Simulation of the scattering properties of a chain-forming triangular prism oceanic diatom

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For publication in the

Journal of Quantitative Spectroscopy & Radiative Transfer

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Abstract

The optical properties of diatom chains in the ocean are studied based on a combination of the many-body iterative T-matrix (MBIT) method and an improved implementation of the ray-by-ray (RBR) geometric optics method. The MBIT, a numerically accurate method, is advantageous for scatterers with linear cells. In contrast to other popular geometric optics methods, the RBR, an approximate method, considers the interference of all outgoing rays. The two methods are verified in comparison with benchmark simulations. The simulation results of diatom chains in a wide size range can be obtained with either or both methods, and each can be applied to any optically soft particle, i.e., in the case when relative refractive index approaches unity.

Keywords: optical properties, diatom chains, many-body iterative T-matrix, ray-by-ray geometric optics method

1. Introduction

The single-scattering properties of soft scatterers (i.e., the refractive index relative to the ambient medium approaches unity) have many practical applications in oceanic optical sensing, in particular, obtaining the characteristics of the scatterers, such as, the particle size distribution, shape, and refractive index by inversion from optical measurements [1-5]. The optical properties for all sizes of either homogeneous spherical scatterers or multi-layer concentric spherical shells can be analytically obtained in terms of the Lorenz-Mie theory [6-10]. Furthermore, the optical properties of an aggregate composed of multiple spheres can be analytically obtained through the multiple sphere T-matrix (MSTM) method [11]. For non-spherical scatterers with certain symmetries (e.g., completely or partially rotational), a semi-analytical method, the T-matrix, can be efficiently used to calculate the scattering properties, and two of the most effective realizations are the extended boundary condition method (EBCM) [12-14] and the invariant imbedding T-matrix (IITM) method [15, 16]. The scattering properties of small sized scatterers can be obtained with numerically accurate methods, such as, the finite-difference time-domain (FDTD) [17, 18], the pseudo-spectral time-domain (PSTD) [19, 20], and the discrete dipole approximation [21-23]. For large sized scatterers, the geometric optics methods can be used to find the single-scattering properties [24-26].

In addition to the aforementioned scattering methods, some approximate methods, such as, Rayleigh-Gans scattering and the anomalous diffraction theory (ADT) [6], are appropriate for extremely soft scatterers, and numerous approximate methods have been employed to study soft scatterers [27-32]. One type of soft scatterer, the red blood cell, has been extensively studied using both accurate [33-37] and approximate methods [38-

43]. The methods used for soft scatterers are only applicable to small-sized or extremely soft cases. In this study, the many-body iterative T-matrix (MBIT) [44, 45] and the geometric optics method using a volume integral equation of the electric field, the ray-by-ray (RBR) [24], are employed to obtain the scattering properties for a range of sizes for “soft” chain-forming triangular prism shaped diatoms found in the ocean.

2. Methods

2.1 MBIT

Based on the T-matrix, the incident and scattered electric field can be expanded in terms of the vector spherical wave functions [14]:

$$\begin{aligned}\mathbf{E}^{inc}(k\vec{r}) &= \sum_{n=1}^{\infty} \sum_{m=-n}^n [a_{mn} Rg\mathbf{M}_{mn}(k\vec{r}) + b_{mn} Rg\mathbf{N}_{mn}(k\vec{r})] \\ \mathbf{E}^{sca}(k\vec{r}) &= \sum_{n=1}^{\infty} \sum_{m=-n}^n [p_{mn} \mathbf{M}_{mn}(k\vec{r}) + q_{mn} \mathbf{N}_{mn}(k\vec{r})], r > r_{>}\end{aligned}\quad (1)$$

where k is the wave number in vacuum; $r_{>}$ is the radius of the smallest circumscribed sphere of a scatterer; $Rg\mathbf{M}, Rg\mathbf{N}, \mathbf{M}, \mathbf{N}$ are the vector spherical wave functions; and, a_{mn}, b_{mn} and p_{mn}, q_{mn} are the expansion coefficients of the incident and scattered fields [14]. Due to the linearity of the Maxwell equations, the transition matrix $\mathbf{T}$ can be formally expressed in terms of the relationship between the incident and scattered expansion coefficients:

$$\begin{pmatrix} p_{mn} \\ q_{mn} \end{pmatrix} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \begin{pmatrix} T_{mm'n'}^{11} & T_{mm'n'}^{12} \\ T_{mm'n'}^{21} & T_{mm'n'}^{22} \end{pmatrix} \begin{pmatrix} a_{m'n'} \\ b_{m'n'} \end{pmatrix} \quad (2)$$

