

1 **Improving low-quality satellite remote sensing reflectance at**
2 **blue bands over coastal and inland waters**

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20 **Abstract**

21 The satellite remote sensing reflectance ($R_{rs}(\lambda)$) at two short blue bands (410 or 412 nm and 443
22 nm) are prone to large uncertainties in coastal and inland waters, prohibiting algorithms from
23 generating reliable ocean color products associated with these bands. In this study, we developed
24 an algorithm to estimate $R_{rs}(41x)$ and $R_{rs}(443)$ when the satellite $R_{rs}(\lambda)$ in blue bands suffer from
25 large uncertainties. The algorithm first determines the $R_{rs}(\lambda)$ spectral shape from the satellite-
26 measured $R_{rs}(\lambda)$ values at three wavelengths of 48x (486, 488, or 490), 55x (547, 551, or 555),
27 and 67x (667, 670, or 671) nm. The algorithm then derives $R_{rs}(41x)$ and $R_{rs}(443)$ from the
28 estimated $R_{rs}(\lambda)$ spectral shape with algebraic formulations. We assessed the algorithm
29 performance with satellite (SeaWiFS, MODISA, and VIIRS-SNPP) and *in situ* $R_{rs}(\lambda)$ matchups
30 from global waters. It is shown that the uncertainties of estimated $R_{rs}(41x)$ and $R_{rs}(443)$ are
31 substantially smaller than the original satellite products when applicable. Besides,
32 implementation of the algorithm contributes to a significant increase in the number of utilizable
33 $R_{rs}(41x)$ and $R_{rs}(443)$ values. The algorithm is relatively stable and is best applicable to the
34 satellite $R_{rs}(\lambda)$ spectra for which the $R_{rs}(48x)$ and $R_{rs}(55x)$ measurements are subject to small
35 uncertainties. The demonstrations support the application of the blue-band estimation algorithm
36 to a wide range of coastal waters.

37 **Keyword:** Remote sensing reflectance; Blue bands; Spectral shape; Atmospheric correction;
38 SeaWiFS; MODIS; VIIRS.

39

40 **1. Introduction**

41 Ocean color satellites provide a means of collecting remote sensing reflectance ($R_{rs}(\lambda)$) on
42 spatial and temporal scales unattainable by conventional *in situ* measurements. The $R_{rs}(\lambda)$ data
43 allow for the derivation of important biological and biogeochemical properties of the upper
44 oceans, such as phytoplankton chlorophyll-a concentration (Chl) (Hu et al., 2012; McClain,
45 2009; Wang and Son, 2016), phytoplankton light absorption (Wang et al., 2017; Wei and Lee,
46 2015), colored dissolved organic matter (CDOM) absorption (Mannino et al., 2014; Wei et al.,
47 2016a; Yu et al., 2016), and primary production (Behrenfeld et al., 2005; Lee et al., 2015a), etc.
48 For reliable estimation of these bio-optical properties, it is vital to obtain accurate $R_{rs}(\lambda)$ product
49 from satellites over a wide spectral domain, particularly at the blue bands of 41x (410 or 412) nm
50 and 443 nm.

51 The ocean color satellites, including the decommissioned Sea-viewing Wide Field-of-view
52 Sensor (SeaWiFS, 1997–2010) and the operational Moderate Resolution Imaging
53 Spectroradiometer (MODIS) onboard the Aqua satellite (MODISA, 2002–present) and Visible
54 Infrared Imaging Radiometer Suite (VIIRS) onboard the Suomi National Polar-orbiting
55 Partnership satellite (VIIRS-SNPP, 2011–present), retrieve $R_{rs}(\lambda)$ from the radiance measured at
56 the top of atmosphere (TOA) through atmospheric correction (AC). Operational AC algorithms
57 usually start with the selection of an aerosol model by assuming null contribution of water-
58 leaving radiance ($L_w(\lambda)$) at the near-infrared (NIR) or shortwave infrared (SWIR) bands (Antoine
59 and Morel, 1999; Gordon and Wang, 1994; Wang, 2007; Wang and Shi, 2007). This “black-
60 pixel” assumption works well in open oceans, but is faced with some difficulties in coastal
61 regions using the NIR and SWIR approach. The strongly absorbing aerosols, for instance, can be
62 prominent in the coastal waters near anthropogenic sources of fossil-burning products, soot, and

63 smog, or under the influence of dust transport. The weakly or strongly absorbing aerosols are
64 hardly discriminable from radiance measurements in the NIR/SWIR domain but quite distinctive
65 at short blue wavelengths (IOCCG, 2010). That being said, the standard AC schemes cannot
66 correctly estimate the strongly absorbing aerosols and often fail to yield robust $R_{rs}(\lambda)$ products at
67 the blue wavelengths in many coastal regions due to lack of aerosol vertical distribution
68 information (IOCCG, 2010; Kahn et al., 2016). As a consequence, and expectedly, the satellite-
69 derived $R_{rs}(41x)$ and $R_{rs}(443)$ products are prone to large uncertainties in the coastal waters
70 (Antoine et al., 2008; Feng et al., 2008; Hlaing et al., 2013; Qin et al., 2017; Zibordi et al., 2009).
71 Apart from atmospheric correction, the large uncertainty in satellite $R_{rs}(41x)$ product is also
72 related to system vicarious calibration and instrument degradation (Franz et al., 2018). The
73 relatively large uncertainties at blue bands and the subsequent lack of utilizable data at these two
74 bands add to the difficulties of satellite ocean color applications in coastal regions (Mouw et al.,
75 2015).

76 To address the blue-band $R_{rs}(\lambda)$ quality issues, a great deal of effort has been invested. Gordon
77 et al. (1997) and Chomko and Gordon (2001) developed an AC procedure to quantify the
78 strongly absorbing aerosol contribution under dust-dominating conditions. Application of their
79 methods, however, remains impractical because the vertical distribution of absorbing aerosols in
80 the atmosphere is not known *a priori* (Banzon et al., 2009; IOCCG, 2010). In another case study,
81 Hu et al. (2000) tested a nearest-neighbor method to account for the aerosol contribution at the
82 NIR bands, with reasonable results. Variants of the standard AC schemes also emerged. Oo et al.
83 (2008) reported improved atmospheric correction for turbid coastal waters by placing constraints
84 onto $R_{rs}(412)$ within their AC procedures. For highly absorptive waters, He et al. (2012)
85 proposed null water-leaving radiance at 412 nm so as to make a guess of the aerosol contribution

86 at that band, which was then used for atmospheric correction. In analogy, Wang and Jiang (2018)
87 forced the negative $R_{rs}(410)$ values from VIIRS-SNPP to zeroes to estimate the aerosol
88 contributions and ultimately to obtain improved $R_{rs}(\lambda)$ products.

89 Besides the above contributions, there exists another line of methodology to deal with the
90 blue-band $R_{rs}(\lambda)$ measurements. Basically, this category of methods attempts to “correct” the
91 problematic blue-band $R_{rs}(\lambda)$ data. In this regard, Ransibrahmanakul and Stumpf (2006) tested a
92 power-law function to account for the spectral artifacts caused by the absorbing aerosols in the
93 northeast U.S. coasts. D'Alimonte et al. (2008) derived multi-linear regression coefficients from
94 satellite and *in situ* $R_{rs}(\lambda)$ matchups and further applied those coefficients to estimate $R_{rs}(412)$ for
95 the same region. Undoubtedly, all strategies mentioned above have demonstrated varying
96 degrees of success, specific to the sensors, dataset, or environments, in improving blue-band
97 $R_{rs}(\lambda)$ quality. Yet, it remains an open question to implement such algorithms as a universal
98 approach to global coastal and inland waters where the satellite $R_{rs}(41x)$ and $R_{rs}(443)$ data are of
99 low quality.

100 The blue-band $R_{rs}(\lambda)$ data are needed for many bio-optical retrievals in the upper water
101 columns. Among others, $R_{rs}(41x)$ and $R_{rs}(443)$ are indispensable for many semi-analytical
102 algorithms to retrieve the phytoplankton and CDOM absorption coefficients from multiband
103 satellite $R_{rs}(\lambda)$ (IOCCG, 2006; Lee et al., 2002; Wei et al., 2019; Werdell et al., 2013). $R_{rs}(443)$
104 data may also be required for Chl estimation in both open and coastal oceans (Hu et al., 2012;
105 O'Reilly et al., 1998; Wang and Son, 2016). Use of $R_{rs}(41x)$ and $R_{rs}(443)$ data with large errors
106 can result in unrealistic retrievals for the water bio-optical properties (Werdell et al., 2018) and
107 biased Chl products (Hyde et al., 2007). It is also risky that merging of such satellite products
108 may generate spurious trends in ocean color time series. In order to best interpret the large-scale

109 and long-term ocean color retrievals, this long-standing problem associated with the blue-band
110 satellite $R_{rs}(\lambda)$ measurements needs to be resolved.

111 In this study, we propose a spectral shape based algorithm to estimate $R_{rs}(41x)$ and $R_{rs}(443)$
112 when the satellite $R_{rs}(\lambda)$ spectra at blue bands are subjected to large uncertainties. Such
113 estimation will help ultimately enhance the bio-optical retrievals with the ocean color algorithms
114 requiring $R_{rs}(41x)$ and/or $R_{rs}(443)$ data. In the following, we first describe the evaluation data
115 from SeaWiFS, MODISA, and VIIRS-SNPP, the proposed algorithm, and relevant analyses
116 (Section 2). Next, we demonstrate the algorithm performance in estimating $R_{rs}(41x)$ and $R_{rs}(443)$
117 by comparison with *in situ* matchup measurements (Section 3). Finally, we discuss the algorithm
118 applicability, uncertainty, potential impacts on satellite bio-optical retrievals, and potential
119 applications to satellite image processing (Section 4).

120

121 **2. Data and methods**

122 **2.1 Satellite and *in situ* $R_{rs}(\lambda)$ matchups**

123 The present study is based on satellite $R_{rs}(\lambda)$ spectra and concurrent *in situ* matchup
124 measurements. There were 2540 and 3639 matchups extracted for SeaWiFS and MODISA,
125 respectively, from the SeaWiFS Bio-optical Archive and Storage (SeaBASS) (Werdell and
126 Bailey, 2005). A total of 2348 matchups were also assembled for VIIRS-SNPP, with the *in situ*
127 and satellite $R_{rs}(\lambda)$ obtained from SeaBASS and NOAA CoastWatch, respectively. The $R_{rs}(\lambda)$
128 matchups were constructed in accordance with the availability of *in situ* data and the filtering
129 criteria for satellite data (Bailey and Werdell, 2006; Mélin et al., 2011; Zibordi et al., 2009).
130 First, the satellite data within a 5×5 pixel box centered at the *in situ* measurement location were
131 considered. Second, the satellite data within the box were checked with the quality-flagging

132 system (QFS), *l2_flags*: all pixels flagged as land, cloud, stray light, high glint, low radiance at
133 555 nm, high TOA radiance, or atmospheric correction failure were excluded from subsequent
134 analysis. The third criterion applied was that at least 50% of the satellite pixels within the box are
135 valid. Then, it was ensured that the solar zenith angle and sensor zenith angle are within 70° and
136 60°, respectively. The maximum time difference between satellite overpass and *in situ* sampling
137 was set to ± 3 hours. The allowed maximum coefficient of variation of $R_{rs}(\lambda)$ inside the pixel box
138 was by default 15%. To make sure of clear sky, the criterion for maximum difference between
139 the *in situ* measured and modeled solar irradiance at sea surface is 20%. Figure 1 shows the
140 geographic locations for the *in situ* and satellite matchups, most of which are located in
141 nearshore regions with water depth shallower than 1000 m. We note that the 5×5 pixel box and
142 the time interval of ± 3 hours are a compromise between the number of matchups and the quality
143 of matchups determined for global waters by SeaBASS. Zibordi et al. (2009) and Mélin et al.
144 (2011) recommended more restricted criteria with a 3×3 pixel box and a time interval of ± 2
145 hours for satellite validations in coastal waters. For the data sets used in this study, we tested the
146 sensitivity of matchups to the different pixel boxes and time intervals but found negligible
147 difference in the uncertainties of the resulted matchups. The criterion of ± 2 h time difference,
148 however, reduced significantly the number of matchups by $< \sim 10\%$. This observation justifies
149 the use of the data filtering criteria of 5×5 pixels and ± 3 hours.

150 SeaWiFS and MODISA $R_{rs}(\lambda)$ data were generated with the *l2gen* package at the NASA
151 Ocean Biology Processing Group (OBPG) during the latest reprocessing (R2018.0). The
152 atmospheric correction was based on the classical scheme of Gordon and Wang (1994) and
153 implemented with an iterative scheme to estimate the aerosol radiance at the NIR bands (Bailey
154 et al., 2010). A total of 80 aerosol distributions were established and used during the processing

155 (Ahmad et al., 2010). The SeaWiFS $R_{rs}(\lambda)$ products have five bands centered at 412, 443, 490,
156 555, and 670 nm, while the MODISA $R_{rs}(\lambda)$ data have approximately the same nominal center
157 wavelengths, including 412, 443, 488, 547, and 667 nm.

