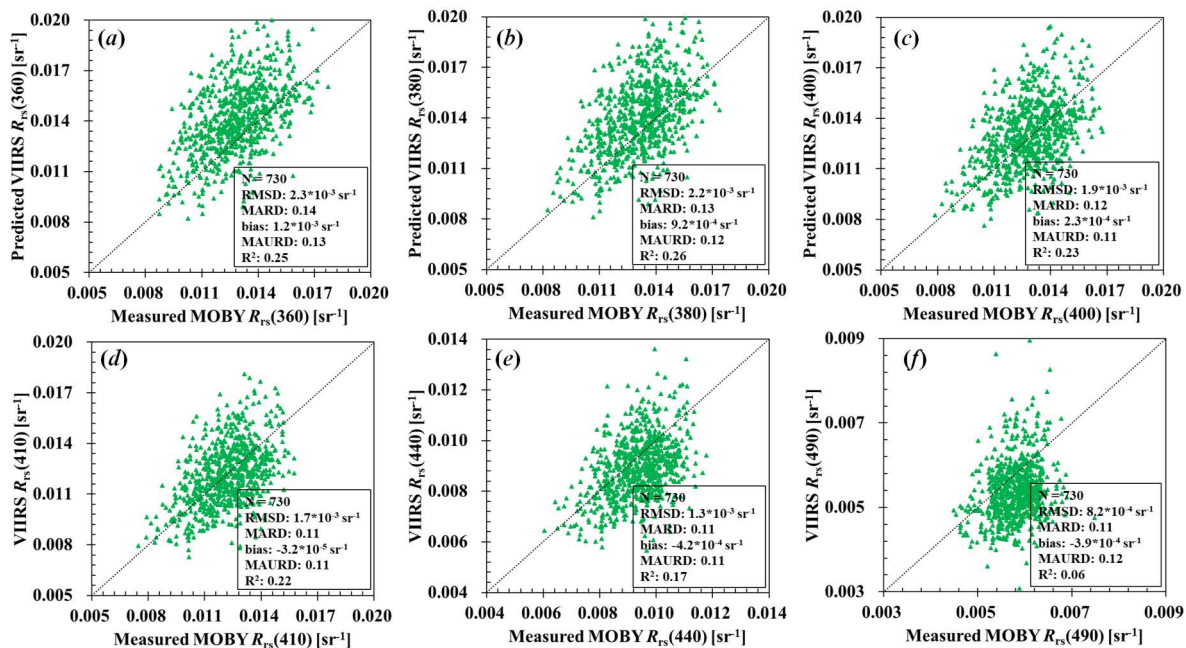
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Fig. 10. Comparison between VIIRS and field measurements SBA R_{rs} : (a) $R_{rs}(360)$, (b) $R_{rs}(380)$, (c) $R_{rs}(400)$, (d) $R_{rs}(410)$, (e) $R_{rs}(440)$, and (f) $R_{rs}(490)$.



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985 Fig. 11. Comparison between VIIRS and field measurements MOBY R_{rs} : (a) $R_{rs}(360)$, (b)

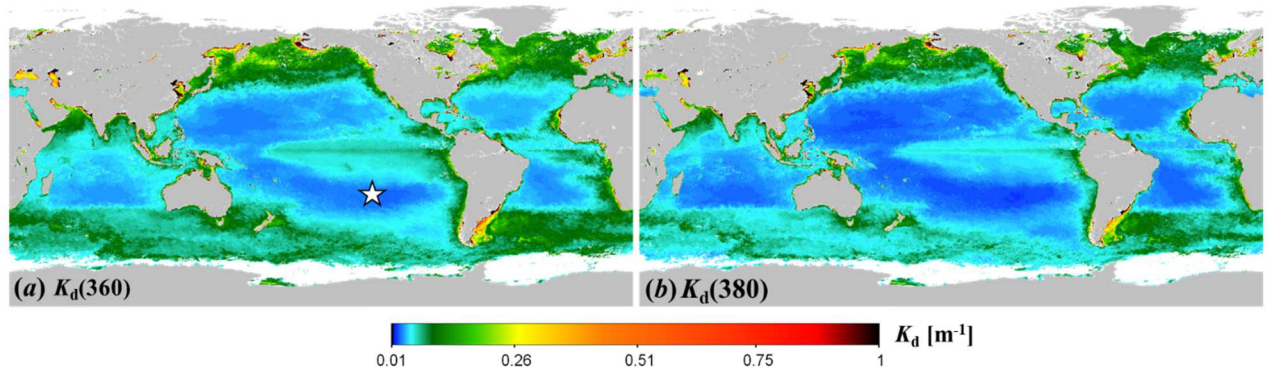
986 $R_{rs}(380)$, (c) $R_{rs}(400)$, (d) $R_{rs}(410)$, (e) $R_{rs}(440)$, and (f) $R_{rs}(490)$.

