Modeling scattering from non-spherical particles

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Optical properties of several Synechococcus (cyanophyceae) species\(^1\) were measured and compared to theoretical predictions. Synechococcus was selected because the simple shapes are a good match to the shapes that can be handled by the existing models and because the light absorbing substances (thylakoid membranes) are well distributed throughout each cell (Fig. 1). Further, these cells lack an outer shell that would require more complicated particle models.

![Fluorescence](image1.png)

**Figure 1:** Bright-field fluorescence microscope image of cyanobacteria CCMP 837 (source: Provasoli-Guillard National Center of Marine Phytoplankton of Bigelow Lab). Cyanobacteria has thylakoid membranes distributed over the cell body – the whole cell body emits fluorescence.

![Reflectance](image2.png)

**Figure 2:** Particle size distribution for CCMP 1629, a good example of a homogeneous sphere. (Size distribution obtained using CASY®-1 Cell Size/Analyzer Counters

We initially consider a spherical-celled species, The optical measurements include size distribution of a spherical cell cyanobacterium (Fig. 2), and the absorption and scattering coefficients (Fig. 3). The spectral, real part of the index of refraction was initially computed using the Ketteler-Helmholtz process (Fig. 4) as implemented in the Ocean Optics Phytoplankton Simulator (OOPS) with the addition of an spectral adjustment for the mean value (Fig. 5).

Even with a nearly ideal phytoplankton cell, the modeled assuming a uniform distribution of absorbing material results compared rather poorly to the measurements (Fig. 6). Hypothesizing that, even in this situation, there is a package effect (PE), an estimate of the PE was made.

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\(^1\) Phytoplankton samples were obtained from the Provasoli-Guillard National Center of Marine Phytoplankton of Bigelow Labs, Boothbay Harbor, ME, USA.
This adjustment resulted in a significant improvement in the fit of the model with measurements, although there are still significant spectral differences in the scattering results (Figs. 8 and 9).

**Figure 3:** Absorption and scattering cross-section for a single particle \([m^2]\). Absorption obtained with an AC-S (Wet Labs, Inc.) and scattering obtained using a Perkin Elmer Lamda-18 with integrating sphere.

**Figure 4:** Computation of the real part of the refractive index using the Ketteler-Helmholtz process as implemented in OOPS.
**Figure 5:** Wavelength adjustment to the K-H estimate of the real refractive index. The real index spectrum is obtained using the K-H process. The center line (red line with black dots) is estimated using the equation $2: A + B/\lambda^4 + C/\lambda^4$. For phytoplankton, A, B, and C correspond to cellular material (protein, carbohydrate, lipid etc). and are estimated for overall best fit. **[Note:]** There is no attempt to optimize the refractive index at each wavelength in order to make a perfect match with measurement.

**Figure 6:** Modeling result with no package effect (PE) correction

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Figure 7: Package effect (PE) for particles of various diameters (D).

\[ PE = \frac{a^*_{\text{model}}}{a^*_{\text{Beer}}} \]

where:

- \( a^*_{\text{Beer}} \) = absorption is the cross-section of cellular pigments computed as \((a_{\text{pigment}} \times \text{cell volume})\).
- \( a^*_{\text{model}} \) = absorption is the cross-section of a cell as computed using Mie code.

Figure 8: Modeling result including the package effect (PE) correction.
Figure 9: Comparison of backscattering spectrum with or w/o PE correction (Due to the lack of \( bb \) measurement, the comparison is made with modeled data. Nonetheless, it demonstrates the significance of PE correction.

Figure 10: Particle size distribution for CCMP 1183 (Synechococcus sp.) – a good example of a homogeneous cylinder.

Figure 11: Absorption and scattering cross-sections for a single CCMP 1183 particle.

As a second example, we considered a species that is a good match for a cylindrical model (Figs. 10 and 11). The standard modeling assumption is that the aspect ratio of the cell remains constant as the size changes. However, observations of this species (CCMP1183) indicated that the diameter remains constant and only the length changes (Fig. 12). The T-matrix code (Mishchenko) was rewritten to match this observation. The computed and measured absorption and scattering coefficients are shown in Fig. 13. Note that, although the match for the spectral absorption coefficients is generally good, the computations with the PE are better. The match is not as good for scattering although the PE correction results in a significant improvement except in the blue.
Finally, estimating the scattering from cylindrical particles using spherical models is problematic. In particular, the backscattering from the cylindrical particles is much greater than that from the spherical particles even though the total scattering from spherical particles is greater (Fig. 14).

Conclusions:
- The packaging effect cannot be safely ignored even for the most ideal real particles.
- Use of spherical models to approximate non-spherical particles is problematic.
Appendix:

The primary software tools used in this paper were the Ocean Optical Plankton Simulator (OOPS), created by Minsu Kim, Cornell University, and the T-matrix code for nonspherical particle by Mischenko http://www.giss.nasa.gov/~ermim/mishchenko.html. The T-Matrix code was modified by Minsu Kim both to make the code more readily usable and to

Specific changes to the T-matrix code included:

1. The code was rewritten in dynamic-memory-allocatable FORTRAN 90, eliminating problems with adjusting array sizes (NMAX, NGAUSS etc).
2. The core computation routine was isolated from the general code. It can now called to operate on any wavelength range, integration of PSD, shape etc.
3. The code has been optimized to be at least 20% faster than the original. The major change occurred in the NMAX convergence routine, but significant changes were made throughout the code.
4. An executable program is now included within OOPS software.

Future goal: Parallelization of the code for cluster super computation.

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