158 The VIIRS-SNPP $R_{rs}(\lambda)$ data were processed with the Multi-Sensor Level-1 to Level-2
159 (*MSL12*) ocean color data processing system at the NOAA Center for Satellite Applications and
160 Research (STAR). *MSL12* is based on the NASA SeaWiFS Data Analysis System (SeaDAS)
161 version 4.6 with modifications. Unlike SeaWiFS and MODISA processing, *MSL12* used the
162 aerosol look-up table (LUT) of 12 aerosol models derived from Shettle and Fenn (1979). The
163 VIIRS-SNPP $R_{rs}(\lambda)$ data were generated with the NIR-SWIR atmospheric correction algorithm
164 (Wang, 2007; Wang and Shi, 2007; Wang et al., 2009). In addition, the algorithm of Wang and
165 Jiang (2018) was used to estimate the blue-band $R_{rs}(\lambda)$ wherever $R_{rs}(410)$ is negative. The
166 resultant VIIRS-SNPP $R_{rs}(\lambda)$ data have five wavelengths at 410, 443, 486, 551, and 671 nm; and
167 no negative $R_{rs}(410)$ and $R_{rs}(443)$ values exist.

168 We computed the quality assurance (QA) scores for each of the satellite $R_{rs}(\lambda)$ spectra to
169 quantitatively assess their data quality. The QA model (Wei et al., 2016b) was initially designed
170 with nine visible bands, collectively representing the heritage and operational ocean color
171 sensors. In the present study, we only considered the five “common” spectral bands centered
172 around 412, 443, 488, 551, and 670 nm. As such, all the QA scores are distributed at six discrete
173 levels of 0, 0.2, 0.4, 0.6, 0.8, and 1, with 1 representing the highest quality and 0 the lowest
174 quality. Use of such common bands for the QA derivation facilitates the subsequent comparison
175 of the obtained QA scores among different ocean color sensors. Recognizing the slight difference
176 between three ocean color sensors’ nominal center wavelengths and the five common bands of
177 the QA model, we stress that this difference has a limited impact on the QA results. In Figure 2,

178 we compare the frequency distribution of QA scores for three satellite sensors. According to the
179 comparison, about 50% of satellite $R_{rs}(\lambda)$ data have the highest quality with QA = 1 and 30% of
180 them show relatively good quality with QA = 0.8. The rest 20%, however, are found with lower
181 quality scores (QA \leq 0.6). In subsequent analysis, the satellite $R_{rs}(\lambda)$ data are divided into three
182 subgroups: high-QA (QA \geq 0.8), moderate-QA (0.4 \leq QA \leq 0.6), and low-QA (QA \leq 0.2) data.
183 The moderate- and low-QA data are the focus of our analysis.

184

185 **2.2 Blue-band estimation algorithm**

186 The blue-band estimation (BBE) algorithm consists of three components: a look-up table for
187 the $R_{rs}(\lambda)$ spectral shapes, spectral matching, and spectral estimation. The three components are
188 described in below with details.

189 (1) $R_{rs}(\lambda)$ spectral shapes

190 The $R_{rs}(\lambda)$ spectral shapes are represented by a total of 1768 normalized remote sensing
191 reflectance spectra, $nR_{rs}(\lambda)$. These spectra were derived from hyperspectral $R_{rs}(\lambda)$ spectra (400–
192 700 nm), which were originated from both *in situ* measurements and radiative transfer
193 simulations. A description of the measurements and simulations can be found in Wei et al.
194 (2016b) and Wei et al. (2019), respectively. The $R_{rs}(\lambda)$ spectra are representative of a wide range
195 of waters with Chl varying from ~ 0.02 mg m^{-3} to > 50 mg m^{-3} . The hyperspectral $R_{rs}(\lambda)$ data
196 were sub-sampled into five discrete bands at 412, 443, 488, 551, and 670 nm. The differences in
197 the nominal center wavelengths among three sets of satellite $R_{rs}(\lambda)$ products are suppressed as
198 they are not critical in the present context. The obtained five-band $R_{rs}(\lambda)$ spectra were then
199 normalized by their respective root of the sum of squares (RSS), leading to

200

$$nR_{rs}(\lambda_i) = \frac{R_{rs}(\lambda_i)}{\left[\sum_{j=1}^5 R_{rs}(\lambda_j)^2 \right]^{1/2}}, \quad i = 1, 2, 3, 4 \text{ and } 5 \quad (1)$$

201 where $nR_{rs}(\lambda)$ is dimensionless and the subscripts 1–5 correspond to the five bands from 412 nm
 202 to 670 nm. The $nR_{rs}(\lambda)$ spectra are characteristic of a few unique features. First, the $nR_{rs}(\lambda)$
 203 spectral ratios at any two random bands remain the same with those of the corresponding $R_{rs}(\lambda)$
 204 spectra. Second, the spectral curvature of $nR_{rs}(\lambda)$ remains unchanged in comparison to $R_{rs}(\lambda)$.
 205 Third, the magnitudes of $nR_{rs}(\lambda)$ always vary between 0 and 1. Last, the sum of squares of $nR_{rs}(\lambda)$
 206 at all five bands is equal to 1. In this context, these $nR_{rs}(\lambda)$ spectra describe the spectral shapes
 207 for the corresponding $R_{rs}(\lambda)$ spectra.

208 In Figure 3, we illustrate the range of variation of the spectral values at 41x and 443 nm and
 209 related spectral ratios for the normalized reflectance of the LUT (denoted $nR_{rs}^{lut}(\lambda)$) and those for
 210 the *in situ* data concurrent with satellite overpass. The evaluation data and the LUT exhibit a
 211 very similar pattern of variation, with the latter spanning over a slightly wider range. Most of the
 212 evaluation data have $nR_{rs}(41x)$ and $nR_{rs}(443)$ lower than 0.7 and 0.6, respectively. The
 213 $nR_{rs}(41x)/nR_{rs}(443)$ and $nR_{rs}(443)/nR_{rs}(55x)$ ratios of the evaluation data are confined within a
 214 much narrower domain (0.6–1.1 and 0.2–1.1, respectively) than the LUT. Outliers do exist,
 215 particularly for the SeaWiFS matchup data. Overall, the range of variation of all data sets shown
 216 in Figure 3 is about the same as that of the compiled data in Valente et al. (2016).

217 (2) Spectral matching

218 For a satellite $R_{rs}(\lambda)$ spectrum in question, the first step is to determine a “true” spectral shape
 219 as a reference. For this purpose, we take advantage of the fact that satellite $R_{rs}(48x)$ and $R_{rs}(55x)$
 220 measurements usually have good quality (Antoine et al., 2008; Hlaing et al., 2013; Zibordi et al.,
 221 2009). The $R_{rs}(67x)$ data are sometimes subjected to large uncertainties, but their impact on the

222 model performance is limited; we will discuss this problem in the sensitivity analysis in Section
 223 3.4. As such, the satellite $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ can be used as a basis for further
 224 processing. First, following the spectral angle mapper (SAM) (Kruse et al., 1993), we quantify
 225 the spectral similarity between satellite-derived $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ values and each
 226 of the $nR_{rs}^{lut}(\lambda)$ spectra by the cosine distance

$$227 \quad d = 1 - \frac{\sum_{i=3}^5 [nR_{rs}^{lut}(\lambda_i) \square R_{rs}(\lambda_i)]}{\sqrt{\sum_{i=3}^5 [nR_{rs}^{lut}(\lambda_i)]^2 \sum_{i=3}^5 [R_{rs}(\lambda_i)]^2}} \quad (2)$$

228 where d is the cosine distance between the vectors of $nR_{rs}^{lut}(\lambda)$ and satellite $R_{rs}(\lambda)$ at 48x, 55x,
 229 and 67x nm bands. Second, we search for the minimum d and locate the corresponding $nR_{rs}^{lut}(\lambda)$
 230 spectrum from the LUT. Such selected $nR_{rs}^{lut}(\lambda)$ spectrum is regarded as the spectral shape for the
 231 satellite $R_{rs}(\lambda)$ in question.

232 (3) Spectral estimation

233 According to Eq. (1), the satellite $R_{rs}(41x)$ and $R_{rs}(443)$ in question can be normalized as
 234 below

$$235 \quad \left\{ \begin{array}{l} \frac{R_{rs}(41x)}{\left[R_{rs}(41x)^2 + R_{rs}(443)^2 + R_{rs}(48x)^2 + R_{rs}(55x)^2 + R_{rs}(67x)^2 \right]^{1/2}} = nR_{rs}(41x) \\ \frac{R_{rs}(443)}{\left[R_{rs}(41x)^2 + R_{rs}(443)^2 + R_{rs}(48x)^2 + R_{rs}(55x)^2 + R_{rs}(67x)^2 \right]^{1/2}} = nR_{rs}(443) \end{array} \right. \quad (3)$$

236 where $R_{rs}(41x)$, $R_{rs}(443)$, $nR_{rs}(41x)$, and $nR_{rs}(443)$ are unknown. Since we have determined the
 237 spectral shape through spectral matching, we substitute $nR_{rs}(41x)$ and $nR_{rs}(443)$ in Eq. (3) with
 238 $nR_{rs}^{lut}(412)$ and $nR_{rs}^{lut}(443)$, respectively. As a result, Eq. (3) can be rewritten as

$$\begin{cases}
R_{rs}(41x) = \left[\frac{R_{rs}(48x)^2 + R_{rs}(55x)^2 + R_{rs}(67x)^2}{nR_{rs}^{lut}(488)^2 + nR_{rs}^{lut}(551)^2 + nR_{rs}^{lut}(670)^2} \right]^{1/2} \times nR_{rs}^{lut}(412) \\
R_{rs}(443) = \left[\frac{R_{rs}(48x)^2 + R_{rs}(55x)^2 + R_{rs}(67x)^2}{nR_{rs}^{lut}(488)^2 + nR_{rs}^{lut}(551)^2 + nR_{rs}^{lut}(670)^2} \right]^{1/2} \times nR_{rs}^{lut}(443)
\end{cases} \quad (4)$$

239 where $R_{rs}(41x)$ and $R_{rs}(443)$ are estimated by both satellite $R_{rs}(\lambda)$ data at the three bands of 48x,
240 55x, and 67x nm and $nR_{rs}^{lut}(\lambda)$ data.
241

242

243 2.3 Metrics for uncertainty evaluation

244 The relative difference (ϵ) was computed to assess the uncertainty of satellite products
245 including $R_{rs}(\lambda)$ spectral values at 41x, 443, 48x, 55x, and 67x nm, and the $R_{rs}(\lambda)$ spectral ratios
246 at 41x and 443 nm band, i.e., R_{443}^{41x} , and the ratios at 443 and 55x nm, i.e., R_{55x}^{443} , as

$$\epsilon = \frac{S_1 - S_2}{S_2} \times 100\% \quad , \quad (5)$$

248 where S_1 and S_2 refer to the satellite-derived values and the corresponding *in situ* values,
249 respectively. The median of the relative difference ($\bar{\epsilon}$) or bias was derived as

$$\bar{\epsilon} = median \left\{ \frac{S_1 - S_2}{S_2} \right\} \times 100\% \quad . \quad (6)$$

251 Further, we derived the absolute percentage difference (APD, denoted as $|\bar{\epsilon}|$) as

$$|\bar{\epsilon}| = median \left\{ \left| \frac{S_1 - S_2}{S_2} \right| \right\} \times 100\% \quad . \quad (7)$$

253 The root-mean-square deviation (RMSD) was also computed to assess the accuracy of satellite
254 products, as

$$RMSD = \sqrt{\frac{1}{N} \sum_{i=1}^N (S_{i,1} - S_{i,2})^2} \quad . \quad (8)$$

256 In analogy to $\bar{\epsilon}$, the unbiased relative difference (denoted as $\bar{\phi}$) was calculated as,

$$257 \quad \bar{\phi} = \frac{2}{N} \sum_{i=1}^N \frac{S_{i,1} - S_{i,2}}{S_{i,1} + S_{i,2}} \times 100\% , \quad (9)$$

258 where $S_{i,1}$ and $S_{i,2}$ are the inherent optical properties derived from the satellite $R_{rs}(\lambda)$ data and *in*
259 *situ* $R_{rs}(\lambda)$ matchup data. The unbiased absolute percentage difference (UPD, denoted as $|\bar{\phi}|$) was

$$260 \quad |\bar{\phi}| = \frac{2}{N} \sum_{i=1}^N \left| \frac{S_{i,1} - S_{i,2}}{S_{i,1} + S_{i,2}} \right| \times 100\% . \quad (10)$$

261

262 **2.4 Sensitivity analysis**

263 The sensitivity of $R_{rs}(41x)$ and $R_{rs}(443)$ estimation to the uncertainties of the algorithm input
264 values of $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ was assessed with the IOCCG (2006) synthetic $R_{rs}(\lambda)$
265 data after adding uncertainties to $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$. The hyperspectral $R_{rs}(\lambda)$ data
266 of IOCCG (2006) were first sampled at 412, 443, 488, 551, and 670 nm. The resultant multiband
267 $R_{rs}(\lambda)$ spectra were then clustered based on the cosine distance as quantified by Eq. (2). To
268 simplify, we assumed three classes to represent these spectra (Classes-1, -2, and -3). As shown in
269 Figure 4, each of three classes is characteristic of a distinctive spectral shape, roughly
270 corresponding to blue, blue-green, and green-yellow colors. For Class-1 water, the maximum
271 spectral values are often present in the blue bands, while $R_{rs}(670)$ is usually very small. In terms
272 of the trophic status, Class-1 is found with low Chl of 0.03–0.7 mg m⁻³ (0.14 mg m⁻³ on
273 average). Class-2 water is characteristic of moderate $R_{rs}(412)$ and $R_{rs}(670)$ values, and generally
274 of moderate Chl, ranging from 0.3 to 10.0 mg m⁻³ (1.6 mg m⁻³ on average). Class-3 waters are
275 representative of relatively turbid environments, with high $R_{rs}(670)$ but relatively small $R_{rs}(412)$
276 values, where Chl are high, varying from 1.5 to 30.0 mg m⁻³ (15 mg m⁻³ on average).

