Supplement of

An estuarine-tuned quasi-analytical algorithm (QAA-V): assessment and application to satellite estimates of SPM in Galveston Bay following Hurricane Harvey

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Section S1

Chlorophyll-a profiles along with depth-dependent mass-specific IOPs are necessary to create Rrs using Hydrolight® four component case-2 models (S1) (Mobley and Sundman 2013; Sathyendranath et al., 1989; Kirk 1994; Bukata et. al., 1995),

\[
a_t(\lambda) = a_w(\lambda) + a_\phi(\lambda) + a_{\text{NAP}}(\lambda) + a_g(\lambda)
\]

\[
b_{bt}(\lambda) = b_{bw}(\lambda) + b_{b\phi}(\lambda) + b_{b\text{NAP}}(\lambda)
\] (S1)

Synthetic chlorophyll concentrations [Chl] (N=730) were obtained with 73 values and ranged between 1 to 40 mg m\(^{-3}\) with 10 repetitions to simulate random variability as observed in natural waters. A total of 730 phytoplankton absorption spectra (a_\phi) were generated using six groups containing 83 in situ normalized a_\phi spectra; random normalized spectrum selection among groups were based on modeled a_\phi440, and the following bio-optical models (Bricaud et al., 1995; Fischer and Fell 1999; Mobley 1994) (Fig. S1; Table S1),

\[
a_\phi^{\text{Normalized}}(\lambda) = \frac{a_\phi(\lambda)}{a_\phi440}
\]

\[
a_\phi440 = 0.06 \times [\text{Chl}]^{0.65} \times \mathcal{R}(1,2)
\]

\[
a_\phi^*(\lambda) = \frac{a_\phi(\lambda)}{[\text{Chl}]}
\] (S2)

Figure S1. (a, b) In situ phytoplankton absorption spectra (N=83) were collected from CDOM-dominated Apalachicola Bay (USA) and sediment-dominated Barataria Bay (USA) to generate 730 simulated spectra for Hydrolight® four-component Case-2 model using Eq. 2, (c) modeled non-algal particle absorption spectra (N = 730) using Eq. 3, and (d) modeled CDOM absorption spectra (N = 730) using (S4).

Table S1: The conditions for allocating in-situ normalized-phytoplankton spectra (a_\phi^{\text{Normalized}}) into 6 groups. a_\phi440 is phytoplankton absorption at 440 nm.
Mass-specific non-algal particle absorption coefficients ($a_{NAP}^*(\lambda)$) were obtained with an exponential model (Roesler et al. 1989; Bricaud et al. 1995), where slope ($S_{NAP}$) used a random value between 0.005 - 0.015 as observed in natural waters ranging from oceanic to estuarine environments (Kirk 1994). The required $a_{NAP} 440$ was modeled using $a_g 440$ based on a constant $p_1 (= a_{NAP} 440 / a_g 440)$ which was set to lie between 1 and 3.5 as generally observed in the two bays, e.g., $p_1 = 1$ represents pigment/CDOM-rich waters and $p_1 = 3.5$ represents sediment/CDOM-rich waters (S3).

\[
a_{NAP} (\lambda) = a_{NAP} 440 \times e^{-S_{NAP} \times (\lambda - 440)}
\]

\[
p_1 = 1 + \frac{2.5 \times a_g 440 \times 9(0.1)}{0.05 + a_g 440}
\]

\[
a_{NAP}^* (\lambda) = \frac{a_g (\lambda)}{[NAP]}
\]

CDOM absorption coefficient was modeled with an exponential model (Bricaud et al. 1981), where spectral slope ($S_g$) was chosen randomly between 0.01 to 0.025 as generally observed in various oceanic to productive estuarine environments (Kirk 1994; Babin et al., 2003) (Fig. S1d). $a_g 440$ was estimated from $a_g 440$ and a constant $p_2 (= a_g 440 / a_g 440)$. $p_2$ was set between 1 to 4.5 based on field data, e.g., $p_2 = 1$ represents phytoplankton/sediment dominated waters and $p_2 = 4.5$ represents CDOM-rich waters (S4).

\[
a_g (\lambda) = a_g 440 \times e^{-S_g \times (\lambda - 440)}
\]

\[
a_g 440 = p_2 \times a_g 440
\]

\[
p_2 = 1 + \frac{3.5 \times a_g 440 \times 9(0.1)}{0.02 + a_g 440}
\]

\[
a_g^* (\lambda) = \frac{a_g (\lambda)}{[Chl]}
\]

Mass-specific phytoplankton backscattering ($b_{NAP}^*$) and non-algal particle back-scattering ($b_{bNAP}^*$) coefficients were obtained based on the oceanic models (IOCCG 2006; please see references therein) with no change, as insufficient observations were available for estuarine environments. Subsequently, these coefficients were then converted to respective back-scattering coefficients by multiplying phase function dependent values “0.005” and “0.0183” (S5 and S6) (Mobley 1994; Mobley and Sundman 2013),

\[
b_{NAP}^* (\lambda) = b_{NAP} (\lambda) \times 0.0183
\]

\[
b_{bNAP}^* (\lambda) = \frac{b_{NAP} (\lambda) \times 0.005}{[NAP]}
\]

\[
b_{bNAP}^* (\lambda) = \frac{b_{NAP} (\lambda) \times 0.005}{[Chl]}
\]

Hydrolight® simulations were then run with a case-2 model to generate Rs using mass-specific IOPs, chlorophyll concentrations, dark bottom sediments, finite depth of 5 meters, sun zenith angle of 30°, no Raman scattering, and no chlorophyll fluorescence. A total of 169 erroneous spectra were suspected.