According to the MBIT method [44, 45], the original scatterer can be divided into N sub-scatterers along the direction of its main axis, and the T-matrix technique can deal

with each sub-scatterer. Consequently, N frame of references exist, each located in the centers of the N sub-scatterers and enumerated from 1 to N. The scattered field expansion coefficients of the original scatterer can be iteratively obtained in terms of the transition matrices of the sub-scatterers:

$$\begin{pmatrix} p_{mn}^{o(i)} \\ q_{mn}^{o(i)} \end{pmatrix} = \begin{pmatrix} p_{mn}^{(i)} \\ q_{mn}^{(i)} \end{pmatrix} + \sum_{\substack{j=1 \\ j \neq i}}^N \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \begin{pmatrix} RgA_{-m'n'}^{-mn}(k\vec{r}_{ij}) & RgB_{-m'n'}^{-mn}(k\vec{r}_{ij}) \\ RgB_{-m'n'}^{-mn}(k\vec{r}_{ij}) & RgA_{-m'n'}^{-mn}(k\vec{r}_{ij}) \end{pmatrix} \begin{pmatrix} p_{m'n'}^{(j)} \\ q_{m'n'}^{(j)} \end{pmatrix}, i=1, \dots, N \quad (3)$$

$$\begin{pmatrix} p_{mn}^{(j)} \\ q_{mn}^{(j)} \end{pmatrix} = \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \begin{pmatrix} T_{mnm'n'}^{11,(j)} & T_{mnm'n'}^{12,(j)} \\ T_{mnm'n'}^{21,(j)} & T_{mnm'n'}^{22,(j)} \end{pmatrix} \begin{pmatrix} a_{m'n'}^{(j)} \\ b_{m'n'}^{(j)} \end{pmatrix}, j=1, \dots, N \quad (4)$$

$$\begin{pmatrix} a_{mn}^{(i)} \\ b_{mn}^{(i)} \end{pmatrix} = \begin{pmatrix} a_{mn}^{o(i)} \\ b_{mn}^{o(i)} \end{pmatrix} + \sum_{\substack{j=1 \\ j \neq i}}^N \sum_{n'=1}^{\infty} \sum_{m'=-n'}^{n'} \begin{pmatrix} A_{-m'n'}^{-mn}(k\vec{r}_{ij}) & B_{-m'n'}^{-mn}(k\vec{r}_{ij}) \\ B_{-m'n'}^{-mn}(k\vec{r}_{ij}) & A_{-m'n'}^{-mn}(k\vec{r}_{ij}) \end{pmatrix} \begin{pmatrix} p_{m'n'}^{(j)} \\ q_{m'n'}^{(j)} \end{pmatrix}, i=1, \dots, N \quad (5)$$

where the superscript “o” represents the expansion coefficients of the original scatterer; the superscripts “i” and “j” indicate the expansion coefficients obtained relative to the i-th and j-th frame of reference; $T^{(j)}$ is the T-matrix of the j-th sub-scatterer relative to its frame of reference; and, RgA, RgB, A, and B are the addition coefficients, which represent the translation of the expansion coefficients between different frames of reference [46-48]. In Eqs. (2) and (4), the IITM is used to calculate the transition matrix of the sub-scatterers, and in Eq. (5), the stabilized bi-conjugate gradient iterative method is employed to accelerate the convergence rate [49-51]. The single-scattering properties of the original scatterer can be obtained in terms of Eqs. (3), (4), and (5).

2.2 RBR

When the characteristic length of a scatterer is much larger than the incident wavelength, the geometric optics method can be employed to find the internal field in terms of the ray

tracing technique. Assuming each ray to have a circular cross section within the scatterer, the internal electric field $\mathbf{E}(\vec{r}')$ can be obtained in terms of the superposition of the electric field values associated with various rays within the particle, that is, the total internal electric field (the near field) can be added ray by ray [24]. The scattered electric field in the far field can be obtained in terms of the volume integral equation:

