A model based on stacked-constraints approach for partitioning the light absorption coefficient of seawater into phytoplankton and non-phytoplankton components

Guangming Zheng and Dariusz Stramski

Marine Physical Laboratory
Scripps Institution of Oceanography
University of California, San Diego
**Background**: Absorption Coefficient of Seawater

\[
\text{Total } a(\lambda) = a_w(\lambda) + a_{ph}(\lambda) + a_d(\lambda) + a_g(\lambda)
\]

- Pure Seawater
- Phytoplankton
- Non-algal Particles
- CDOM

Total non-water \( a_{nw}(\lambda) \)
Existing Partitioning Models

Involve highly restrictive assumptions on spectral shape of $a_{ph}(\lambda)$ and/or spectral slope of $a_{dg}(\lambda)$, which limit the performance of these models.

<table>
<thead>
<tr>
<th>Model</th>
<th>Minimum Input</th>
<th>Key Assumptions for Phytoplankton Absorption</th>
<th>Key Assumptions for Non-Phytoplankton Absorption</th>
</tr>
</thead>
</table>
| **Roesler et al., 1989**                | [Chl-a], [Pheo] and $a_m(\lambda)$ at 436, 676 nm | 1. The ratio $a_{ph}(436):a_{ph}(676)$ is a specified function of the ratio [Pheo]:[Chl a].
2. $a_{ph}(676) = a_{m}(676)$ | $a_{dg}(\lambda)$ is an exponential function of $\lambda$ with fixed slope, $S_{dg} = 0.015$ nm$^{-1}$. |
| **Lee et al., 2002, 2007**              | $a_{m}(\lambda)$ at 410, 440 nm, and $r_{m}(\lambda)$ at 440, 555 nm | The ratio $a_{ph}(410):a_{ph}(440)$ is a function of the ratio $r_{m}(440):r_{m}(555)$. | $a_{dg}(\lambda)$ is an exponential function of $\lambda$ with fixed slope, $S_{dg} = 0.015$ nm$^{-1}$. |
| **Maritorena et al., 2002**             | $a_{m}(\lambda)$ at 412, 443, 490, 510, 555, 670 nm | The Chl-specific absorption coefficients for phytoplankton are specified. | $a_{dg}(\lambda)$ is an exponential function of $\lambda$ with fixed slope, $S_{dg} = 0.015$ nm$^{-1}$. |
| **Gallegos and Neale, 2002**            | $a_{m}(\lambda)$ at 412, 440, 488, 676, 715 nm | $a_{ph}(\lambda)$ are specified linear functions of $a_{m}(676)$. | $a_{l}(\lambda)$ and $a_{d}(\lambda)$ are specified linear functions of $a_{l}(440)$ and $a_{d}(440)$, respectively. |
| **Schofield et al., 2004**             | $a_{m}(\lambda)$ at 412, 440, 488, 510, 555, 630, 650, 676, 715 nm | $a_{ph}(\lambda)$ is a linear combination of three specified absorption spectra representing phytoplankton containing Chl $\alpha$-c, phycobilin, and Chl $\alpha$-$b$, respectively. | 1. Both $a_{l}(\lambda)$ and $a_{d}(\lambda)$ are exponential functions of $\lambda$ with variable slopes, $S_{l}$ and $S_{d}$.  
2. $S_{l} > S_{d}$  
3. $a_{l}(676) = a_{d}(676)$ |
| **Ciotti and Bricaud, 2006**            | [Chl] and $a_{m}(\lambda)$ at 412, 443, 490, 510, 555 nm | 1. $a_{ph}(490)/a_{ph}(412) = 0.919$ [Chl]$^{0.012}$  
2. $a_{ph}(510)/a_{ph}(412) = 0.581$ [Chl]$^{0.047}$ | $a_{dg}(\lambda)$ is an exponential function of $\lambda$ with variable slope, $S_{dg}$. |
1. $a_{ph}(\lambda)$ is a linear combination of two specified absorption spectra representing picoplankton and microplankton, respectively.  
2. $a_{ph}(505) = 0.0185$ [Chl]$^{0.684}$ |
Objective

Develop a partitioning model that

- does not require highly restrictive assumptions on $a_{ph}(\lambda)$ and $a_{dg}(\lambda)$
- can be applied to data at past and current satellite ocean color bands, as well as data with higher spectral resolution including future satellite data
Calculate $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$

MBS Algorithm

Step 1

Matrix B

$B_{ij} = (x_i, y_j)$

Step 2

Calculate $S$ and $A$

Input: $a_{nw}(\lambda)$

Step 2

Matrix C

$C_{ij} = (S_{ij}, A_{ij})$

Step 3

Calculate $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$

Step 3

Matrix D

$D_{ij} = (a_{dg}(\lambda)_{ij}, a_{ph}(\lambda)_{ij})$

Step 4

Satisfy constraints

#4 - #8

Yes

Step 4

Output:

Optimal Solution

Range of Feasible Solutions

Step 5

Matrix A

Feasible Solutions

Stacked-Constraints Algorithm

Flowchart

Derive a large number of speculative solutions.