277 In the following, the $R_{rs}(\lambda)$ spectra within each of three classes were used to synthesize error-
 278 disturbed reflectance, $\tilde{R}_{rs}(\lambda)$. We investigated a simplified situation where only one of $R_{rs}(488)$,
 279 $R_{rs}(551)$, or $R_{rs}(670)$ values was subjected to uncertainty, while the other two were error-free.
 280 The error-disturbed $\tilde{R}_{rs}(\lambda)$ value was simulated as below

$$281 \quad \tilde{R}_{rs}(\lambda_i) = R_{rs}(\lambda_i) \times (1 + 2\varepsilon \cdot \mathfrak{R}) \quad (11)$$

282 where λ_i refers to 488, 551, or 670 nm, ε is the relative error varying from -50% to 50% (with a
 283 5% step), and \mathfrak{R} is a random value between 0 and 1. For each ε , Eq. (11) was repeated 100 times,
 284 leading to a total of 17300, 13700, and 19000 error-disturbed $\tilde{R}_{rs}(\lambda_i)$ values for Classes-1, -2, and
 285 -3, respectively. From these synthetic reflectance, new $R_{rs}(412)$ and $R_{rs}(443)$ values were
 286 estimated with the BBE algorithm and then compared with known values to quantify their
 287 difference.

288 It is noted that the uncertainty of satellite-derived $R_{rs}(\lambda)$ products remains difficult to
 289 characterize as it is not only spectrally variable but dependent on environmental conditions as
 290 well as instrumental calibration (Antoine et al., 2008; Hu et al., 2013; Wei et al., 2018). To gain
 291 further perspective, we considered four simplistic scenarios with different combinations of
 292 uncertainties simultaneously assigned to $R_{rs}(488)$, $R_{rs}(551)$, and $R_{rs}(670)$. Table 1 lists the
 293 amplitudes of the absolute percentage errors commonly observed in the ocean color satellite
 294 $R_{rs}(\lambda)$ products (Antoine et al., 2008; Hlaing et al., 2013; Zibordi et al., 2009). In addition, we
 295 also considered a particular scenario with zero uncertainty for the purpose of comparison. The
 296 following model was used to create error-disturbed $\tilde{R}_{rs}(\lambda)$ at 488, 551, and 670 nm,

$$297 \quad \tilde{R}_{rs}(488, 551, 670) = R_{rs}(488, 551, 670) \cdot \left[1 + 2(2\mathfrak{R} - 1) \cdot |\bar{\varepsilon}|_{488, 551, 670} \right] \quad (12)$$

298 where $|\bar{\varepsilon}|_{488, 551, 670}$ refers to the absolute percentage errors at 488, 551, and 670 nm in Table 1 and

299 \mathfrak{R} is a random number between 0 and 1. Eq. (12) predicts spectrally coherent uncertainties,
300 where the relative errors share the same positive or negative signs at 488, 551, and 670 nm. As
301 the above, Eq. (12) was repeated 100 times for each $R_{rs}(\lambda)$ spectrum within each water class to
302 generate the corresponding $\tilde{R}_{rs}(\lambda)$ values.

303

304 **3. Results**

305 **3.1 Comparison of satellite and *in situ* $R_{rs}(\lambda)$ matchups**

306 We first assessed the satellite $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ uncertainties based on the
307 satellite and *in situ* matchups as the $R_{rs}(\lambda)$ data quality at these three bands is important for the
308 implementation of the BBE algorithm. Comparisons of three groups of analyses in Table 2
309 indicate that the satellite $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ are prone to increasingly larger
310 uncertainties with the decrease of QA scores, and *vice versa*. For the high-QA satellite data,
311 specifically, $R_{rs}(48x)$ and $R_{rs}(55x)$ only suffer an absolute relative difference of 10%–13% and a
312 negative bias varying between 0% and –10%. Even at the red band of 67x nm, the analyses show
313 a fairly small uncertainty for the reflectance values, with $|\bar{\epsilon}|$ varying between 11% and 22% and $\bar{\epsilon}$
314 between –16% and 2%. In comparison to high-QA data, the moderate-QA group has much fewer
315 data points. Also, $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ measurements in this group are found with
316 increased uncertainties, particularly for $|\bar{\epsilon}|$. The low-QA group only accounts for a very small
317 portion of the satellite measurements used herein. Their $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$
318 measurements are susceptible to almost doubled relative differences (with $|\bar{\epsilon}|$ up to 45%) and
319 biases (with $\bar{\epsilon}$ beyond –44%), in comparison to the high-QA group.

320 Similar to $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$, the uncertainties of satellite $R_{rs}(41x)$ and $R_{rs}(443)$
321 are also found to increase with decreasing QA scores (Table 3). Taking MODISA as an example,

322 the $R_{rs}(412)$ uncertainty increased from $|\bar{\epsilon}| = 27\%$ in high-QA group to $|\bar{\epsilon}| = 51\%$ for moderate-
323 QA group, and finally to $|\bar{\epsilon}| = 89\%$ for low-QA data. It is also noted that many SeaWiFS and
324 MODISA $R_{rs}(412)$ values in these datasets are negative, but it is rare to observe negative
325 $R_{rs}(410)$ values for VIIRS-SNPP due to a recent improvement made by Wang and Jiang (2018).
326 Exclusion of these negative $R_{rs}(41x)$ data from evaluation, however, has resulted in a significant
327 reduction in the total numbers of available matchups for $R_{rs}(41x)$. Particularly for SeaWiFS and
328 MODISA, the numbers of $R_{rs}(412)$ matchups for moderate- and low-QA subgroups are about
329 15%–30% less than $R_{rs}(443)$. The uncertainties of satellite $R_{rs}(41x)$ and $R_{rs}(443)$ are generally
330 greater than the corresponding $R_{rs}(48x)$ and $R_{rs}(55x)$, which is consistent with earlier analyses
331 (Hlaing et al., 2013; Qin et al., 2017; Zibordi et al., 2009). This feature can be partly attributable
332 to the relatively small values of $R_{rs}(41x)$ and $R_{rs}(443)$ in the evaluation data, and partly to the
333 relatively large uncertainty of *in situ* measurements at these two bands in coastal waters (also see
334 Hooker et al., 2002).

335 The correspondence between increasing uncertainties and decreasing QA scores for satellite
336 $R_{rs}(\lambda)$ measurements has several implications. Firstly, it provides a first-hand evidence that the
337 QA scores are a useful measure of the overall data quality for satellite-derived $R_{rs}(\lambda)$ spectra.
338 Secondly, it is important to note that the satellite validation analyses (e.g., Hlaing et al., 2013;
339 Qin et al., 2017; Wei et al., 2018) tend to consider all available matchups as a whole, in which
340 the satellite $R_{rs}(\lambda)$ spectra with different QA scores are mixed. Since the moderate- and low-QA
341 score data often account for a relatively small percentage of the available data (see Figure 2),
342 their relatively larger uncertainties are often suppressed and less likely to dominate the overall
343 uncertainty. The above analyses provided a feasible way to identify specific subgroups of the
344 satellite $R_{rs}(\lambda)$ measurements based on their QA scores.

345

346 **3.2 Estimated $R_{rs}(41x)$ and $R_{rs}(443)$**

347 The evaluation results for BBE-estimated $R_{rs}(41x)$ and $R_{rs}(443)$ are also included in Table 3
348 for direct comparison with the original satellite products. Notably, all those initially negative
349 $R_{rs}(41x)$ and $R_{rs}(443)$ values for SeaWiFS and MODISA are now restored to positive values,
350 leading to a significant increase in the total number of utilizable $R_{rs}(41x)$ and $R_{rs}(443)$ data. The
351 larger numbers of positive $R_{rs}(41x)$ values could enhance the effectiveness of subsequent bio-
352 optical retrievals as many semi-analytical inversion algorithms (Carder et al., 1999; Lee et al.,
353 2002; Wei and Lee, 2015; Werdell et al., 2013) require $R_{rs}(410)$ or $R_{rs}(412)$ as input to separate
354 phytoplankton and CDOM, which will be discussed later in Section 4. Partly because of the
355 change of the number of observations, however, the BBE-estimated $R_{rs}(412)$ for SeaWiFS did
356 not show a reduction in its uncertainties, rather experienced some degree of increase in $|\bar{\epsilon}|$, from
357 22% to 36% for the moderate-QA group. In comparison to MODISA, the estimated $R_{rs}(412)$ data
358 exhibited a slight increase in the biases ($\bar{\epsilon}$ increased from -6% to -8% for moderate-QA group);
359 this is to a large degree a result of the large biases associated with $R_{rs}(488)$, $R_{rs}(547)$, and
360 $R_{rs}(667)$ (Table 2). On the other hand, without much change to the total number of the VIIRS-
361 SNPP observations, the estimated $R_{rs}(410)$ and $R_{rs}(443)$ data show much reduced uncertainties
362 for both moderate- and low-QA groups. Overall, very limited improvements were found for the
363 high-QA data of three satellites. This phenomenon may be further explained from the following
364 two perspectives. First, the high QA scores imply that the R_{rs} spectra are already of high quality.
365 Estimations with the BBE algorithm may thus be superfluous for high-QA data. Second, part of
366 the normalized remote sensing reflectance spectra within the LUT are also used by the QA
367 model (Wei et al., 2016b); it is technically difficult to further improve the spectral shapes of

368 satellite $R_{rs}(\lambda)$ data by the BBE algorithm. As a matter of fact, as indicated in Table 3, the
369 original high-QA satellite data appear most accurate. They will less likely benefit from an
370 estimation scheme as developed here.

371 To further highlight the model performance, we contrasted the satellite $R_{rs}(41x)$ and $R_{rs}(443)$
372 with *in situ* matchups for the moderate-QA group of data in scatterplots (Figure 5), with the
373 BBE-estimated $R_{rs}(41x)$ and $R_{rs}(443)$ overlaid for comparison. Note that these illustrations have
374 included all available matchup data in this subgroup, including positive and negative values. As
375 shown in the plots, many SeaWiFS and MODISA $R_{rs}(412)$ values are negative, and even some of
376 the corresponding $R_{rs}(443)$ data are negative as well. Unlike SeaWiFS and MODISA, the BBE
377 estimates of $R_{rs}(412)$ and $R_{rs}(443)$ are all physically meaningful values. The estimated $R_{rs}(412)$
378 and $R_{rs}(443)$ are distributed much more tightly around the 1:1 line than the original satellite data
379 (for SeaWiFS, MODISA, and VIIRS-SNPP). As a result, the linear regression slopes for the
380 BBE estimates and the *in situ* matchups are generally much closer to unity.

381

382 **3.3 $R_{rs}(\lambda)$ spectral ratios**

383 Since the BBE algorithm is based on the knowledge of the $R_{rs}(\lambda)$ spectral shapes, it is
384 expected that such estimated $R_{rs}(41x)$ and $R_{rs}(443)$ should yield improvement on the $R_{rs}(\lambda)$
385 spectral ratios. We derived the ratios of $R_{rs}(443)$ to $R_{rs}(55x)$ and $R_{rs}(41x)$ to $R_{rs}(443)$ and
386 compared them with those of *in situ* matchup data in Table 4. Among three subgroups of data,
387 very limited differences are observed in R_{443}^{41x} and R_{55x}^{443} for the high-QA group, which is consistent
388 with the analyses of $R_{rs}(41x)$ and $R_{rs}(443)$ uncertainties in Table 3. For the moderate-QA data,
389 the presence of many negative $R_{rs}(41x)$ and $R_{rs}(443)$ data have resulted in either negative R_{443}^{412} or
390 sometimes positive outliers and some negative R_{55x}^{443} values (see scatterplots in Figure 6). The

391 BBE algorithm improved both R_{443}^{41x} and R_{55x}^{443} with overall reduced uncertainties and significantly
392 increased the number of utilizable data (by as much as ~20% for the moderate-QA data). The
393 improvement in the spectral band ratios, along with estimated spectral values, is important for
394 bio-optical inversion, in that they are indispensable for many empirical ocean color algorithms
395 (Morel and Gentili, 2009; O'Reilly et al., 1998) and semi-analytical algorithms (IOCCG, 2006;
396 Werdell et al., 2018). We will discuss the potential impact on bio-optical retrievals in Section
397 4.3.