$$\mathbf{E}^{sca}(k\vec{r})|_{kr \rightarrow \infty} = \frac{\exp(ikr)}{-ikr} \frac{-ik^3}{4\pi} \iiint_V (\epsilon - 1) [\mathbf{E}(\vec{r}') - \hat{r}(\hat{r} \cdot \mathbf{E}(\vec{r}'))] \exp(-ik\hat{r} \cdot \vec{r}') d^3r' \quad (6)$$

where $\mathbf{E}(\vec{r}')$ is the internal field within the scatterer, k is the wavenumber in vacuum, $\hat{r}$ is the unit vector of the scattering direction, and ϵ is the isotropic permittivity of the scatterer. The volume integral equation in Eq. (6) can be replaced by a summation over number of rays and scattering orders in a geometric optics approximation as follows:

$$\mathbf{E}^{sca}(k\vec{r})|_{kr \rightarrow \infty} = \frac{\exp(ikr)}{-ikr} \frac{ik^3}{4\pi} \sum_{\gamma} \sum_p (1 - \epsilon) q_{\gamma,p}(\hat{r}) \mathbf{U}_{\gamma,p} \mathbf{E}^{int} \quad (7)$$

where γ denotes the number of rays, which can cover all the illuminated side of the scatterer, p , from 0 to ∞ , denotes the scattering order, where the incident point is defined as order 0 and then order from 1 to ∞ ; $\mathbf{E}^{int}$ is the incident field; $\mathbf{U}_{\gamma,p}$ is the Fresnel coefficient associated with a series of reflection and refraction processes; $q_{\gamma,p}$ is the phase integral associated with the phase of electric field and the scattering direction over the volume past by a ray γ from the order p to the order $(p+1)$. The single scattering properties can be obtained by Eq. (7) in terms of a ray-by-ray algorithm (RBR). The RBR actually is a geometric-physical optics method, where the near field is obtained by ray-tracing and the far field by accurately mapping the near field to in terms of the Eqs. (6) and (7). Moreover, implicitly included into the calculation is the diffraction, a significant

component of forward scattering for soft scatterers [40]. In Eq. (7), the interferences of the diffraction and the different rays are all automatically taken into consideration, which is important for the scattering of soft scatterers [43]. For homogeneous facet scatterers, the ray-tracing process can be obtained analytically by the physical-geometric optics hybrid (PGOH) method [26], which can be used to verify the RBR process.

3. Simulation results and discussion

Diatoms, a type of ocean phytoplankton, are a significant part of the oceanic ecosystem. In 3D *in situ* holographic imaging observations [52-54], some diatoms not only show large aspect ratios, but also link together to form linear chains. In a plethora of diatom cell shapes, the present simulations of the optical properties of chain-forming triangular prism diatoms are focused on the Mueller Matrix elements [6, 7].

Figure 1 shows images of the triangular prism *Ditylum sp.*: (a) of linear chains in the ocean where they tend to align in the direction of the ocean currents, (b) of a single chain, and (c) of a single diatom cell. A single cell is composed of three layers: the outer hard shell with two spines, the cytoplasm, and the cell nucleus. Based on the materials of the three layers, the refractive indices relative to water are respectively set to be $1.1+i0.0$, $1.03+i0.0001$, and $1.06+i0.025$ [55, 56].

Figure 2 (a) shows the simulation model in terms of a diatom cell structure with dimensions taken from microscopic analysis with two concentric triangular prisms for the two outer layers, two cylinders for the two spines, and a sphere in the center for the core. Diatom chains are formed by linearly connecting the cells. Figure 2 (b) shows the laboratory frame of reference with the z-axis along the prism main axis and the x-axis perpendicular to one of the prism side surfaces and pointing inside toward the

corresponding edge of the prism, and the interpretation of the incident relative angles. H indicates the prism height and r is the distance from the prism lower center to the vertex.

3.1 Validation of the present computational methods

The transition matrix is necessary input for the MBIT and is indicated by Eq. (4). The IITM is employed to find the T-matrix of the inhomogeneous diatom cell shown in Figure 2. The Amsterdam discrete dipole approximation (ADDA) code is used as a benchmark method to validate the simulations.

