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Absorption and scattering by fractal aggregates and by their equivalent coated spheres

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ABSTRACT

This paper demonstrates that the absorption and scattering cross-sections and the asymmetry factor of randomly oriented fractal aggregates of spherical monomers can be rapidly estimated as those of coated spheres with equivalent volume and average projected area. This was established for fractal aggregates with fractal dimension ranging from 2.0 to 3.0 and composed of up to 1000 monodisperse or polydisperse monomers with a wide range of size parameter and relative complex index of refraction. This equivalent coated sphere approximation was able to capture the effects of both multiple scattering and shading among constituent monomers on the integral radiation characteristics of the aggregates. It was shown to be superior to the Rayleigh–Debye–Gans approximation and to the equivalent coated sphere approximation proposed by Latimer. However, the scattering matrix element ratios of equivalent coated spheres featured large angular oscillations caused by internal reflection in the coating which were not observed in those of the corresponding fractal aggregates. Finally, the scattering phase function and the scattering matrix elements of aggregates with large monomer size parameter were found to have unique features that could be used in remote sensing applications.

1. Introduction

Particle aggregation and coagulation is a frequent occurrence in numerous applications such as combustion systems [1], atmospheric science [2,3], astronomy and astrophysics [4], chemistry [5], and biotechnology [6–8]. Small particles aggregate to form fractal-like structures changing the light absorption and scattering properties of the suspension [2]. For example, Fig. 1a, b, c, d, e, and f shows micrographs of soot [9], snow [10], cosmic dust [11], gold nanoparticles [12], bacteria [13], and microalgae aggregates, respectively. In all these systems, knowledge of the radiation characteristics of the fractal aggregates are of prime importance for radiation transfer analysis and remote sensing applications. The radiation characteristics of soot and aerosol aggregates have been studied extensively as reviewed by Sorensen [2]. However, to the best of our knowledge, those pertaining to aggregates composed of larger monomers such as microalgae colonies have not been studied.

Microalgae are single cell photosynthetic microorganisms growing in freshwater or seawater. They can be grown in photobioreactors (PBRs) exposed to solar radiation to produce biofuels as well as various pharmaceuticals and biochemicals [14]. For example, *Botryococcus braunii* (Fig. 1f) can be used for producing biofuels for powering jet engines [14]. This species secretes exopolysaccharides (EPS), a viscous substance coating the cell surface and causing their aggregation into colonies. EPS production is part of a protection mechanism activated in response to environmental conditions such as limited