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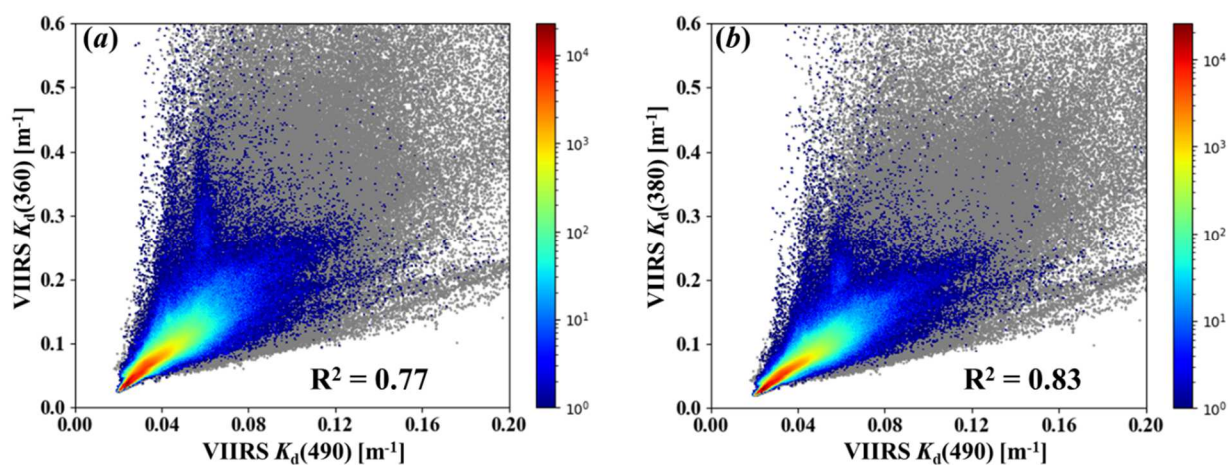
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993 Fig. 12. Global distribution of seasonal composite $K_d(\text{nbUV})$ for the period of October to
994 December 2012 obtained from VIIRS: (a) $K_d(360)$, and (b) $K_d(380)$.

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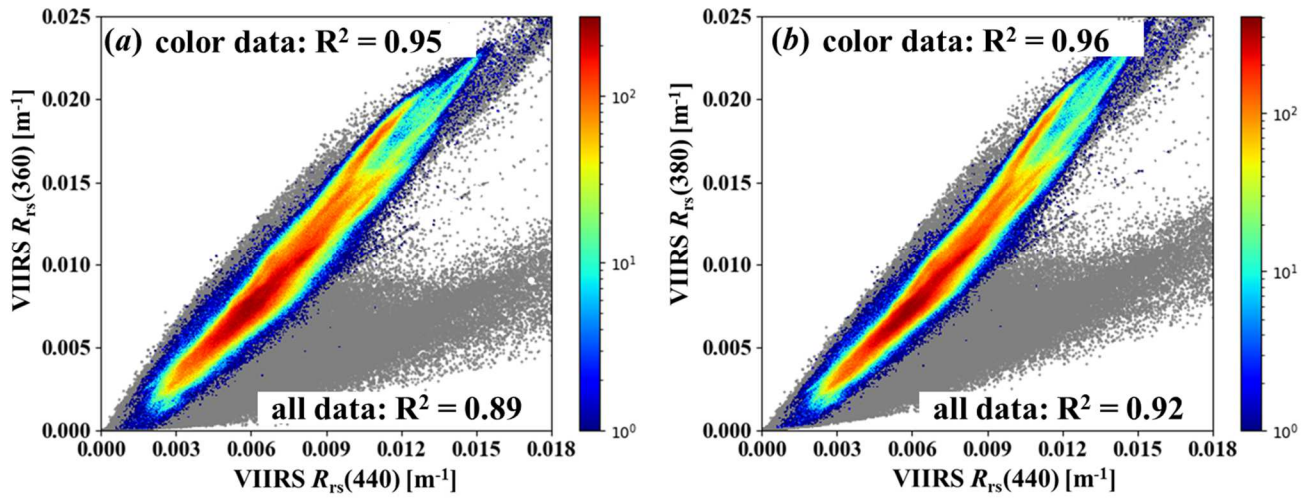
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Fig. 13. Relationships between $K_d(\text{nbUV})$ and $K_d(490)$ of global waters obtained from VIIRS: (a) $K_d(360)$ vs $K_d(490)$, and (b) $K_d(380)$ vs $K_d(490)$. Color dots are for bottom depth > 1,000 m, and gray dots, for bottom depth < 1,000 m. The R^2 values are for the data with depth > 1,000 m.