398

399 **3.4 Sensitivity of $R_{rs}(41x)$ and $R_{rs}(443)$ estimation**

400 The sensitivity of $R_{rs}(41x)$ and $R_{rs}(443)$ estimation to the input $R_{rs}(\lambda)$ values at 48x, 55x, or
401 67x nm is illustrated in Figure 7. Several important conclusions can be readily reached from the
402 comparisons. First, the minimum uncertainty of estimated $R_{rs}(41x)$ and $R_{rs}(443)$ ($|\bar{\epsilon}| \approx 15\%$) is
403 observable with error-free input $R_{rs}(\lambda)$ data for all classes of waters, which can be considered as
404 the inherent uncertainty for the BBE algorithm. Second, it is found that the estimations for
405 $R_{rs}(41x)$ and $R_{rs}(443)$ are most sensitive to the uncertainty of $R_{rs}(48x)$. For instance, when
406 $R_{rs}(48x)$ has $\epsilon = 30\%$, the BBE-estimated $R_{rs}(41x)$ can be subjected to an uncertainty as large as
407 $|\bar{\epsilon}| = 50\%–60\%$ over three classes of waters. The uncertainty of input $R_{rs}(55x)$ plays a secondary
408 role; according to our analysis, an error of $\epsilon = 30\%$ with $R_{rs}(55x)$ will result in a smaller
409 uncertainty for $R_{rs}(41x)$, with $|\bar{\epsilon}|$ less than 35%. In contrast, the uncertainty of $R_{rs}(67x)$ appears to
410 be the least important element to influence the $R_{rs}(41x)$ and $R_{rs}(443)$ uncertainties.

411 The above-revealed differential dependency of the algorithm uncertainty on specific
412 wavelengths can be explained by the uncertainty propagation of the BBE algorithm. In Eq. (13),
413 the uncertainty of $R_{rs}(41x)$ is expressed as a function of the input $R_{rs}(\lambda)$ and $nR_{rs}^{lut}(\lambda)$ values and

414 the associated uncertainty at a specific band λ_j (48x, 55x, or 67x nm), following the principle of
 415 uncertainty propagation,

$$\begin{aligned}
 u(41x) = & \frac{1}{\sqrt{R_{rs}(48x)^2 + R_{rs}(55x)^2 + R_{rs}(67x)^2}} \cdot R_{rs}(\lambda_j) \cdot u(\lambda_j) \\
 & \cdot \frac{nR_{rs}^{lut}(412)}{\sqrt{nR_{rs}^{lut}(488)^2 + nR_{rs}^{lut}(551)^2 + nR_{rs}^{lut}(670)^2}}
 \end{aligned} \tag{13}$$

417 In Eq. (13), we assumed zero uncertainty for $nR_{rs}^{lut}(\lambda)$ and uncorrelated input quantities. As the
 418 two fractional terms in Eq. (13) are certain for a given satellite reflectance spectrum, $u(41x)$ is
 419 sensitive to the input value for $R_{rs}(\lambda_j)$ and associated uncertainty $u(\lambda_j)$. Recalling Figure 4,
 420 $R_{rs}(67x)$ are usually smaller than $R_{rs}(48x)$ and/or $R_{rs}(55x)$ in the test data, the uncertainty
 421 propagation of the $R_{rs}(67x)$ uncertainty to the total uncertainty is thus relatively less critical. In
 422 extremely turbid waters, the $R_{rs}(67x)$ values can be very large; but the corresponding
 423 uncertainties tend to be small. For Class-1 waters, $R_{rs}(48x)$ are almost always higher than
 424 $R_{rs}(55x)$, thus playing a dominant role in the resulted $R_{rs}(41x)$ and $R_{rs}(443)$. For Class-2 waters,
 425 there are some instances where $R_{rs}(55x)$ are comparable to or even higher than $R_{rs}(48x)$; under
 426 these situations, $R_{rs}(55x)$ may play a more important role (e.g., Figure 7c). Based on this
 427 analysis, the BBE algorithm may be applicable to a wide range of environments.

428 According to the five combinations of uncertainties (Table 1), the increase of the uncertainties
 429 in input $R_{rs}(\lambda)$ leads to increased uncertainties in estimated $R_{rs}(41x)$ and $R_{rs}(443)$ (Table 5). In
 430 particular, the absolute percentage differences for $R_{rs}(41x)$ herein experienced a huge jump, from
 431 9% to 56%. But, recall that the $|\bar{\epsilon}|$ for moderate-QA satellite $R_{rs}(48x)$ and $R_{rs}(55x)$ data are
 432 generally between 12% and 23% (Table 2). That is to say, the simulation No. 3 best describes the
 433 realistic situations, in which the $|\bar{\epsilon}|$ for estimated $R_{rs}(41x)$ varies between 25% and 37%, a range
 434 close to the evaluation results in Table 3. Besides, our analyses indicate a weak dependency of

435 $R_{rs}(41x)$ uncertainty on the class of water. The BBE algorithm tends to bias the estimation of
 436 $R_{rs}(41x)$ and $R_{rs}(443)$ for Class-3, for which the $nR_{rs}(41x)$ and $nR_{rs}(443)$ values are often
 437 relatively smaller (recall Figure 4).

438

439 **4. Discussion**

440 **4.1 Why the algorithm works**

441 The BBE algorithm infers the $R_{rs}(\lambda)$ spectral shapes through a spectral matching procedure
 442 using initial satellite $R_{rs}(\lambda)$ values measured at 48x, 55x, and 67x nm and subsequently estimates
 443 $R_{rs}(41x)$ and $R_{rs}(443)$. It is based on an implicit assumption that the normalized satellite $R_{rs}(\lambda)$
 444 values at 41x and 443 nm are approximately equal to those selected from the LUT after the
 445 spectral matching. According to the validation results, this assumption is reliable for the
 446 estimation of $R_{rs}(\lambda)$ at blue bands. The algorithm's success benefits from the following two facts.
 447 First, the $R_{rs}(48x)$ and $R_{rs}(55x)$ values generated from satellites are relatively accurate (Table 2)
 448 (also see Antoine et al., 2008; Hlaing et al., 2013; Qin et al., 2017; Zibordi et al., 2009). Second,
 449 the algorithm remains least sensitive to $R_{rs}(67x)$ for most waters (Figure 7). These factors favor
 450 and facilitate the optimal performance of the BBE algorithm.

451 The light absorption and scattering properties of optically active constituents determine the
 452 $R_{rs}(\lambda)$ spectra, simplified as the following (Gordon et al., 1988),

$$453 \quad R_{rs}(\lambda) \propto \frac{b_{bp}(\lambda) + b_{bw}(\lambda)}{a_{ph}(\lambda) + a_{dg}(\lambda) + a_w(\lambda) + b_{bp}(\lambda) + b_{bw}(\lambda)} \quad (14)$$

454 where $b_{bp}(\lambda)$ and $b_{bw}(\lambda)$ are the scattering coefficients due to particulates and pure seawater,
 455 respectively; $a_{ph}(\lambda)$, $a_{dg}(\lambda)$ and $a_w(\lambda)$ refer to the absorption coefficients of phytoplankton,
 456 colored detrital material (including CDOM and detritus), and pure seawater, respectively; and,

457 $a_w(\lambda)$ and $b_{bw}(\lambda)$ are often taken as wavelength-specific constants (Lee et al., 2015b; Mason et al.,
458 2016; Zhang and Hu, 2009). Among all these inherent optical properties (IOPs), the $b_{bp}(\lambda)$
459 spectrum is monotonous under most circumstances and can be described by a power-law
460 function. Thus, the spectral variability of $R_{rs}(\lambda)$ is mostly dominated by light absorption spectra.
461 The light absorption of phytoplankton is contributed by various pigments (Bricaud et al., 1995;
462 Bricaud et al., 2004). In the visible domain, $a_{ph}(\lambda)$ values are spectrally interdependent (Bricaud
463 et al., 1998; Lee et al., 1998; Sathyendranath et al., 1987). Further, the light absorption of colored
464 detrital material is also spectrally dependent and can be simplified by an exponential decay
465 model. Given the spectral dependency of IOPs, $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ values are as a
466 matter of fact interconnected with $R_{rs}(41x)$ and $R_{rs}(443)$. This is the basis on which $R_{rs}(41x)$ and
467 $R_{rs}(443)$ can be estimated from Eq. (14). The accuracy of model estimation will primarily depend
468 on the degree of our understanding of the IOPs and the IOP- R_{rs} relationships.

469

470 **4.2 Algorithm limitations**

471 We reiterate that the BBE algorithm is by no means intended to replace the measurements of
472 $R_{rs}(41x)$ and $R_{rs}(443)$ from satellite ocean color sensors. Rather, it provides a workaround to
473 estimate $R_{rs}(41x)$ and $R_{rs}(443)$ when the satellite-derived $R_{rs}(\lambda)$ spectra are highly questionable
474 and are almost useless in blue bands. Like other remote sensing algorithms, the BBE algorithm is
475 subject to uncertainties and limitations. Fully understanding the estimation uncertainty will
476 require advanced statistical methodologies (Jay et al., 2018; Wang et al., 2005) and knowledge of
477 the satellite $R_{rs}(\lambda)$ uncertainty in various waters (e.g., Hu et al., 2013). According to our
478 preliminary analyses, the error propagation from $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ can be a
479 primary source of uncertainty for model-estimated $R_{rs}(41x)$ and $R_{rs}(443)$. Besides, a few other

480 contributing factors merit further discussion. First, the proposed spectral matching procedure
481 uses the reflectance at three base wavelengths of 48x, 55x, and 67x nm. The use of a subset of
482 wavelengths for water optical classification may introduce uncertainties, which further propagate
483 to the estimation of the $R_{rs}(\lambda)$ spectral shapes, and finally to the estimated $R_{rs}(41x)$ and $R_{rs}(443)$.
484 The results in Figure 7 and Table 5 are based upon the IOCCG (2006) data, which are well
485 represented by the LUT. The uncertainties ($|\bar{\epsilon}| \leq 13\%$, $-10\% \leq \epsilon \leq 1\%$, and $0.0004 < \text{RMSD} <$
486 0.002 sr^{-1}) derived with error-free $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ are basically equivalent to the
487 algorithm residual uncertainties originated from the use of three-band reflectance. Second, it is
488 difficult (if not impossible) for the LUT to characterize all $R_{rs}(\lambda)$ spectral shapes occurring in
489 natural waters. In spite of the satisfactory validation results presented herein, there might exist
490 peculiar waters not represented by the current LUT. Thus, it is necessary to continue to enrich
491 the LUT towards a universal application. Third, the $R_{rs}(\lambda)$ spectrum is determined by the water
492 IOPs including the spectral slope (S_{dg}) for $a_{dg}(\lambda)$. Variation of S_{dg} alone can cause substantial
493 variability for $R_{rs}(\lambda)$ in short blue bands (Wei et al., 2016a), in which case the estimation of
494 $R_{rs}(41x)$ and $R_{rs}(443)$ will suffer from uncertainty. Lastly, the BBE algorithm has simplified the
495 spectral settings to five common bands (412, 443, 488, 551, and 670 nm), which ignored the
496 discrepancy of center wavelengths among SeaWiFS, MODISA, and VIIRS-SNPP. Based on
497 IOCCG (2006) data, we evaluated the potential impact on $R_{rs}(\lambda)$ values due to this ignorance.
498 Comparing with the common bands, the $R_{rs}(41x)$, $R_{rs}(48x)$, $R_{rs}(55x)$, and $R_{rs}(67x)$ are subject to
499 relatively small differences, with $|\bar{\epsilon}| = 1.1\%$, 1.7% , 4% , and 3.6% , respectively. These
500 uncertainties are much smaller than the inherent uncertainties of the BBE algorithm and/or those
501 from measurements, thus not important in this context. Although IOCCG synthetic data are not
502 inclusive of every types of waters in nature, the uncertainty analysis based on them should

503 provide a representative assessment. The algorithm uncertainty can be further explored when the
504 uncertainty of satellite-derived $R_{rs}(\lambda)$ spectra is better known.

505

506 **4.3 Potential improvement on bio-optical retrievals**

507 The primary purpose of maintaining high-quality satellite $R_{rs}(\lambda)$ measurements is to provide
508 the aquatic science community with reliable bio-optical retrievals. To demonstrate the
509 contributions of the algorithm, we derived $a_{ph}(443)$ and $a_{dg}(443)$ from the original satellite $R_{rs}(\lambda)$
510 data, estimated $R_{rs}(\lambda)$ data at blue bands, and *in situ* $R_{rs}(\lambda)$ matchups, using the quasi-analytical
511 algorithm (QAA) (Lee et al., 2002). According to the results of uncertainty analysis (Table 6),
512 the implementation of the BBE algorithm has exerted negligible impacts on the $a_{ph}(443)$ and
513 $a_{dg}(443)$ retrievals for the high-QA satellite data. This is consistent with the observation in
514 Section 3 in which the BBE algorithm was shown unable to make substantial improvements to
515 $R_{rs}(41x)$ and $R_{rs}(443)$ for the high-QA satellite data (Table 3). For the moderate-QA data, the
516 retrievals of $a_{dg}(443)$ from BBE-estimated R_{rs} spectra are much more accurate than those from
517 the original satellite $R_{rs}(\lambda)$ data (except for SeaWiFS), with much reduced $|\bar{\Phi}|$, $\bar{\Phi}$, and RMSD.
518 Also inspiringly, the total number of valid $a_{ph}(443)$ and $a_{dg}(443)$ retrievals from SeaWiFS and
519 MODISA are increased by as much as 15%–30%. This improvement is significant as accurate,
520 and potentially more representative, data points will be accounted for in relevant ocean color
521 applications. Similar increases in the number of bio-optical products and decreases in $a_{dg}(443)$
522 uncertainty are also found in the low-QA SeaWiFS and MODISA data. In contrast, no significant
523 change in the total numbers of $a_{ph}(443)$ and $a_{dg}(443)$ retrievals are observed for VIIRS-SNPP,
524 mostly because VIIRS-SNPP has nearly no negative $R_{rs}(410)$ or $R_{rs}(443)$ values (see Figure 5
525 and Figure 6).