Figure 3 shows a comparison between the Mueller matrix elements computed with the IITM and the ADDA for the diatom cell shown in Figure 2(a). In Figure 2(b), the outer prism height H and radius r are $3\mu\text{m}$ and $0.75\mu\text{m}$, the inner prism height H and radius r are $2.86\mu\text{m}$ and $0.68\mu\text{m}$, the core radius is $0.19\mu\text{m}$, and the spine length and diameter are $0.6\mu\text{m}$ and $0.15\mu\text{m}$, the incident wavelength is $0.475\mu\text{m}$, and the incident angles are $\theta_i = 40^\circ, \phi_i = 30^\circ$. The results computed from the two methods are identical, and indicate the MBIT can successfully use the transition matrix to obtain the single-scattering properties of many diatom cells.

Figure 4 shows a comparison between the Mueller matrix elements computed with the MBIT and the ADDA for two diatom cells. Two diatom cells are linearly connected along the direction of the z -axis in the laboratory frame of reference. For each cell, all the parameters are the same as in Figure 3. The MBIT uses an iterative technique to calculate the scattering properties of the two diatom cells while the ADDA generates dipoles of the two diatom cells and treats them as a whole. The perfect agreement indicates the accuracy of the MBIT.

Figure 5 shows a comparison between the Mueller Matrix elements computed with the PGOH and the RBR for the homogeneous triangular prism shown in Figure 2(b). The prism height and radius are $9\mu\text{m}$ and $2.25\mu\text{m}$, the refractive index is $1.1+i0.0$, the incident wavelength is $0.475\mu\text{m}$, and the incident angles are $\theta_i = 40^\circ, \phi_i = 40^\circ$. The PGOH and the RBR are both geometric optics methods, but the ray-tracing part of the PGOH is analytically obtained while the RBR uses a number of rays to approximate the incident cross section. Exact results for the homogeneous prism indicate the correctness of the RBR process.

3.2 Simulation of the optical properties of diatom particles

The relative refractive indices of a diatom cell are close to unity, and the interactions between different diatom cells are weak. If no interaction between the cells is assumed, the scattered electromagnetic field of different cells relative to a standard has a phase difference $\exp(ik_0(\hat{n}_i - \hat{n}_s) \cdot \vec{r}_{j0})$, where $k_0, \hat{n}_i, \hat{n}_s, \vec{r}_{j0}$ are, respectively, the wavenumber in a vacuum, the unit vectors of the incident and scattering directions, and the displacement vector of the j-th cell relative to the standard.

Figure 6 compares the Mueller Matrix elements of three cells calculated by the MBIT and IITM, plus the phase differences with the assumption of no interaction between the cells. For one cell, the outer prism height H and radius r are $3\mu\text{m}$ and $0.75\mu\text{m}$, the inner prism height H and radius r are $2.86\mu\text{m}$ and $0.68\mu\text{m}$, the core radius is $0.19\mu\text{m}$, the spine length and diameter are $0.6\mu\text{m}$ and $0.15\mu\text{m}$, and the incident wavelength is $0.475\mu\text{m}$. An average of 273 orientations are taken in order to do a random orientation average. The

discrepancy between the numerically accurate and the assumed samples is negligible, which indicates the weak interactions between diatom cells.

Figure 7 compares the Mueller Matrix elements of one cell computed by the IITM and RBR. The outer prism height H and radius r are $6\mu\text{m}$ and $1.5\mu\text{m}$, the inner prism height H and radius r are $5.72\mu\text{m}$ and $1.36\mu\text{m}$, the core radius is $0.38\mu\text{m}$, the spine length and diameter are $1.2\mu\text{m}$ and $0.3\mu\text{m}$, the incident wavelength is $0.475\mu\text{m}$, and the incident angles are $\theta_i = 90^\circ, \phi_i = 0^\circ$. For the backscattering of P_{11} , a high specular peak occurs due to the flat surface of the outer prism. The elements $P_{12}/P_{11}, P_{22}/P_{11}, P_{33}/P_{11}, P_{44}/P_{11}$ have the features of soft scatterers.

Figure 8 shows a comparison between the Mueller Matrix elements of one cell calculated by the ADDA and the RBR. The outer prism height H and radius r are $9\mu\text{m}$ and $4.5\mu\text{m}$, the inner prism height H and radius r are $8.58\mu\text{m}$ and $4.29\mu\text{m}$, the core radius is $0.57\mu\text{m}$, the spine length and diameter are $1.8\mu\text{m}$ and $0.45\mu\text{m}$, the incident wavelength is $0.475\mu\text{m}$, and the incident angles are $\theta_i = 90^\circ, \phi_i = 45^\circ$. The phase function peaks are due to the geometric optics effect. The right four panels show the features of soft scatterers. The simulation results become more accurate with an increase in cell size.