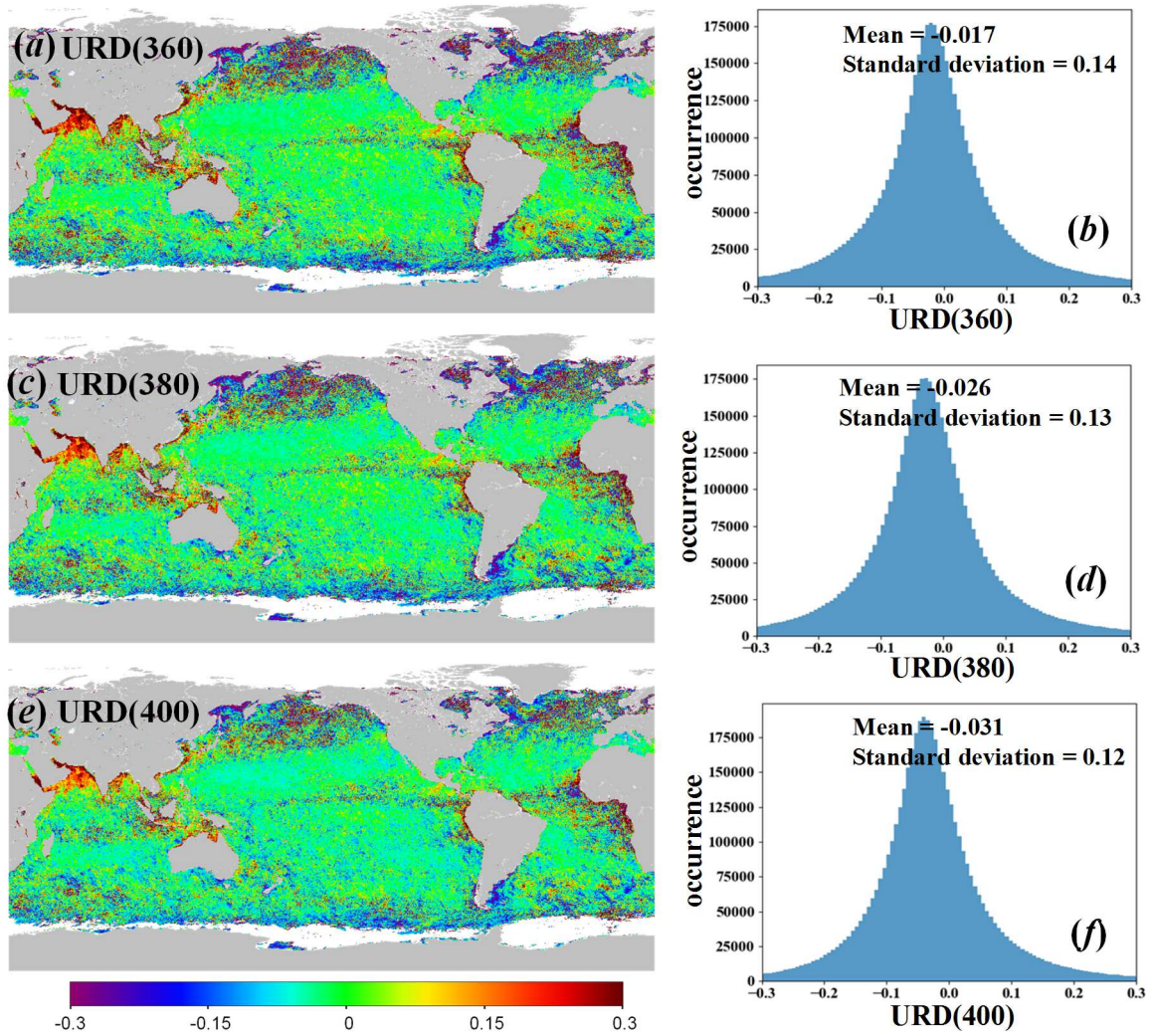
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Fig. 14. Same as Fig. 13, except between $R_{rs}(\text{nbUV})$ and $R_{rs}(440)$: (a) $R_{rs}(360)$ vs $R_{rs}(440)$, and (b) $R_{rs}(380)$ vs $R_{rs}(440)$. Color dots are for data with bottom depth $> 1,000$ m, and gray points for data with bottom depth $< 1,000$ m.