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0022-4073/

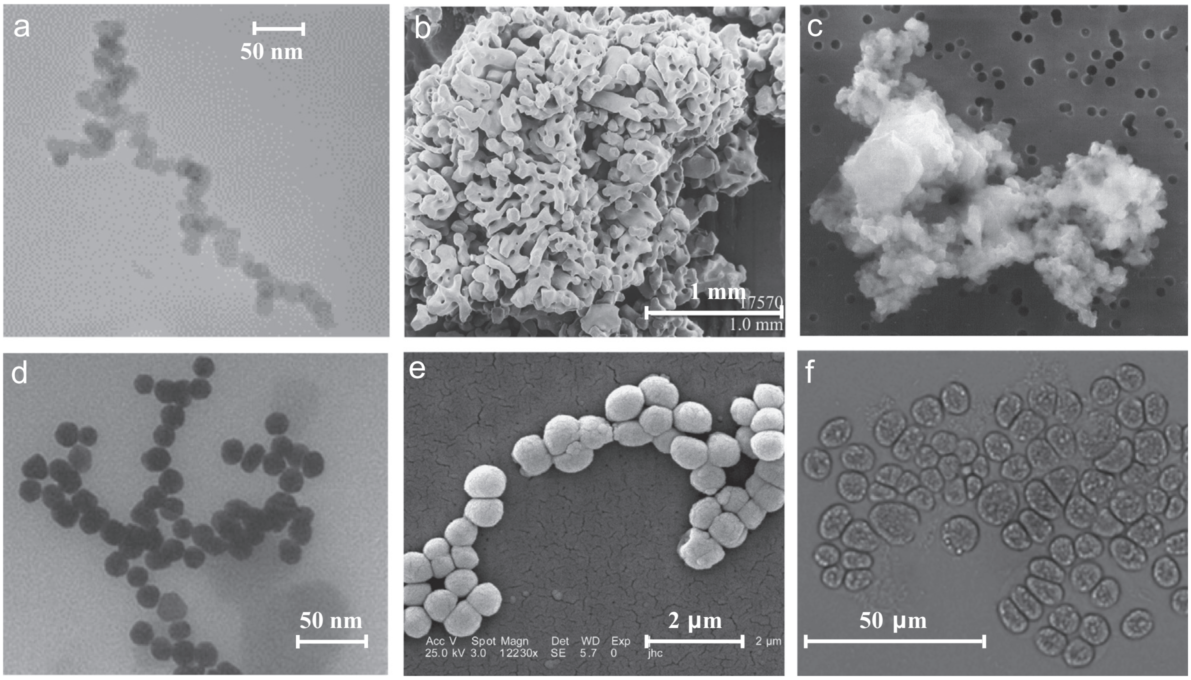

Fig. 1. Micrographs of fractal aggregates of (a) soot [9], (b) snow [10], (c) cosmic dust [11], (d) gold nanoparticles [12], (e) the bacteria *M. luteus* [13], and (f) colonie of the microalgae *B. braunii*.

illumination [15], non-optimal temperature [16], high salinity [16], and limited nutrient availability [17]. In addition, a recent study demonstrated reversible cell aggregation in concentrated *Chlorella vulgaris* cultures used for protein, starch, and lipid production [18]. The authors hypothesized that aggregation occurred at large cell concentration due to the proximity of the cells to one another. Since larger microalgae cells possess a larger surface charge density compared to smaller cells, the electrostatic repulsion between larger cells is much stronger than that between a large and a small cell [18]. This leads to aggregation of the smaller cells in the space created by the electrostatic repulsion between the larger cells.

To achieve maximum biomass and biofuel productivities, light transfer in the PBRs must be optimized [19–21]. For example, a flat-plate PBR should be designed and operated such that the fluence rate at the backwall corresponds to the photosynthetic compensation point, i.e., the minimum amount of energy required to maintain cell metabolism [21]. The latter was reported to be 10 $\mu mol_{h\nu}/m^2$ s for the microalgae *Chlamydomonas reinhardtii* [22] and 2 $\mu mol_{h\nu}/m^2$ s for the cyanobacteria *Arthrospira platensis* [19]. Optimizing PBRs for maximum biomass productivity requires the solution to the radiative transfer equation and the knowledge of the absorption and scattering cross-sections as well as the scattering phase function of the microalgal suspension [20]. Moreover, the scattering matrix elements of the microalgal suspension may be measured for remote sensing of the PBR [23]. The radiation characteristics of suspensions composed of single cells can be predicted theoretically [24–27] or measured experimentally [20,28]. However, theoretical or experimental characterization of the radiation characteristics of suspensions consisting of microalgae colonies have received less attention.

Several numerical methods exist to estimate the radiation characteristics of aggregates consisting of spherical monomers. They include the superposition T-matrix method [29], the generalized multiparticle-Mie theory [30], and the volume integral method [31]. However, depending on the size of the aggregate, calculations can be time consuming and require significant computational resources [4]. Thus, it would be computationally far more efficient to approximate the radiation characteristics of aggregates with complex morphology by those of particles with simple shapes such as spheres, coated spheres, or cylinders whose radiation characteristics can be computed relatively rapidly [32]. For example, Drolen and Tien [33] approximated the absorption and scattering cross-sections of soot particle aggregates as those of a volume equivalent solid sphere. More recently, Lee and Pilon [34] demonstrated that the absorption and scattering cross-sections per unit length of randomly oriented linear chains of spheres can be approximated as those of randomly oriented infinitely long cylinders with equivalent volume per unit length. Alternatively, the Rayleigh–Debye–Gans (RDG) approximation provides an analytical expression for the absorption and scattering cross-sections and the scattering phase function of aggregates based on the assumption that the size of the monomers is much smaller than the incident radiation wavelength [35].

This study aims to identify approximations and equivalent particles for rapidly and accurately predicting the absorption and scattering cross-sections and, if possible, the scattering matrix elements of fractal aggregates composed of relatively large monodisperse or polydisperse optically soft spherical monomers. The goal is to facilitate the predictions of radiation characteristics of fractal