Inherent optical properties of pollen particles: a case study for the morning glory pollen

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Abstract: Biological aerosols, such as bacteria, fungal spores, and pollens, play an important role on various atmospheric processes, whereas their inherent optical property is one of the most uncertainties that limit our ability to assess their effects on weather and climate. A numerical model with core-shell structure, hexagonal grids and barbs is developed to represent one kind of realistic pollen particles, and their inherent optical properties are simulated using a pseudo-spectral time domain method. Both the hexagonal grids and barbs substantially affect the modeled pollen optical properties. Results based on the realistic particle model are compared with two equivalent spherical approximations, and the significant differences indicate the importance of considering pollen geometries for their optical properties.

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1. Introduction

Biological particles, such as bacteria, fungal spores, and pollens, show significant impacts on atmospheric processes (e.g. direct radiative effects and severing as cloud condensation nuclei or ice forming nuclei), and have been investigated with increasing intensity [1–4]. Biological aerosols occupy up to 30% of total aerosol loading over continental areas [5,6], and the percentage can be even higher in certain locations or certain seasons [1]. Thus, they may significantly affect radiative forcing by directly absorbing and scattering radiation. However, the inherent optical properties of those particles are among the most uncertain quantities for aerosol researches, and, thus, limit our ability to assess their effects on environment and climate [1,2]. The necessity and importance to study biological optical properties have been carefully stressed by Després et al. [1].

Pollen particles are one of the largest biological particles, and their equivalent diameters may reach 100μm [1,7]. The concentration, size distribution, dispersion, transportation and residence time of pollen particles have been intensively studied by in situ measurement [1,8–10]. Various networks are built to advance our knowledge of pollen particles, including the Pollen Monitoring Program in Europe [9] and Pollen Biology Research Coordination Network in the United States [10]. Although having relatively large sizes [1,11], pollen particles can also travel long distances and be lifted into upper layers of the atmosphere [4,12–14]. It is noticed by Sassen [15] that boreal tree pollen may generate strong laser depolarization, and those biogenic depolarization could lead to confusion in the CALIPSO lidar observations [15]. Spänkuch et al. [7] show that the high concentration of pine pollen significantly increases the down-welling infrared flux. Overall, pollen particles should be of importance to atmospheric radiation and remote sensing (especially on regional scale). However, studies on the optical properties of pollen particles are relatively limited, and only spherical and spheroidal models are used to explain the pollen corona [16–19]. Because shapes of pollen particles from different plant families and species can be significantly variable and irregular [11,20–22], accurate modeling of their optical properties becomes extremely difficult. Furthermore, it is perhaps beyond our current ability to mathematically describe the exact geometries of those naturally occurring particles.

Meanwhile, as an essential component of atmospheric radiative transfer and remote sensing, aerosol optical properties, such as the extinction efficiency, single-scattering albedo, asymmetry factor and scattering phase matrix, have been widely studied. Aerosol particles normally have complicated and irregular geometries, and both numerical and observational investigations indicate that simple spherical models are not accurate enough for atmospheric applications [23,24]. Those studies focus on particles, such as dust, black carbon and sea salt. Among them, dust particles are the most intensively investigated aerosol, and various complex and irregular models have been developed, such as Poisson-Voronoi tessellation [25], agglomerate debris particles [26], and fractal polyhedra [27]. Those models show much improved performances on representing the optical properties of natural dust. However, similar work on biological particles is missing [1,2].

As a result, this study takes pollen as an example. We develop a non-spherical and inhomogenous model for one kind of pollen particles, and investigate their inherent optical properties numerically. The remainder of this paper is organized as follows. The numerical models to represent the pollen particles and to simulate their inherent optical properties are described in Section 2. Section 3 presents results to show the resulting optical properties and compares them with those from two simple spherical approximations. The conclusions of this study are discussed in Section 4.
2. Numerical models for pollen particles

One of the toughest problems that limits our understanding on the optical properties of pollen particles (as well as other aerosols) is the variation on their geometries, for particles either from different plants or within one plant. Fortunately, similar features do exist for their geometries, such as internal lipidic structures coated by elaborate extracellular pollen wall. The overall shapes are either spherical or irregular, and the pollen wall can have quite complicated structures [21,28]. This study considers an example of pollen particles from the images taken by the Dartmouth Electron Microscope Facility [29], i.e. a scanning electron microscope image of morning glory pollen (in the genus ipomoea purpurea and family convolvulaceae). It should be noticed that we only focus on this single but general example, whereas the model is flexible enough to be modified and generalized to account pollen particles of other kinds due to the geometrical similarity.