<table>
<thead>
<tr>
<th>Groups</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (n=18)</td>
<td>$a_g 440 &lt; 0.1$</td>
</tr>
<tr>
<td>2 (n=15)</td>
<td>$a_g 440 \geq 0.1$ &amp; $a_g 440 &lt; 0.2$</td>
</tr>
<tr>
<td>3 (n=12)</td>
<td>$a_g 440 \geq 0.2$ &amp; $a_g 440 &lt; 0.3$</td>
</tr>
<tr>
<td>4 (n=11)</td>
<td>$a_g 440 \geq 0.3$ &amp; $a_g 440 &lt; 0.5$</td>
</tr>
<tr>
<td>5 (n=16)</td>
<td>$a_g 440 \geq 0.5$ &amp; $a_g 440 &lt; 1.0$</td>
</tr>
<tr>
<td>6 (n=11)</td>
<td>$a_g 440 \geq 1.0$</td>
</tr>
</tbody>
</table>
possibly due to atypical combinations of CDOM, non-algal particles, and bottom reflectance; these were not used in further analysis.

References


Section S2

Table S2: Comparison statistics between the QAA-V and QAA-v6 algorithms based on simulated Hydrolight® dataset (HL) and in-situ estuarine and near-shore dataset (IES). N= number of observations, RMSE=Root mean square error, MRE= mean relative error.

<table>
<thead>
<tr>
<th>N</th>
<th>Bias_{log10} (m⁻¹)</th>
<th>RMSE_{log10} (m⁻¹)</th>
<th>MRE (%)</th>
<th>R²</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>QAA-V</td>
<td>QAA-v6</td>
<td>QAA-V</td>
<td>QAA-v6</td>
</tr>
<tr>
<td></td>
<td></td>
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<td>QAA-V</td>
<td>QAA-v6</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>QAA-V</td>
<td>QAA-v6</td>
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</tbody>
</table>

**Synthetic data**

<p>| | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>a_{tnw} 411</td>
<td>561</td>
<td>-0.028</td>
<td>-0.088</td>
<td>0.074</td>
<td>0.117</td>
<td>12.7</td>
<td>19.7</td>
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<tr>
<td>a_{tnw} 489</td>
<td>561</td>
<td>-0.006</td>
<td>-0.071</td>
<td>0.071</td>
<td>0.106</td>
<td>12.7</td>
<td>17.7</td>
</tr>
<tr>
<td>a_{tnw} 555</td>
<td>561</td>
<td>-0.003</td>
<td>-0.076</td>
<td>0.072</td>
<td>0.110</td>
<td>13.0</td>
<td>18.0</td>
</tr>
<tr>
<td>b_{tnw} 411</td>
<td>561</td>
<td>-0.020</td>
<td>-0.118</td>
<td>0.096</td>
<td>0.149</td>
<td>16.3</td>
<td>23.9</td>
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<tr>
<td>b_{tnw} 443</td>
<td>561</td>
<td>-0.041</td>
<td>-0.159</td>
<td>0.097</td>
<td>0.173</td>
<td>15.5</td>
<td>28.9</td>
</tr>
<tr>
<td>b_{tnw} 489</td>
<td>561</td>
<td>-0.025</td>
<td>-0.130</td>
<td>0.086</td>
<td>0.152</td>
<td>14.4</td>
<td>25.3</td>
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<tr>
<td>b_{tnw} 555</td>
<td>561</td>
<td>-0.017</td>
<td>-0.119</td>
<td>0.082</td>
<td>0.146</td>
<td>14.1</td>
<td>23.9</td>
</tr>
</tbody>
</table>

**IES dataset (Testing set: N = 219)**

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<thead>
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</thead>
<tbody>
<tr>
<td>a_{tnw} 443</td>
<td>209</td>
<td>-0.023</td>
<td>-0.091</td>
<td>0.142</td>
<td>0.180</td>
<td>22.7</td>
<td>25.8</td>
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<tr>
<td>a_{tnw} 555</td>
<td>209</td>
<td>-0.029</td>
<td>-0.124</td>
<td>0.190</td>
<td>0.249</td>
<td>34.3</td>
<td>47.5</td>
</tr>
<tr>
<td>b_{tnw} 532</td>
<td>89</td>
<td>0.038</td>
<td>-0.049</td>
<td>0.173</td>
<td>0.174</td>
<td>26.0</td>
<td>34.6</td>
</tr>
</tbody>
</table>

Section S3

![Figure S2](image)

Figure S2: A comparison of SPM concentration obtained with 0.2 µm Nylon filter and 0.7 µm GFF filters.
Figure S3: Validation of the atmospheric corrected images that were used for generating maps of $a_{\text{mwa}443}$ and $b_{\text{mwa}470}$ in Fig. 10 of the manuscript.