526

527 **4.4 Condition of applicability**

528 It is important to understand the condition of applicability under which the BBE algorithm
529 can be best used to estimate $R_{rs}(41x)$ and $R_{rs}(443)$. The quality flagging system is the quality-
530 control measure adopted by space agencies like NASA and NOAA to generate scientific quality
531 data (Bailey and Werdell, 2006; Mikelsons et al., 2020). In practice, the often-used filtering flags
532 include land, cloud, stray light, high glint, low radiance at 55x nm, high TOA radiance, and
533 atmospheric correction failure, etc. The pixels passing the flag check will be regarded as good
534 quality and included in the higher-level products. The satellite $R_{rs}(\lambda)$ data used for our analyses
535 have been checked for valid quality flags also. The QA scoring system (Wei et al., 2016b) is a
536 quantitative measure for the quality of each $R_{rs}(\lambda)$ spectrum, which can further help to identify
537 questionable data. The present study has considered both the flags and the QA scores. According
538 to Figure 2, about 20% of the satellite data available for validation analysis, which have passed
539 the quality flag filtering, are found to have moderate- or low-QA scores ($QA \leq 0.6$). This portion
540 of satellite $R_{rs}(\lambda)$ spectra is characteristic of high uncertainties and can be further improved by
541 the BBE algorithm. In Figure 8, we illustrate the percentage of moderate- and low-QA satellite
542 $R_{rs}(\lambda)$ in the U.S. coastal and inland waters. Within each plot, the pixels have passed the quality
543 flag filtering. Obviously, the “correctable” satellite $R_{rs}(\lambda)$ products are mostly found in the
544 nearshore waters, where the atmospheric conditions and water optical properties are most likely
545 complex. Despite the positive results (Table 3 and Table 4), it is without doubt that estimating
546 $R_{rs}(41x)$ and $R_{rs}(443)$ with the BBE algorithm in such complex waters can sometimes be
547 challenging, especially when the LUT does not sufficiently characterize the complex water
548 optical variations. There is a continuous need for accumulation and inclusion of representative *in*
549 *situ* $R_{rs}(\lambda)$ spectra in the LUT.

550

551 **4.5 Satellite ocean color image processing**

552 The coastal waters are typical of high absorption and scattering properties, with non-
553 negligible water-leaving radiance at the NIR bands (Siegel et al., 2000; Wang and Shi, 2005).
554 Close to sources of air pollutions, the types of aerosols are complex and more difficult to predict
555 (IOCCG, 2010). The oceanic and atmospheric conditions together render a very critical situation
556 for atmospheric correction. Here, we used an imagery of the northern Gulf of Mexico captured
557 by VIIRS-SNPP to demonstrate the BBE algorithm performance. As shown in Figure 9a, the
558 original image was processed with the latest *MSL12* ocean color data processing system, which
559 incorporated the Wang and Jiang (2018) algorithm. It is shown that the $R_{rs}(410)$ values are
560 extremely low in the northern shelf waters, many of which are infinitesimally close to zero.
561 According to the quality flags, there possibly existed strongly absorbing aerosols over a great
562 number of pixels in these waters (highlighted by the dashed line in Figure 9a). To implement the
563 BBE algorithm, all the pixels were first subjected to the quality check for land, cloud, stray light,
564 high glint, and high TOA, etc. Then, the moderate- and low-QA pixels were identified and
565 finally $R_{rs}(410)$ and $R_{rs}(443)$ were estimated with the proposed algorithm. The new $R_{rs}(410)$
566 image is presented in Figure 9b, which includes the model-estimated $R_{rs}(410)$ values at low- and
567 moderate-QA pixels and the original values at high-QA pixels. It is obvious that the close-to-
568 zero pixels are rectified to much larger values; some originally higher $R_{rs}(410)$ values are
569 decreased. As a result, the estimated $R_{rs}(410)$ image over the Mississippi Delta waters has shown
570 characteristics of spatial pattern with realistic gradients and amplitudes.

571

572 **5. Conclusions**

573 Accurate retrieval of remote sensing reflectance in the two short blue bands of 41x nm and
574 443 nm in coastal and inland waters from ocean color satellites has been a challenge because of
575 the complex oceanic and atmospheric properties. Whereas great effort has been put in, a
576 considerable proportion of satellite reflectance products are still found susceptible to large
577 uncertainties. In this study, we developed a spectral shape based algorithm to estimate $R_{rs}(41x)$
578 and $R_{rs}(443)$. The algorithm uses a spectral-matching procedure to determine the spectral shapes
579 for the satellite $R_{rs}(\lambda)$ spectra in question based on the initial satellite $R_{rs}(\lambda)$ measurements at the
580 three wavelengths of 48x, 55x, and 67x. This is a novel attempt to complement and enhance the
581 existing efforts for atmospheric correction. Evaluation with satellite (SeaWiFS, MODISA, and
582 VIIRS-SNPP) and *in situ* $R_{rs}(\lambda)$ matchups in global oceans, with most of the data located within
583 coastal waters, shows that the estimated $R_{rs}(41x)$ and $R_{rs}(443)$ have much-reduced uncertainties
584 with respect to the initial satellite data. It can be expected that such estimated $R_{rs}(41x)$ and
585 $R_{rs}(443)$ data will enhance the quality of bio-optical retrievals for the absorption coefficients of
586 phytoplankton and CDOM and detritus, and increase the quantities of utilizable bio-optical
587 products. Despite the inherent uncertainty (~10%), the algorithm is shown to be applicable to a
588 wide range of waters. Recognizing that the current algorithm cannot characterize every spectral
589 shapes in nature, we stress the necessity to further enrich the data pool included in the LUT.

590

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602 or U.S. Government position, policy, or decision.

603 The evaluation data used in this study are available upon request. Matlab scripts are provided
604 to facilitate further assessment ([https://github.com/Ocean-Color-Remote-Sensing-
605 Algorithm/BBE/blob/master/blue_band_estimation.m](https://github.com/Ocean-Color-Remote-Sensing-Algorithm/BBE/blob/master/blue_band_estimation.m) and [https://github.com/Ocean-Color-
606 Remote-Sensing-Algorithm/BBE/blob/master/QAscores_5Bands.m](https://github.com/Ocean-Color-Remote-Sensing-Algorithm/BBE/blob/master/QAscores_5Bands.m)).

607

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List of Figure Captions

799 Figure 1. Satellite matchup stations for SeaWiFS (denoted by open circles “○”), MODISA
800 (denoted by crosses “+”), and VIIRS-SNPP (denoted by open diamonds “◇”) in the global
801 oceans. The background image refers to the annual chlorophyll-a concentration for 2010 derived
802 from SeaWiFS.

803 Figure 2. Frequency distribution of the QA scores for SeaWiFS, MODISA, and VIIRS-SNPP
804 $R_{rs}(\lambda)$ data. The QA scores are calculated based on the five “common” bands of 41x, 443, 48x,
805 55x, and 67x nm.

806 Figure 3. Ranges of $nR_{rs}(\lambda)$ values used in different data sets. Note that the in situ matchup data
807 are used to describe the variability of corresponding satellite missions in order to avoid the
808 negative $nR_{rs}(41x)$ values.

809 Figure 4. Normalized remote sensing reflectance spectra representative of three distinctive
810 optical water classes based on the IOCCG (2006) $R_{rs}(\lambda)$ data at 412, 443, 488, 551, and 670 nm.
811 The shaded areas describe the range of variation of the spectral values of $nR_{rs}(\lambda)$.

812 Figure 5. Comparison of moderate-QA (0.4 \leq QA \leq 0.6) $R_{rs}(\lambda)$ data and in situ
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815 also plotted for two data sets. Note that the scatterplots have included all available data points,
816 positive and negative.

817 Figure 6. Comparison of moderate-QA (0.4 \leq QA \leq 0.6) satellite $R_{rs}(\lambda)$ spectral ratios with in
818 situ matchups. The symbols of red and blue denote the available data points, positive and negative. the
819 implementation of the BBE algorithm. Linear regression results are also plotted for two data sets.
820 Note that the scatterplots have included all available data points, positive and negative.

821 Figure 7. Uncertainty of estimated $R_{rs}(412)$ and $R_{rs}(443)$ induced by erroneous $R_{rs}(\lambda)$ at 488,
822 551, or 670 nm bands. The first, second, and third rows refer to Class 1, Class 2, and Class 3
823 waters, respectively, corresponding to Figure 4.

824 Figure 8. Percentage of moderate-QA and low-QA satellite data in (a) the U.S. west coasts (b)
825 the U.S. east coasts. The two highlighted areas are (c) the Vancouver Island and (d)
826 Massachusetts Bay and the Gulf of Maine. The percentage data shown here are derived from the
827 MODISA Level 3 mapped (9 km) daily remote sensing reflectance products in 2003, with the
828 QA scores computed based on the $R_{rs}(\lambda)$ at five bands (412, 443, 488, 547, and 667 nm).

829 Figure 9. (a) VIIRS-SNPP $R_{rs}(410)$ image in the northern Gulf of Mexico (Image id:
830 V2016048190213_NPP_SCINIR_L2). (b) The same image but with estimated $R_{rs}(410)$ for
831 moderate- and low-QA pixels. White pixels indicate the failure of quality checks for land, cloud,

832 stray light, high glint, and/or high TOA, etc. The dashed line in (a) indicates where the strongly
833 absorbing aerosols occur, and the negative $R_{rs}(410)$ values are likely to present, according to the
834 quality flags.

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836 Table 1. Synthesized combinations of absolute percentage errors $|\bar{\epsilon}|$ for $R_{rs}(488)$,
837 $R_{rs}(551)$, and $R_{rs}(670)$ data for uncertainty analysis.

	Class 1 (N = 173)			Class 2 (N = 137)			Class 3 (N = 190)		
	$R_{rs}(488)$	$R_{rs}(551)$	$R_{rs}(670)$	$R_{rs}(488)$	$R_{rs}(551)$	$R_{rs}(670)$	$R_{rs}(488)$	$R_{rs}(551)$	$R_{rs}(670)$
1	0	0	0	0	0	0	0	0	0
2	5%	5%	20%	15%	10%	20%	15%	10%	15%
3	10%	15%	30%	20%	15%	30%	20%	15%	20%
4	20%	20%	45%	25%	20%	35%	25%	20%	25%
5	30%	20%	60%	30%	20%	40%	30%	25%	30%

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839 * The chlorophyll-a concentration (\pm standard deviation) for each water class is as below: Class 1, Chl =
840 $0.14 (\pm 0.13) \text{ mg m}^{-3}$; Class 2, Chl = $1.6 (\pm 1.8) \text{ mg m}^{-3}$; Class 3, Chl = $15 (\pm 9) \text{ mg m}^{-3}$.

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844 Table 2. Uncertainties of satellite $R_{rs}(\lambda)$ values at three wavelengths (48x, 55x,
 845 and 67x nm) generated from SeaWiFS, MODISA, and VIIRS-SNPP in the global
 846 waters. The uncertainties are calculated based upon the satellite and *in situ*
 847 matchups. The data are divided into three subgroups according to the QA scores
 848 of the satellite $R_{rs}(\lambda)$ spectra. Negative values are excluded from analysis.

		SeaWiFS			MODISA			VIIRS-SNPP		
		$R_{rs}(490)$	$R_{rs}(555)$	$R_{rs}(670)$	$R_{rs}(488)$	$R_{rs}(547)$	$R_{rs}(667)$	$R_{rs}(486)$	$R_{rs}(551)$	$R_{rs}(671)$
QA \leq 0.2	$ \bar{\epsilon} $	46%	23%	21%	40%	22%	28%	34%	27%	48%
	$\bar{\epsilon}$	-45%	-23%	-19%	-37%	-21%	-26%	-19%	-17%	-24%
	RMSD ¹	0.0011	0.0006	0.0002	0.0007	0.0006	0.0002	0.0009	0.0005	0.0002
	N *	92	95	81	101	101	91	24	24	22
0.4 \leq QA \leq 0.6	$ \bar{\epsilon} $	18%	15%	11%	24%	16%	37%	18%	11%	23%
	$\bar{\epsilon}$	-10%	-7%	0%	-20%	-15%	-31%	-5%	-5%	-1%
	RMSD	0.0006	0.0004	0.0000	0.0007	0.0005	0.0002	0.0004	0.0003	0.0002
	N	359	359	321	576	576	515	239	239	236
QA \geq 0.8	$ \bar{\epsilon} $	10%	11%	11%	13%	11%	22%	13%	11%	20%
	$\bar{\epsilon}$	0%	-4%	0%	-10%	-9%	-16%	-10%	-9%	2%
	RMSD	0.0004	0.0004	0.0001	0.0005	0.0005	0.0002	0.0006	0.0005	0.0002
	N	2055	2055	1999	2932	2932	2866	2148	2148	2134

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850 ¹ RMSD is given in absolute units of sr⁻¹.