![Fig. 1. A pollen image and procedures to generate a pollen model.](image)

The pollen particle we considered is shown in Fig. 1(a) [29], and this study intends to build a numerical model similar to the real one. Generally, three steps used to generate the numerical model correspond to three particle features, i.e. the core-shell structure, hexagonal grids and barbs on the surface, and the procedure is illustrated in Fig. 1. Firstly, concentric core-shell spheres are used, i.e. Figure 1(b), and a smooth spherical particle is generated. The core part corresponds to the internal lipidic material of pollen particles, and the spherical shell is the pollen wall of the first layer. Secondly, hexagonal grids are added outside the smooth sphere, and the resulting particle is illustrated in Fig. 1(c). There are also some pentagon elements in the mesh grids, and particles with hexagons and pentagons have been used to simulate light scattering properties of small ice crystals [30]. The hexagonal grids are assumed to have the same height and width, and the details of generating them will be given in the following paragraph. The last step is to add “barbs” on each vertex of hexagonal grids, and they are assumed to be cylinders with the same size. Following the aforementioned procedures, the numerical pollen particle generated is shown in Fig. 1(d). The parameters of
the model particle will be given later. Furthermore, each vertex of the hexagonal grids as well as attached barbs can be randomly moved, and Figs. 1(e) and 1(f) are two examples of the randomized pollen particles. To be consistent with real pollen particles, our numerical model is inhomogeneous. The spherical core from the first step is a kind of material representing internal lipidic part, and all other elements, including the spherical shell from the first step, the hexagonal grids added in the second step and the barbs, are treated as a homogeneous part, representing an extracellular “pollen wall”. It is clearly shown that our numerical generated particle is highly similar to the realistic one in Fig. 1(a) [29].

As shown in the image of Fig. 1(a), the pollen surface is discretized by hexagonal grids, and the hexagonal elements are quite regular and similar-sized. Thus, the second step discussed above is designed to generate similar grids numerically. To our knowledge, hexagonal grids are widely used for geodesic discrete global grid system [31]. The scheme developed by Williamson [31,32] is adopted in this study. The scheme starts from a regular icosahedron, i.e. polyhedron with twenty same-sized regular triangles and twelve vertices, which is shown in Fig. 2(a), and all vertices are on the same sphere. Then, each triangle is discretized in the way illustrated in Fig. 2(b), i.e. separated into four regular hexagons, three half-hexagons and three triangles (all discretized sides have the same length). After the discretization, the new vertices are projected to the circumsphere of the icosahedron, and the hexagonal surfaces are kept. The two connected half-hexagons are combined as a whole, and the five triangles around each original vertex can build a regular pentagon surface (with the original vertex removed). Overall, the sphere is discretized into 110 hexagons and twelve pentagons, which is shown in Fig. 2(c). Each side on the discretized surface can be changed into a “wall” by projecting to a larger spherical shell and widening, and the resulting meshed sphere is shown in Fig. 2(d).

The relative sizes of the model elements, including radius of the core \((r_c)\), thickness of the spherical shell \((h_s)\), height/thickness and width of the hexagonal grids \((h_h \text{ and } w_h)\), diameter and height of the cylindrical barbs \((d_b \text{ and } h_b)\), are roughly approximated based on the image given in Fig. 1(a). Figure 3 and Table 1 illustrate the length parameters used in the model. The concentric spheres in Fig. 3(a) indicate the four layers of the model, i.e. core, spherical shell, hexagonal grids and barbs. In Fig. 3(a), \(R\) is the particle overall radius, and all size
parameters are given in unit of $R$ in Table 1. Figures 3(b) and 3(c) give the basic hexagonal and cylindrical element of the model, respectively.

![Diagram](Image)

**Fig. 3.** (a) A cross section indicating four layers of the modeled particles (i.e. core, spherical shell, hexagonal grids and barbs). (b) A hexagonal grid element. (c) A cylinder representing the barbs on the pollen surface. The parameters to determine the particle geometries are all listed in the figure.

### Table 1. Length Parameter Used to Generate the Pollen Particle

| Symbol | Quantity                        | Value used in the model |
|--------|---------------------------------|--------------------------|
| $r_c$  | Radius of the internal core     | $0.70R$                  |
| $h_s$  | Thickness of the spherical shell| $0.05R$                  |
| $h_h$  | Thickness of the hexagonal grid | $0.10R$                  |
| $w_h$  | Width of the hexagonal grid     | $0.05R$                  |
| $d_b$  | Diameter of the cylindrical barb| $0.05R$                  |
| $h_b$  | Height of the cylindrical barb  | $0.15R$                  |
| $R$    | Overall radius                  | $R$                      |
| $D$    | Overall diameter                | $2R$                     |