First identifies feasible solutions, then optimal solution and range of feasible solutions.
Input and Output

- **Input**
  - $a_{nw}(\lambda)$ at a minimum of six wavelengths
    - 412 nm, 443 nm, 490 nm, 510 nm, 555 nm, and 670 nm
  - or $a_{nw}(\lambda)$ with higher spectral resolution

- **Output**
  - $a_{dg}(\lambda)$ with arbitrarily high spectral resolution because
    \[ a_{dg}(\lambda) = A \exp(-S\lambda) \]
  - $a_{ph}(\lambda)$ with same spectral resolution as input $a_{nw}(\lambda)$
Calculate $a_{dg}(\lambda)^{i,j}$ and $a_{ph}(\lambda)^{i,j}$

**MBS Algorithm**

- **Step 1**: Input: $\{x_i\} = \{y_j\} = \{0.01, 0.02, \ldots, 1\}$
- **Step 2**: Calculate $S$ and $A$
- **Step 2**: Matrix $B$
  - $B_{i,j} = (x_i, y_j)$
- **Step 3**: Matrix $C$
  - $C_{i,j} = (S_{i,j}, A_{i,j})$
- **Step 3**: Matrix $D$
  - $D_{i,j} = (a_{dg}(\lambda)^{i,j}, a_{ph}(\lambda)^{i,j})$
- **Input**: $a_{nw}(\lambda)$
- **Output**: Optimal Solution, Range of Feasible Solutions

**Stacked-Constraints Algorithm**

- **Step 4**: Satisfy constraints
  - #4 - #8
- **Yes**: Feasible Solutions
- **Yes**: Matrix $A$

**Flowchart**

- Derive a large number of speculative solutions.
- First identifies feasible solutions, then optimal solution and range of feasible solutions.
Absorption coefficients data collected from 505 open ocean and coastal surface stations from low to high latitudes.

### Inequality Constraints

<table>
<thead>
<tr>
<th>#</th>
<th>Constraint</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$0 &lt; \frac{a_{ph}(412)}{a_{ph}(443)} &lt; 1$</td>
</tr>
<tr>
<td>2</td>
<td>$0 &lt; \frac{a_{ph}(510)}{a_{ph}(490)} &lt; 1$</td>
</tr>
<tr>
<td>3</td>
<td>$0.006 \text{ nm}^{-1} &lt; S &lt; 0.03 \text{ nm}^{-1}$</td>
</tr>
<tr>
<td>4</td>
<td>$0.74 &lt; \frac{a_{ph}(467)}{a_{ph}(412)} &lt; 1.54$</td>
</tr>
<tr>
<td>5</td>
<td>$1.3 &lt; \frac{a_{ph}(510)}{a_{ph}(555)} &lt; 10$</td>
</tr>
<tr>
<td>6</td>
<td>$1.4 &lt; \frac{a_{ph}(443)}{a_{ph}(670)} &lt; 9.1$</td>
</tr>
<tr>
<td>7</td>
<td>$0.33 \frac{a_{nw}(412)}{a_{nw}(443)} &lt; \frac{a_{dg}(412)}{a_{nw}(412)} &lt; 0.78 \frac{a_{nw}(412)}{a_{nw}(443)}$</td>
</tr>
<tr>
<td>8</td>
<td>$0.003 &lt; \frac{(na_{ph}(510) - na_{ph}(555))}{(555 - 510)} &lt; 0.0087$</td>
</tr>
</tbody>
</table>

Hyperspectral measurements spanning a wide range of variability in spectral shape and magnitude.

Account for the wide range of variability.
Calculate $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$

MBS Algorithm

Stacked-Constraints Algorithm

Satisfy constraints #4 - #8

Output:
Optimal Solution
Range of Feasible Solutions

Input:
$a_{nw}(\lambda)$

Feasible Solutions

Matrix A

Step 1

$\{x_i\} = \{y_j\} = \{0.01, 0.02, \ldots, 1\}$

Step 2

Calculate $S$ and $A$

Step 2

Calculate $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$

Step 3

Matrix D

$D_{i,j} = (a_{dg}(\lambda)_{i,j}, a_{ph}(\lambda)_{i,j})$

Step 4

Yes

Step 4

Satisfy constraints #4 - #8

Step 5

Matrix B

$B_{i,j} = (x_i, y_j)$

Step 1

First identifies feasible solutions, then optimal solution and range of feasible solutions.