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Table 3. Uncertainties of satellite $R_{rs}(\lambda)$ values at two blue bands (41x and 443 nm) generated from SeaWiFS, MODISA, and VIIRS-SNPP in the global waters. The uncertainties are calculated based upon the satellite and *in situ* matchups. The data are divided into three subgroups according to the QA scores of the satellite $R_{rs}(\lambda)$ spectra. Negative values are excluded from analysis.

Original data							
		SeaWiFS		MODISA		VIIRS-SNPP	
		$R_{rs}(412)$	$R_{rs}(443)$	$R_{rs}(412)$	$R_{rs}(443)$	$R_{rs}(410)$	$R_{rs}(443)$
QA ≤ 0.2	$ \bar{\epsilon} $	82%	71%	89%	62%	80%	32%
	$\bar{\epsilon}$	-52%	-64%	10%	-52%	42%	11%
	RMSD	0.0024	0.0017	0.0018	0.0007	0.0016	0.0008
	N	29	61	35	75	23	23
0.4 ≤ QA ≤ 0.6	$ \bar{\epsilon} $	22%	31%	51%	38%	83%	38%
	$\bar{\epsilon}$	0%	-14%	-8%	-11%	36%	20%
	RMSD	0.0009	0.0008	0.0010	0.0007	0.0013	0.0007
	N	279	346	450	561	235	239
QA ≥ 0.8	$ \bar{\epsilon} $	17%	18%	27%	17%	28%	19%
	$\bar{\epsilon}$	0%	4%	3%	3%	7%	5%
	RMSD	0.0007	0.0007	0.0006	0.0005	0.0008	0.0006
	N	2049	2055	2913	2932	2148	2148
BBE-estimated data							
		SeaWiFS		MODISA		VIIRS-SNPP	
		$R_{rs}(412)$	$R_{rs}(443)$	$R_{rs}(412)$	$R_{rs}(443)$	$R_{rs}(410)$	$R_{rs}(443)$
QA ≤ 0.2	$ \bar{\epsilon} $	59%	39%	51%	36%	52%	42%
	$\bar{\epsilon}$	30%	-17%	-3%	-17%	21%	4%
	RMSD	0.0008	0.0006	0.0004	0.0004	0.0012	0.0009
	N	95	95	101	101	24	24
0.4 ≤ QA ≤ 0.6	$ \bar{\epsilon} $	36%	23%	39%	30%	41%	28%
	$\bar{\epsilon}$	8%	-4%	-6%	-13%	18%	10%
	RMSD	0.0009	0.0007	0.0006	0.0005	0.0006	0.0005
	N	359	359	576	576	239	239
QA ≥ 0.8	$ \bar{\epsilon} $	22%	17%	28%	18%	27%	19%
	$\bar{\epsilon}$	-1%	-2%	0%	-2%	1%	0%
	RMSD	0.0009	0.0007	0.0006	0.0005	0.0007	0.0005
	N	2055	2055	2932	2932	2148	2148

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Table 4. Uncertainties of satellite retrieved $R_{rs}(\lambda)$ spectral ratios, R_{443}^{41x} and R_{55x}^{443} , for SeaWiFS, MODISA, and VIIRS-SNPP in the global waters. The uncertainties are calculated based upon the satellite and *in situ* matchups. The data are divided into three subgroups according to the QA scores of the satellite $R_{rs}(\lambda)$ spectra. Negative values are excluded from analysis.

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		With original $R_{rs}(41x)$ and $R_{rs}(443)$ data					
		SeaWiFS		MODISA		VIIRS-SNPP	
		R_{555}^{443}	R_{443}^{412}	R_{547}^{443}	R_{443}^{412}	R_{551}^{443}	R_{443}^{410}
QA \leq 0.2	$ \bar{\epsilon} $	62%	60%	53%	58%	44%	39%
	$\bar{\epsilon}$	-52%	-32%	-38%	34%	44%	33%
	RMSD	0.4495	0.4718	0.2224	0.5126	0.4925	0.4135
	N	61	29	75	35	23	23
0.4 \leq QA \leq 0.6	$ \bar{\epsilon} $	24%	16%	36%	25%	37%	43%
	$\bar{\epsilon}$	-4%	-3%	3%	-7%	30%	10%
	RMSD	0.2452	0.1455	0.1982	0.2159	0.2358	0.3329
	N	346	279	561	450	239	235
QA \geq 0.8	$ \bar{\epsilon} $	17%	9%	17%	12%	18%	12%
	$\bar{\epsilon}$	11%	-1%	13%	-1%	15%	1%
	RMSD	0.1848	0.0812	0.1053	0.1015	0.1272	0.1002
	N	2055	2049	2932	2913	2148	2148
		With BBE-estimated $R_{rs}(41x)$ and $R_{rs}(443)$ data					
		SeaWiFS		MODISA		VIIRS-SNPP	
		R_{555}^{443}	R_{443}^{412}	R_{547}^{443}	R_{443}^{412}	R_{551}^{443}	R_{443}^{410}
QA \leq 0.2	$ \bar{\epsilon} $	35%	41%	29%	29%	31%	23%
	$\bar{\epsilon}$	6%	36%	-3%	25%	16%	3%
	RMSD	0.1615	0.3145	0.0940	0.2298	0.3699	0.2163
	N	95	95	101	101	24	24
0.4 \leq QA \leq 0.6	$ \bar{\epsilon} $	18%	20%	22%	16%	25%	18%
	$\bar{\epsilon}$	0%	11%	1%	5%	18%	5%
	RMSD	0.1988	0.1838	0.1288	0.1390	0.1405	0.1672
	N	359	359	576	576	239	239
QA \geq 0.8	$ \bar{\epsilon} $	15%	12%	16%	13%	16%	13%
	$\bar{\epsilon}$	4%	0%	7%	1%	9%	1%
	RMSD	0.1594	0.1125	0.0938	0.1123	0.1057	0.1149
	N	2055	2055	2932	2932	2148	2148

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Table 5. Combined uncertainty for the estimated $R_{rs}(412)$ and $R_{rs}(443)$ as a result of the uncertainty propagation from the input $R_{rs}(\lambda)$ spectra at 488, 551, and 670 nm. The uncertainties for the input $R_{rs}(\lambda)$ spectra are tabulated in Table 1.

Chl	No.	$R_{rs}(412)$				$R_{rs}(443)$			
		$ \bar{\epsilon} $	$\bar{\epsilon}$	RMSD	N	$ \bar{\epsilon} $	$\bar{\epsilon}$	RMSD	N
Class 1 0.14 ± 0.13 mg m^{-3}	1	13%	-10%	0.0020	173	7%	-5%	0.0009	173
	2	16%	-6%	0.0021		10%	-4%	0.0011	
	3	25%	-4%	0.0035		17%	-2%	0.0021	
	4	40%	-1%	0.0057		32%	0%	0.0036	
	5	56%	-1%	0.0077		47%	1%	0.0051	
Class 2 1.6 ± 1.8 mg m^{-3}	1	9%	-2%	0.0008	137	4%	-1%	0.0004	137
	2	28%	-3%	0.0015		22%	0%	0.0012	
	3	35%	-3%	0.0019		29%	-1%	0.0016	
	4	41%	-2%	0.0023		35%	-1%	0.0020	
	5	46%	-2%	0.0027		40%	-1%	0.0023	
Class 3 15 ± 9 mg m^{-3}	1	13%	1%	0.0008	190	6%	0%	0.0005	190
	2	30%	11%	0.0011		22%	8%	0.0009	
	3	37%	18%	0.0013		27%	12%	0.0011	
	4	43%	24%	0.0016		31%	16%	0.0014	
	5	47%	30%	0.0018		35%	20%	0.0016	

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Table 6. Uncertainties of $a_{ph}(443)$ and $a_{dg}(443)$ derived from the original satellite $R_{rs}(\lambda)$ data and estimated $R_{rs}(\lambda)$ data at blue bands. The uncertainties are calculated with regard to the retrievals from corresponding *in situ* $R_{rs}(\lambda)$. All negative $R_{rs}(41x)$ and $R_{rs}(443)$ values and negative $a_{ph}(443)$ and $a_{dg}(443)$ retrievals are excluded from the comparison. Negative values are excluded from analysis.

		With original $R_{rs}(41x)$ and $R_{rs}(443)$ data					
		SeaWiFS		MODISA		VIIRS-SNPP	
		$a_{ph}(443)$	$a_{dg}(443)$	$a_{ph}(443)$	$a_{dg}(443)$	$a_{ph}(443)$	$a_{dg}(443)$
QA \leq 0.2	$ \bar{\phi} $	46%	136%	56%	142%	38%	132%
	$\bar{\phi}$	0%	34%	-12%	4%	-4%	-91%
	RMSD	0.0213	0.2878	0.0464	0.3031	0.0195	0.0359
	N	7	29	16	28	15	19
0.4 \leq QA \leq 0.6	$ \bar{\phi} $	48%	64%	67%	89%	47%	117%
	$\bar{\phi}$	-26%	15%	-42%	-3%	-10%	-24%
	RMSD	0.0070	0.0179	0.0324	0.0679	0.0334	0.2291
	N	169	268	261	418	116	190
QA \geq 0.8	$ \bar{\phi} $	44%	42%	49%	58%	41%	57%
	$\bar{\phi}$	-21%	-4%	-21%	-13%	-10%	-11%
	RMSD	0.0155	0.0144	0.0314	0.0494	0.0260	0.0477
	N	1786	2024	2258	2873	1685	2088
		With BBE-estimated $R_{rs}(41x)$ and $R_{rs}(443)$ data					
		SeaWiFS		MODISA		VIIRS-SNPP	
		$a_{ph}(443)$	$a_{dg}(443)$	$a_{ph}(443)$	$a_{dg}(443)$	$a_{ph}(443)$	$a_{dg}(443)$
QA \leq 0.2	$ \bar{\phi} $	87%	105%	78%	82%	58%	72%
	$\bar{\phi}$	34%	-15%	33%	-14%	-55%	12%
	RMSD	0.1908	0.3423	0.1680	0.2426	0.0249	0.0524
	N	55	107	66	118	15	20
0.4 \leq QA \leq 0.6	$ \bar{\phi} $	51%	66%	59%	59%	62%	69%
	$\bar{\phi}$	5%	-16%	-19%	5%	-32%	-21%
	RMSD	0.0102	0.0333	0.0367	0.0694	0.0435	0.0868
	N	202	345	327	548	118	219
QA \geq 0.8	$ \bar{\phi} $	45%	48%	50%	57%	49%	56%
	$\bar{\phi}$	-13%	0%	-13%	-11%	-8%	-7%
	RMSD	0.0155	0.0211	0.0320	0.0566	0.0306	0.0532
	N	1791	2030	2268	2907	1685	2102

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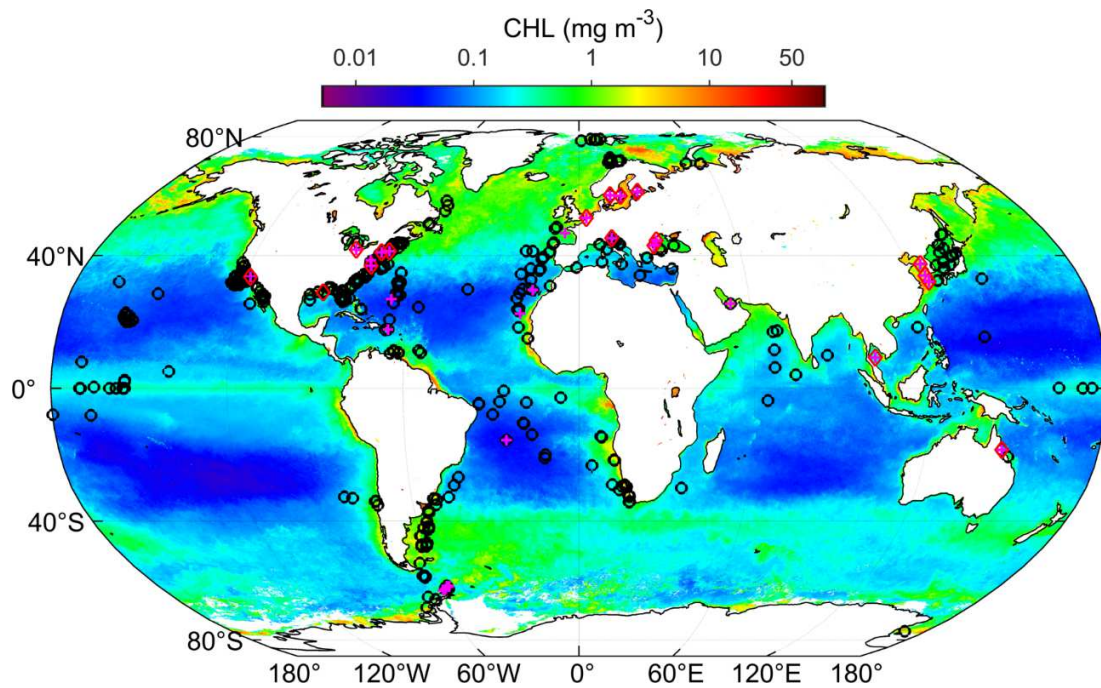
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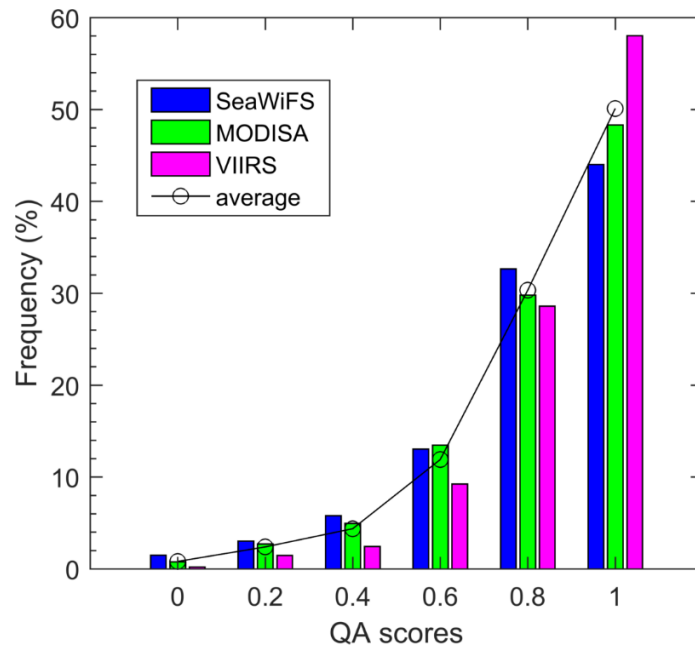