With the geometry of the pollen particle mathematically defined, it is straightforward to calculate their optical properties. The pseudo-spectral time domain (PSTD) method, pioneered by Liu [33], is used. Differing from the traditional finite-difference time domain method (FDTD) [34–36], the PSTD uses a spectral method to approximate the spatial derivatives in Maxwell’s curl equations, and was first applied to simulate optical properties of atmospheric particles by Chen et al. [37]. The method as well as the computational implementation has been significantly improved by Liu et al. [38]. The current PSTD implementation is carefully validated for both homogenous and inhomogeneous particles [39,40], and applied for optical properties of randomly oriented hexagonal columns with a size parameter of 100 (defined as $\pi L/\lambda$, where $L$ is the length of the column and $\lambda$ is the incident wavelength.) [37]. Thus, the PSTD is used to simulate the optical properties of the particles described above, and the details on the accuracy and efficiency of the implementation can be found in [41]. The incident wavelength is chosen to be 0.65$\mu$m. There are still significant uncertainties on the refractive indices of biological particles [42,43]. For simplification, both the internal lipidic sphere and pollen wall (including the spherical shell, hexagonal grids and barbs) are assumed to be non-absorptive, i.e. their imaginary parts of refractive indices being zero, and the real parts are set to be 1.3 and 1.5, respectively. The PSTD discretizes the space with cubic cells, and each cell is given the corresponding refractive index to define the modeled particle. With the geometric parameters given in Table 1, the volume fractions of the internal and wall parts are approximately 53% and 47%, respectively. This study emphasizes the geometries of the pollen particle, whereas more accurate refractive indices should be determined for further applications. All optical properties discussed in this study are those of randomly oriented particles, and results are
obtained by averaging those from particles with different orientations. With the symmetry of the modeled pollen particle (the same as that of regular icosohedron), only 60 different particle orientations are enough to give the averaged properties, whereas much more may be needed for non-symmetric particles as noticed by other studies [44,45].

3. Results and discussions

Figure 4 shows the non-zero phase matrix elements of pollen particle with an overall diameter \( D = 20 \mu m \), and the size parameter of the final modeled particle \((\pi D/\lambda)\) is 97. As discussed in Section 2, three steps are used to generate the particle, and the resulting phase matrix elements corresponding to the particle after each step are illustrated in the figure. The comparison shows the influence of each geometrical element on pollen optical properties. The computational domain used for the PSTD simulation includes \(300 \times 300 \times 300 \) grid cells, which are fine enough to describe the particle we defined (e.g. a barb is discretized into over 4000 cubic cells).

With only the concentric core-shell structure (particle in Fig. 1(b)), it should be expected that the phase function \((P_{11})\) and the ratios of other elements to the phase function are highly oscillated (except \(P_{22}/P_{11}\) being 1). The curves labeled “with hexagonal grids” in Fig. 4 represent results for the particle with hexagonal grids added (particle in Fig. 1(c)). Besides the strong forward peak on the phase function, the hexagonal grids smooth out the oscillations on all the phase matrix elements. \(P_{12}/P_{11}\) becomes close to zero, and \(P_{22}/P_{11}\) is significantly smaller than 1. It should be noticed that, to be consistent, the ratio \(P_{12}/P_{11}\), not the linear polarization \(-P_{12}/P_{11}\), is given in the figure. The red curves in the figure are the phase matrix elements of our modeled pollen (the final pollen particle in Fig. 1(d)) with a diameter of 20\(\mu m\). The phase matrix elements of the particle “with hexagonal grids” and “modeled pollen” show little difference, and this may be due to the relatively small fraction of the barbs (approximately 7% of the overall volume). Relatively strong backward scattering peaks at scattering angle of 180° are noticed, and they are similar to other non-spherical particles at non-absorptive wavelengths [46,47]. The extinction efficiency (\(Q_{ext}\)) and asymmetry (\(g\)) factors of the particle are listed in the figure. Although the barbs have little influence on the
phase matrix elements, they increase the extinction efficiency (i.e. scattering efficiency at this case) by approximately 20%.

Figure 4 indicates that the hexagonal grids do significantly influence the phase matrix of pollen particles. However, it is almost impossible to model the hexagonal grids accurately considering the irregularity and variation of natural particles. Figure 5 illustrates the importance of the detailed grid structure by comparing the phase matrices of pollen particles with regular and irregular hexagonal grids. As mentioned in Section 2, the vertices of the hexagonal grids can be randomly moved on the spherical surface to generate irregular grids. To define the degree of modeled irregularity, we introduce a criterion that limits the maximum length between the randomized vertex and the original one. The irregularity criterion, \( \alpha \), is the ratio of the maximum length moved to the length of the shortest side on the regular hexagonal grids. Considering that the real pollen particle has quite regular hexagonal grids, \( \alpha \) values of 0 (regular case), 0.125 and 0.25 (two slightly irregular cases) and a diameter of 20\( \mu \)m (size parameter of 97) are used for the simulations in Fig. 5, and the corresponding particles are given in Figs. 1(e) and 1(f). With close agreements on the phase matrix elements of the three pollen particles (i.e. \( \alpha = 0, 0.125 \) and 0.25), Fig. 5 indicates that the minor movements of the hexagonal grids have little effect on the phase matrices of the pollen particles. The integral optical properties, i.e. extinction efficiencies and asymmetry factors (listed in the figure), are also very close with each other. As a result, as long as the general grid structure exists, the detailed adjustments can hardly influence the pollen optical properties.