Derive a large number of speculative solutions.
Modified Bricaud & Stramski (MBS) Algorithm

Original Bricaud and Stramski [1990] Algorithm

\[ a_d(\lambda) = A \exp(-S \lambda) \]

\[ a_{ph}(505)/a_{ph}(380) = 0.99 \]
\[ a_{ph}(580)/a_{ph}(693) = 0.92 \]

\[ S, A \rightarrow a_d(\lambda) \rightarrow a_{ph}(\lambda) \]

Modified Bricaud & Stramski Algorithm, MBS

\[ a_{dg}(\lambda) = A \exp(-S \lambda) \]

\[ a_{ph}(412)/a_{ph}(443) = x \]
\[ a_{ph}(510)/a_{ph}(490) = y \]

\[ S, A \rightarrow a_{dg}(\lambda) \rightarrow a_{ph}(\lambda) \]

**Inequality Constraints**

<table>
<thead>
<tr>
<th>#</th>
<th>Constraint</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( 0 &lt; x = a_{ph}(412)/a_{ph}(443) &lt; 1 )</td>
</tr>
<tr>
<td>2</td>
<td>( 0 &lt; y = a_{ph}(510)/a_{ph}(490) &lt; 1 )</td>
</tr>
<tr>
<td>3</td>
<td>( 0.006 \text{ nm}^{-1} &lt; S &lt; 0.03 \text{ nm}^{-1} )</td>
</tr>
</tbody>
</table>
Calculate $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$

**MBS Algorithm**

- **Input:** $a_{nw}(\lambda)$
- **Calculate $S$ and $A$**
- **Calculate $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$**
- **Satisfy constraints #4 - #8?**
- **Output:** Optimal Solution
- **Range of Feasible Solutions**

**Flowchart**

Derive a large number of speculative solutions.

First identifies feasible solutions, then optimal solution and range of feasible solutions.
Example Partitioning Results

The **Optimal Solutions** are very close to the actual measured spectra.

The **Range of Feasible Solutions** is a unique feature of our model.
Evaluation of the Model for 505 Samples

Measured $a_{dg}(\lambda)$ [m$^{-1}$]  

Modeled $a_{dg}(\lambda)$ [m$^{-1}$]  

Measured $a_{ph}(\lambda)$ [m$^{-1}$]  

Modeled $a_{ph}(\lambda)$ [m$^{-1}$]
Example Error Statistics for Optimal Solutions at Two Wavelengths

<table>
<thead>
<tr>
<th>Output Variables</th>
<th>R</th>
<th>Median Ratio Modeled : Measured</th>
<th>Median Absolute Percent Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_{dg}(443)$</td>
<td>0.985</td>
<td>1.004</td>
<td>6.50</td>
</tr>
<tr>
<td>$a_{ph}(443)$</td>
<td>0.963</td>
<td>0.988</td>
<td>12.04</td>
</tr>
<tr>
<td>$a_{dg}(670)$</td>
<td>0.899</td>
<td>0.815</td>
<td>21.43</td>
</tr>
<tr>
<td>$a_{ph}(670)$</td>
<td>0.997</td>
<td>1.043</td>
<td>4.82</td>
</tr>
</tbody>
</table>

Both systematic and random errors are generally small.
Spectral Dependence for the Median and Quartile Ratios of Modeled:Measured $a_{dg}(\lambda)$ and $a_{ph}(\lambda)$ — Optimal Solutions

$MR$, median ratio

$QR_1$, 1st quartile ratio

$QR_3$, 3rd quartile ratio

$MR$, $QR_1$, and $QR_3$ are calculated based on 505 samples
Summary and Conclusions

- We have formulated a model that successfully relaxes the widely used highly restrictive assumptions on both the spectral slope $S$ of $a_{dg}(\lambda)$ and the spectral shape of $a_{ph}(\lambda)$.
  - Our assumptions include exponential shape of $a_{dg}(\lambda)$ and eight inequality constraints that account for a wide range of variability in absorption coefficients.
  - The model requires input of $a_{nw}(\lambda)$ at a minimum of six wavelengths, but can also work with data with higher spectral resolution.
- Evaluation of the model performance with field data from diverse environments shows good error statistics.
- These results support the prospect of good performance of our model on data provided by various remote-sensing and in situ platforms.
Acknowledgements

- This work was supported by NASA Ocean Biology and Biogeochemistry Program (Grants NNG04GO02G and NNX10AG05G) and NASA Cryosphere Program (Grant NNX07AR20G).

- We thank all scientists and personnel who contributed to the collection and processing of field data of absorption coefficients used in this study. In particular, we thank K. Carder, G. Cota, M. Kahru, G. Mitchell, N. Nelson, D. Siegel, A. Subramaniam, and R. Zimmerman who made the data available through the NASA's SeaWiFS Bio-Optical Archive and Storage System (SeaBASS); M. Babin, A. Bricaud, and H. Claustre who made the data available through the BIOSOPE database; and M. Babin, L. Clementson, A. Matsuoka, and R. Röttgers who shared the data through personal communication.

- We extend our gratitude to Rick Reynolds for valuable discussions.