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907 Figure 1. Satellite matchup stations for SeaWiFS (denoted by open circles “o”),
908 MODISA (denoted by crosses “+”), and VIIRS-SNPP (denoted by open diamonds
909 “◇”) in the global oceans. The background image refers to the annual chlorophyll-
910 a concentration for 2010 derived from SeaWiFS.

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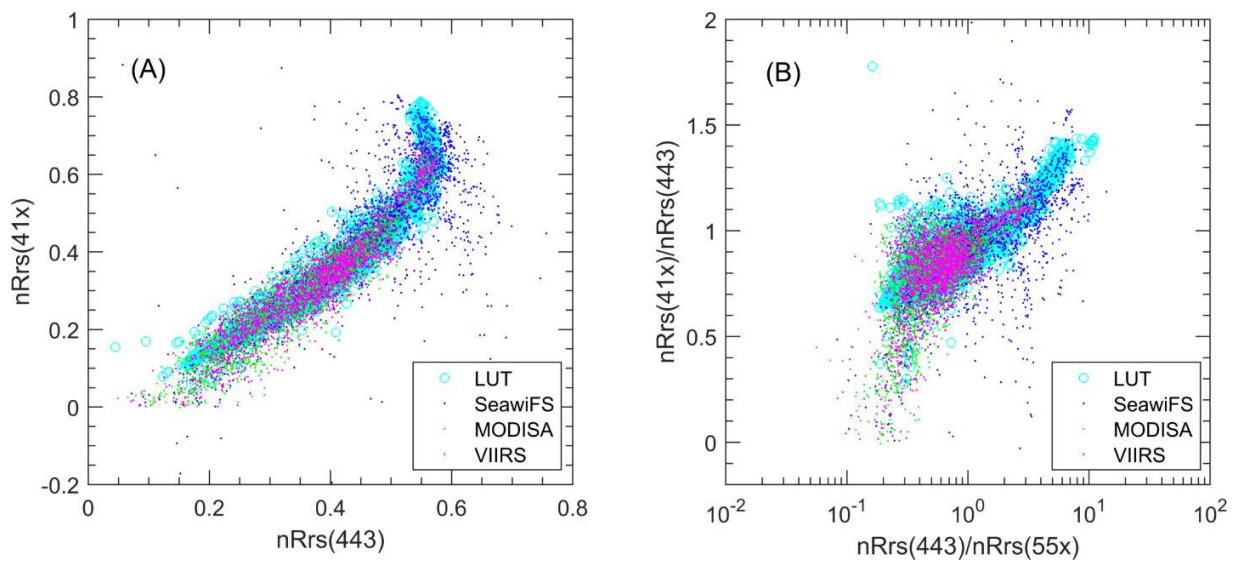
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Figure 2. Frequency distribution of the QA scores for SeaWiFS, MODISA, and VIIRS-SNPP $R_{rs}(\lambda)$ data. The QA scores are calculated based on the five “common” bands of 41x, 443, 48x, 55x, and 67x nm.

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921 Figure 3. Ranges of $nR_{rs}(\lambda)$ values used in different data sets. Note that the *in situ*
922 matchup data are used to describe the variability of corresponding satellite
923 missions in order to avoid the negative $nR_{rs}(41x)$ values.

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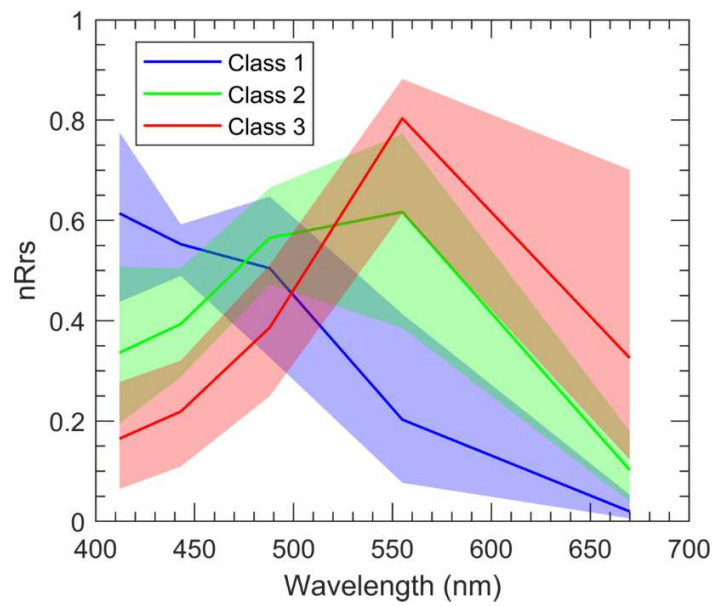
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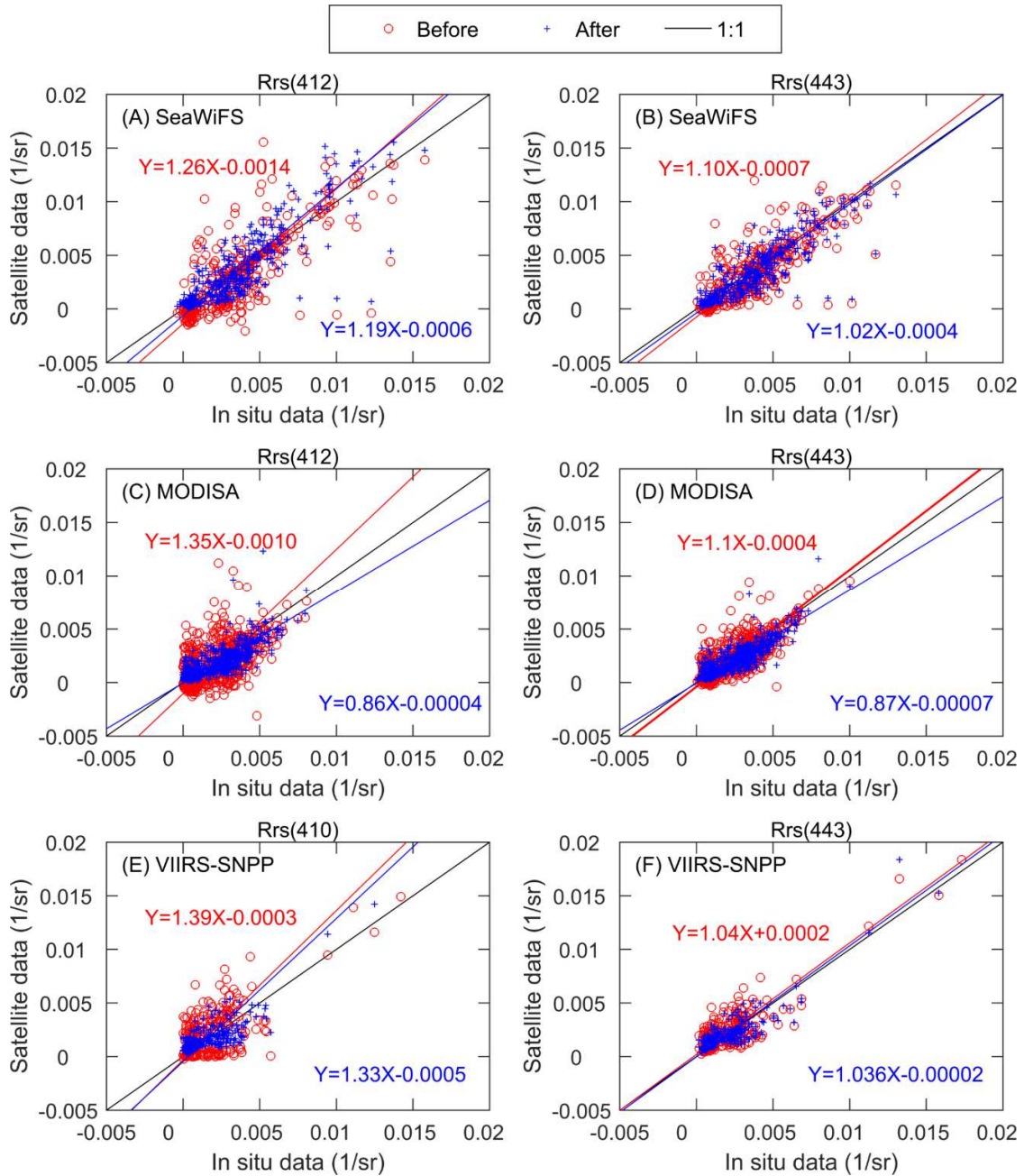
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Figure 4. Normalized remote sensing reflectance spectra representative of three distinctive optical water classes based on the IOCCG (2006) $R_{rs}(\lambda)$ data at 412, 443, 488, 551, and 670 nm. The shaded areas describe the range of variation of the spectral values of $nR_{rs}(\lambda)$.



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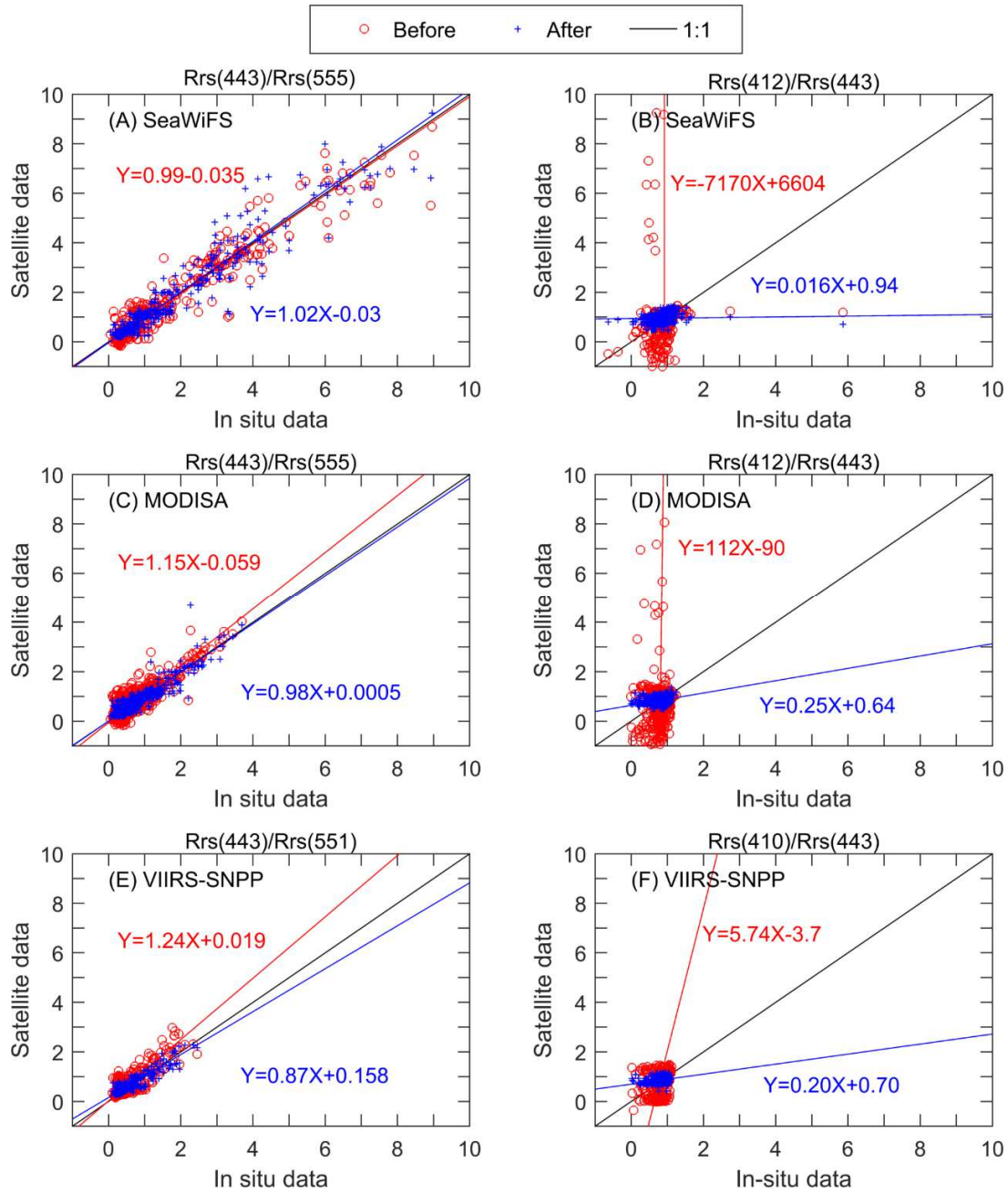
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Figure 5. Comparison of moderate-QA ($0.4 \leq QA \leq 0.6$) satellite $R_{rs}(\lambda)$ data and *in situ* measurements at 41x and 443 nm bands. The symbols of red “o” and blue “+” denote the results before and after the implementation of the BBE algorithm. Linear regression results are also plotted for two data sets. Note that the scatterplots have included all available data points, positive and negative.