Figure 9 shows a comparison between the Mueller Matrix elements of one cell calculated by the ADDA and the RBR. The incident angles are $\theta_i = 70^\circ, \phi_i = 0^\circ$, and the other parameters are the same as in Figure 8. The elements agree very well except for P_{43}/P_{11} which has discrepancies in the scattering angles around 90° .

Figure 10 shows a comparison between the Mueller Matrix elements of one cell computed with the IITM and the RBR. The outer prism height H and radius r are $9\mu\text{m}$

and $2.25\mu\text{m}$, the inner prism height H and radius r are $8.58\mu\text{m}$ and $2.04\mu\text{m}$, the core radius is $0.57\mu\text{m}$, and the spine length and diameter are $1.8\mu\text{m}$ and $0.45\mu\text{m}$, and the incident wavelength is $0.475\mu\text{m}$. The incident zenith angle θ_i is 90° and the result is averaged by the incident azimuthal angles ϕ_i from 0° to 60° . In this case, the elements P_{12}/P_{11} , P_{33}/P_{11} , and P_{44}/P_{11} show perfect Rayleigh scattering features.

Figure 11 shows a comparison between the Mueller Matrix elements of two diatom cells computed with the MBIT and the RBR. All the parameters are the same as in Figure 10 except two cells are considered. The RBR ray tracing occurs on only one cell, but the ray tracing part of the other cells can be obtained in terms of the periodic boundary conditions. The elements are similar to Figure 10 because the interactions between two cells are weak, and the same conclusion is reached as that shown in Figure 6.

The refractive indices of all three layers of a single cell are soft so that the elements P_{12}/P_{11} , P_{22}/P_{11} , P_{33}/P_{11} and P_{44}/P_{11} have show similar Rayleigh scattering features in small and intermediate sizes. It indicates that these elements in the case of soft refractive indices and intermediate sizes are not sensitive to its shape and inhomogeneity.

4. Conclusion

In this study, the scattering properties of the diatom chains in the ocean are simulated in terms of two numerically accurate methods, the IITM and the MBIT, and an approximate method, the RBR. The application of the three methods to diatom chains is verified in comparison with the simulations based on the ADDA and the PGOH methods. The particle model and the refractive indices are based on the actual shape and composition of diatoms. In order to obtain reasonable results, the interference between soft particles' outgoing rays must be taken into consideration. The MBIT effectively deals with linear

diatom cell chains with the transition matrix of one cell and the iterative technique. The RBR method calculates the near field by using the ray-tracing technique, and the far field by using a volume integral equation that maps the near field to the far field. For multiple diatom cells, the RBR traces one cell and the result is applied to all other cells in terms of the periodic boundary conditions. The simulation results of the diatom chains are shown for different aspect ratios, sizes, incident angles, and diatom numbers. Compared to the results calculated by the accurate methods, the overall agreement of the Mueller matrix elements has been obtained by the RBR. For soft particles, the MBIT and the RBR can be combined to obtain the scattering properties for a complete range of sizes.

Acknowledgement

The authors thank that Tamotsu Nagumo allows us to use his *Ditylum brightwelli* figure in Fig. 1(c). The authors thank Drs. Maxim Yurkin and A.G. Hoekstra for the use of their ADDA code. The authors acknowledge the Texas A&M Supercomputing Facility for computing resources. George Kattawar acknowledges support by the ONR MURI program (N00014-09-1-1054) and the National Science Foundation Grant # OCE-1130906. Ping Yang acknowledges the support by a NASA grant (NNX11AK37G). Bingqiang Sun was supported by ONR Coastal Geophysics. M. Twardowski and J. Sullivan gratefully acknowledge support from the National Ocean Partnership Program, ONR Coastal Geophysics, and the Harbor Branch Oceanographic Institute Foundation. The authors thank the anonymous reviewers for constructive comments.

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(a)

(b)

(c)

Figure 1. Different scale views of the diatom *Ditylum*: (a) linear chains of diatoms in the ocean; (b) a single diatom chain; and, (c) a single diatom cell.

Figure 2(a). Simulation model in terms of diatom cell structure: two concentric triangular prisms represent the two outer layers and a center sphere represents the core. Chains are formed by linearly linking the diatom cells. (b). The laboratory frame of reference with the z-axis along the prism's main axis and the x-axis perpendicular to one of the prism side surfaces and pointing inside to the corresponding prism edge, and an interpretation of the relative incident angles. H indicates the prism height and r is the distance from the prism lower center to the vertex.