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1021 Fig. 15. Global distribution (left) and histogram (right) of URD(nbUV) between MODIS and

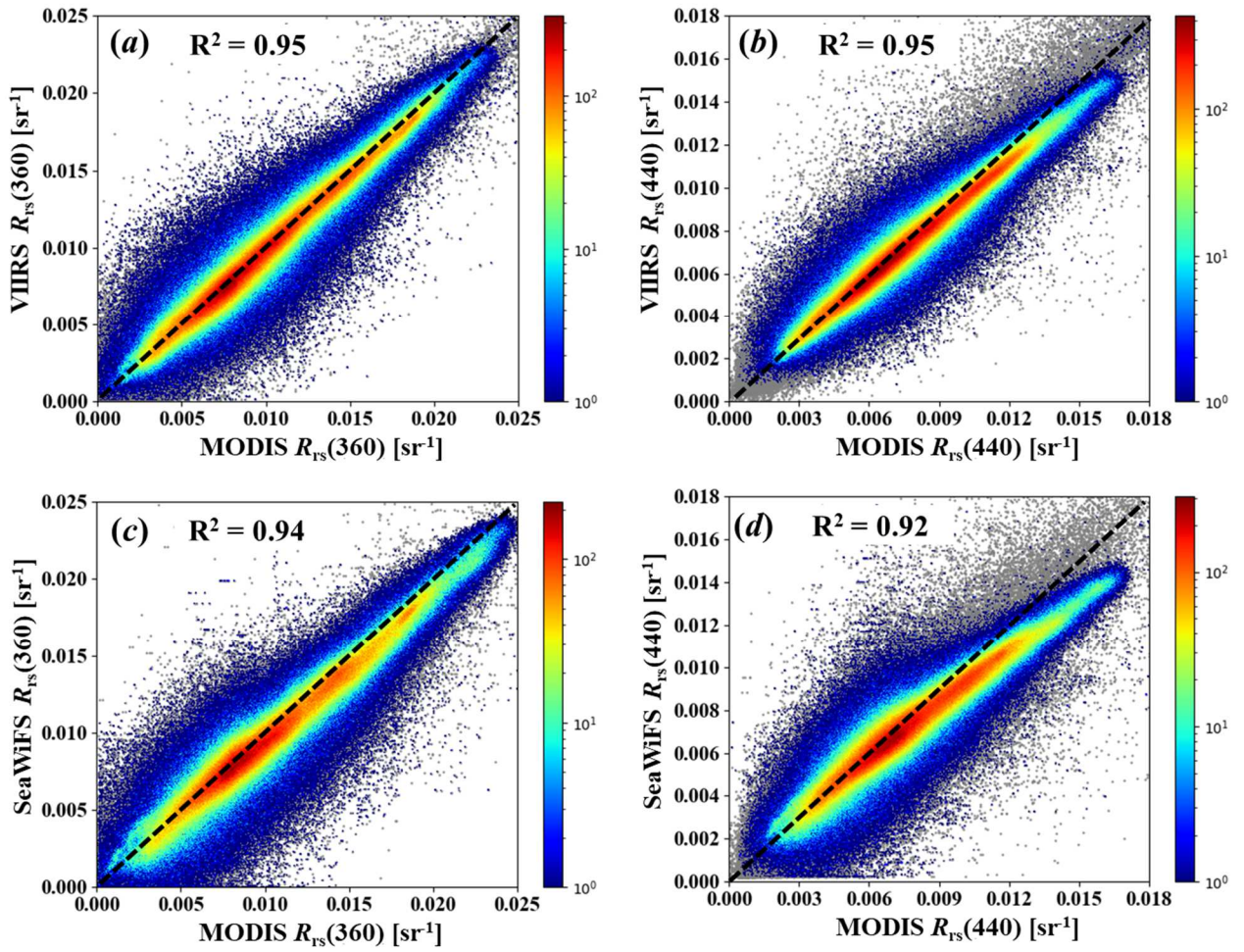
1022 VIIRS for seasonal data of October–December 2012: (a) 360 nm, (b) 380 nm, and (c) 400

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Fig. 16. Comparison of R_{rs} between MODIS and VIIRS (a, b), and between MODIS and SeaWiFS (c, d).