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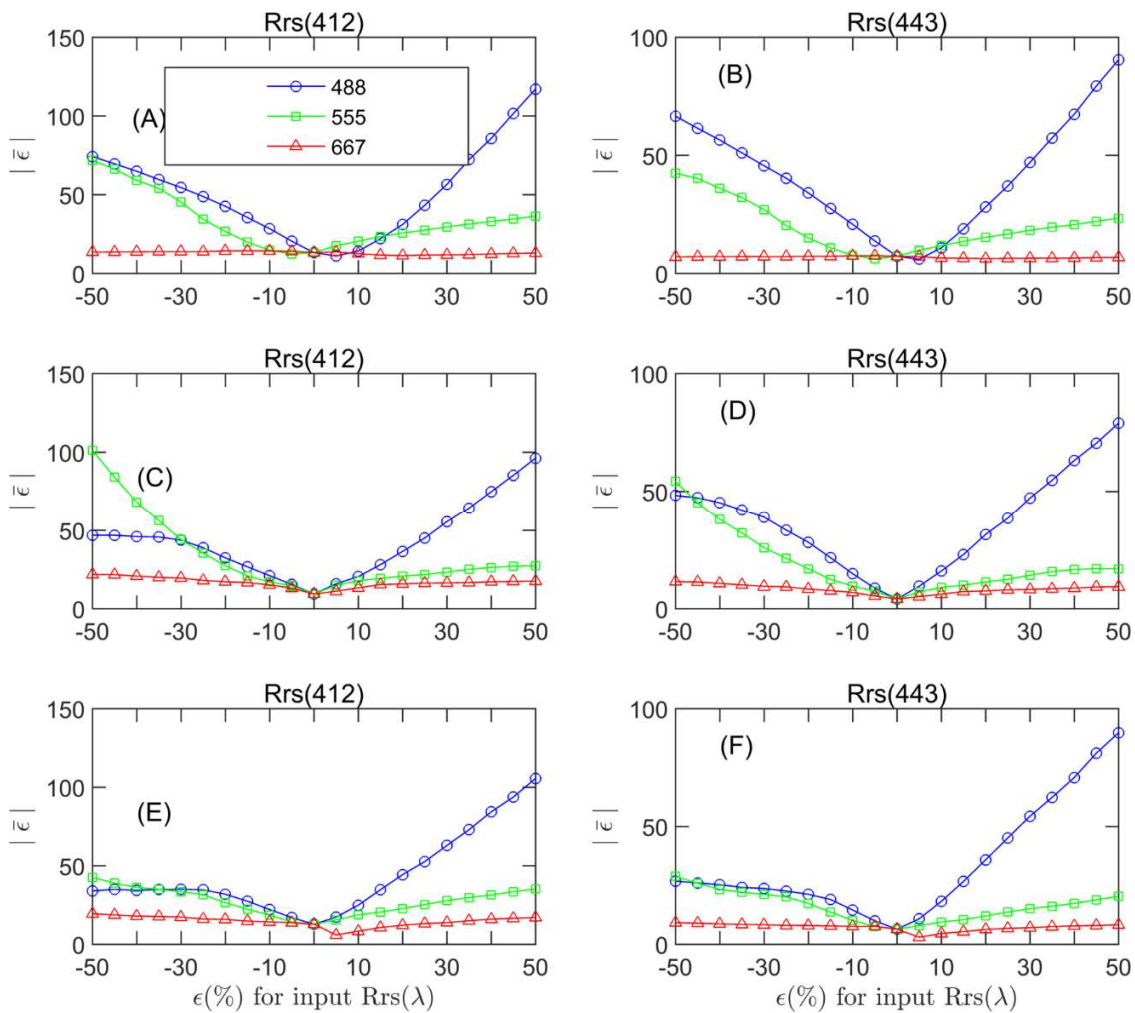
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Figure 6. Comparison of moderate-QA ($0.4 \leq QA \leq 0.6$) satellite $R_{rs}(\lambda)$ spectral ratios with *in situ* matchups. The symbols of red “o” and blue “+” denote the results before and after the implementation of the BBE algorithm. Linear regression results are also plotted for two data sets. Note that the scatterplots have included all available data points, positive and negative.

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959 Figure 7. Uncertainty of estimated $R_{rs}(412)$ and $R_{rs}(443)$ induced by erroneous

960 $R_{rs}(\lambda)$ at 488, 551, or 670 nm bands. The first, second, and third rows refer to

961 Class 1, Class 2, and Class 3 waters, respectively, corresponding to Figure 4.

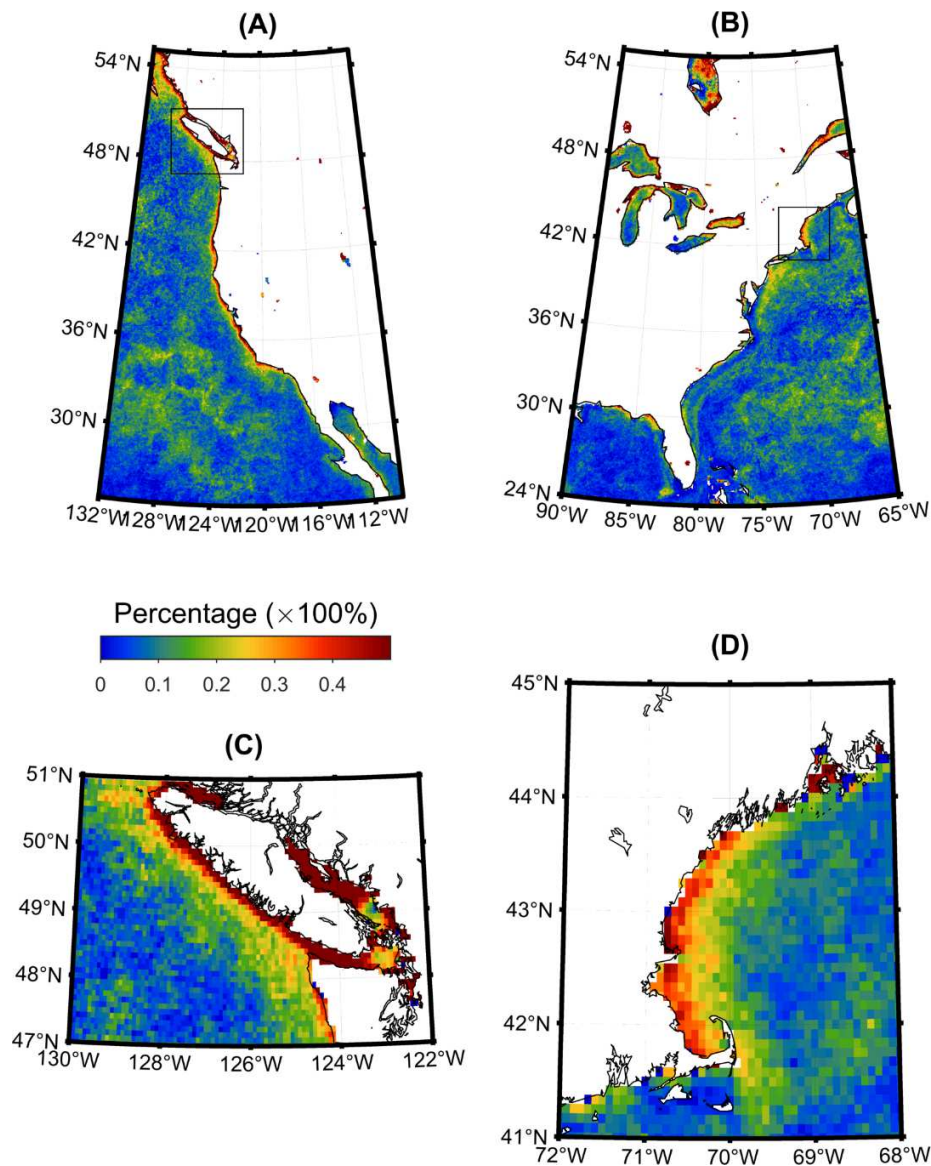
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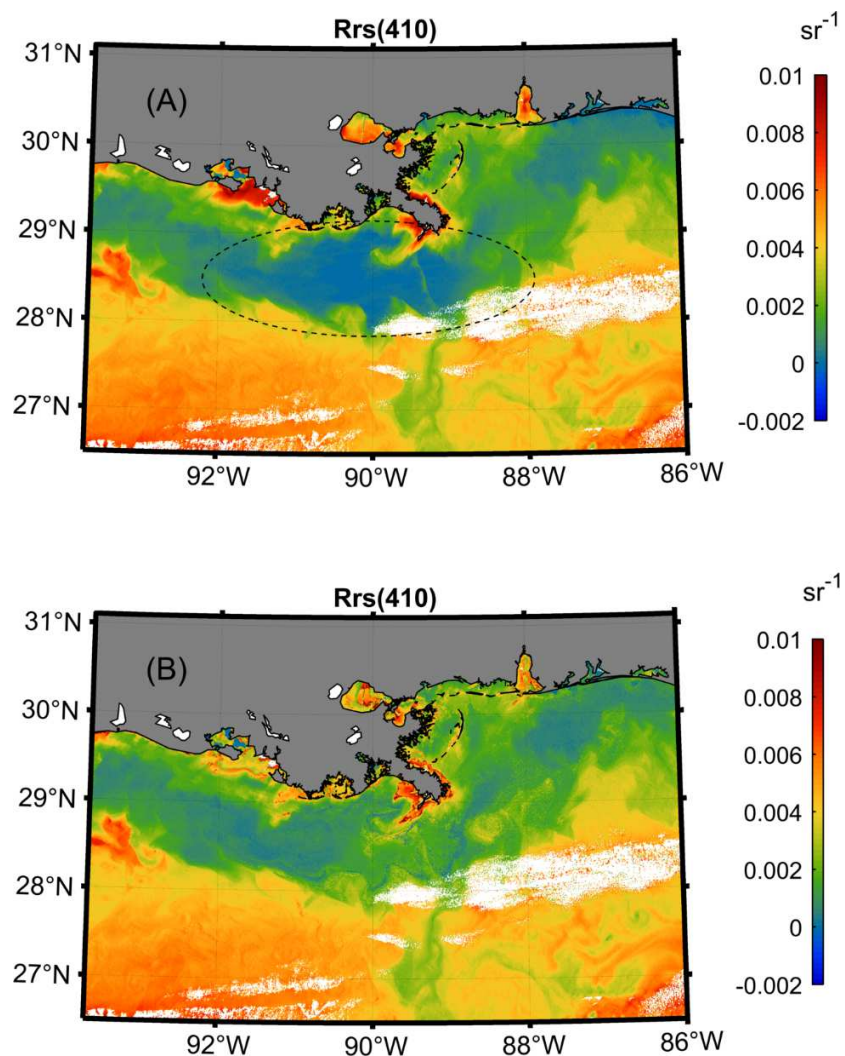
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Figure 8. Percentage of moderate-QA and low-QA satellite data in (a) the U.S. west coasts and inland waters; and (b) the U.S. east coasts and inland waters. The two highlighted areas are (c) the Vancouver Island and (d) Massachusetts Bay and the Gulf of Maine. The percentage data shown here are derived from the MODISA Level 3 mapped (9 km) daily remote sensing reflectance products in 2003, with the QA scores computed based on the R_{rs} at five bands (412, 443, 488, 547, and 667 nm).



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Figure 9. (a) VIIRS-SNPP $R_{rs}(410)$ image in the northern Gulf of Mexico (Image id: V2016048190213_NPP_SCINIR_L2). (b) The same image but with estimated $R_{rs}(410)$ for moderate- and low-QA pixels. White pixels indicate the failure of quality checks for land, cloud, stray light, high glint, and/or high TOA, etc. The dashed line in (a) indicates where the strongly absorbing aerosols occur, and the negative $R_{rs}(410)$ values are likely to present, according to the quality flags.