Figure 3. Comparison between the Mueller matrix elements calculated by the IITM and the ADDA for the diatom cell shown in Figure 2. The outer prism height H and radius r are $3\mu\text{m}$ and $0.75\mu\text{m}$, the inner prism height H and radius r are $2.86\mu\text{m}$ and $0.68\mu\text{m}$, the core radius is $0.19\mu\text{m}$, the spine length and diameter are $0.6\mu\text{m}$ and $0.15\mu\text{m}$, the incident wavelength is $0.475\mu\text{m}$, and the incident angles are $\theta_i = 40^\circ, \phi_i = 30^\circ$.

Figure 4. Comparison between the Mueller matrix elements of two diatom cells calculated by the MBIT and the ADDA. Two diatom cells are linearly connected along the direction of the z-axis of the laboratory frame of reference. For one cell, all the parameters are the same as in Figure 3.

Figure 5. Comparison between the Mueller Matrix elements calculated by the PGOH and the RBR for the homogeneous triangular prism shown in Figure 2b. The prism height and radius are $9\mu\text{m}$ and $2.25\mu\text{m}$, the refractive index is $1.1+i0.0$, the incident wavelength is $0.475\mu\text{m}$, and the incident angles are $\theta_i = 40^\circ, \phi_i = 40^\circ$.

Figure 6. Comparison between the Mueller matrix elements of three cells calculated by the MBIT and by IITM, plus the phase difference with the assumption of no interaction between the cells. For one cell, the outer prism height H and radius r are $3\mu\text{m}$ and $0.75\mu\text{m}$, the inner prism height H and radius r are $2.86\mu\text{m}$ and $0.68\mu\text{m}$, the core radius is $0.19\mu\text{m}$, the spine length and the diameter are $0.6\mu\text{m}$ and $0.15\mu\text{m}$, and the incident wavelength is $0.475\mu\text{m}$. An average of 273 orientations are taken to obtain random orientation results.

Figure 7. Comparison between the Mueller Matrix elements of one cell calculated by the IITM and RBR. The outer prism height H and radius r are $6\mu\text{m}$ and $1.5\mu\text{m}$, the inner prism height H and radius r are $5.72\mu\text{m}$ and $1.36\mu\text{m}$, the core radius is $0.38\mu\text{m}$, the spine length and diameter are $1.2\mu\text{m}$ and $0.3\mu\text{m}$, the incident wavelength is $0.475\mu\text{m}$, and the incident angles are $\theta_i = 90^\circ, \phi_i = 0^\circ$.

Figure 8. Comparison between the Mueller Matrix elements of one cell calculated by the ADDA and the RBR. The outer prism height H and radius r are $9\mu\text{m}$ and $4.5\mu\text{m}$, the inner prism height H and radius r are $8.58\mu\text{m}$ and $4.29\mu\text{m}$, the core radius is $0.57\mu\text{m}$, the spine length and diameter are $1.8\mu\text{m}$ and $0.45\mu\text{m}$, the incident wavelength is $0.475\mu\text{m}$, and the incident angles are $\theta_i = 90^\circ, \phi_i = 45^\circ$.

Figure 9. Comparison between the Mueller Matrix elements of one cell calculated by the ADDA and the RBR. The incident angles are $\theta_i = 70^\circ, \phi_i = 0^\circ$, and the other parameters are the same as in Figure 8.

Figure 10. Comparison between the Mueller Matrix elements of one cell calculated by the IITM and the RBR. The outer prism height H and radius r are $9\mu\text{m}$ and $2.25\mu\text{m}$, the inner prism height H and radius r are $8.58\mu\text{m}$ and $2.04\mu\text{m}$, the core radius is $0.57\mu\text{m}$, and the spine length and diameter are $1.8\mu\text{m}$ and $0.45\mu\text{m}$, the incident wavelength is $0.475\mu\text{m}$, and the incident zenith angle θ_i is 90° with the result averaged by the incident azimuthal angles ϕ_i from 0° to 60° .

Figure 11. Comparison between the Mueller Matrix elements of two diatom cells calculated by the MBIT and the RBR. All the parameters are the same as in Figure 10 except that two cells are considered.