We are capable of calculating the optical properties of complicated particles accurately, at least for those with a size parameter up to almost two hundred [38], whereas it becomes time-consuming as the particles become larger. As a result, even knowing that the optical properties of spherical and realistic non-spherical particles are quite different, most atmospheric aerosols are treated as spheres, because the optical properties of spheres can be efficiently calculated using the Mie theory [48]. To illustrate the importance and necessity of the non-spherical and complicated geometries on pollen optical properties, we compare the results with two simplified spherical models. The first model uses homogeneous spheres with
equivalent volumes, one of the simplest models that can be applied. We use the Bruggeman theory to give an effective refractive index for the inhomogeneous pollen particle we considered [40,49]. With the fixed volume fractions and refractive indices, an effective index of 1.39 is obtained. The second model considers core-shell spheres, and, in other words, the complicated pollen wall (Fig. 1(d)) is replaced by a spherical shell. To be more specific, the spherical core is the same as that of our pollen model, whereas a concentric spherical shell that has the same volume as the pollen wall (the original shell as well as the hexagonal grids and barbs) is used. The optical properties of the core-shell sphere can also be handled efficiently using a modified Mie theory [50].

![Fig. 6. The extinction efficiencies and asymmetry factors of the modeled pollen particles and the two spherical approximations (homogeneous and inhomogeneous) as functions of pollen diameter.](image)

The extinction efficiencies and asymmetry factors of the pollen particles and two spherical approximations are given in Fig. 6. The x-axis is the diameter of pollen particles, and, at each pollen diameter, the homogeneous and inhomogeneous spheres with the same volume are considered. The project areas of equivalent-volume spheres are used to calculate the extinction efficiency for all three cases. Figure 6 clearly shows that the optical properties of modeled pollen particles are substantially different from those of either homogeneous or inhomogeneous spheres. When the particle diameters are less than 10μm, similar oscillations are noticed for the extinction efficiency of all three cases. However, as the diameter becomes larger, the pollen particles show larger extinction efficiency than those of the two spherical approximations. The asymmetry factors of the pollen model are smaller than those of the two spherical approximations. Compared with the optical properties of the homogenous spheres, the extinction efficiencies of the inhomogeneous spheres have weaker oscillations, and their asymmetry factor is slightly larger.

The bulk phase matrices of the modeled pollen particles and the two spherical approximations are compared in Fig. 7. A lognormal size distribution with a geometric mean diameter of 15μm and a standard deviation of 1.4 is assumed [18]. As the bulk optical properties are averaged over different particle sizes, the oscillations for the spherical particles are smoothed out. However, the phase matrix elements of the pollen particles with realistic geometries are significantly different from those based on spherical approximations. The modeled pollen particles show very smooth variations on the phase function ($P_{11}$), which are quite different from those of spheres. $P_{12}/P_{11}$ and $P_{34}/P_{11}$ of the modeled pollen particles are close to 0, whereas the values can reach to over 0.5 for the two spherical approximations. The
other obvious difference is on the ratio of $P_{22}$ to $P_{11}$, because, for spherical particles, $P_{22}/P_{11} = 1$. The bulk extinction efficiencies and asymmetry factors are also listed in the upper left panel of the figure. As we can expect based on values shown in Fig. 6, the pollen model gives much stronger extinction efficiency (almost 20% larger than those of both spherical models) and much smaller asymmetry factors. The differences on the bulk optical properties would definitely show different influences on their interaction with the solar radiation, which will be investigated in further studies.

Fig. 7. Comparison of the non-zero phase matrix elements of modeled pollen particles and two spherical approximations.

4. Summary

This study develops a numerical model to investigate the inherent optical properties of a kind of pollen particles, and the nonspherical, inhomogeneous model exhibits quite different optical properties from those simplified spherical ones. Thus, the complicated geometry should be considered for applications related to the atmospheric radiative transfer and remote sensing. However, uncertainties on the detailed geometries and refractive indices still exist for the pollen particles, and their effects on local radiative forcing should be investigated in further studies.

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