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Porous effect on the radiative properties of fly ash particles: A discrete dipole approximation investigation

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ABSTRACT

Fly ash particles, one of the primary atmospheric pollutants, generally possess internal porous structure. In this work, porous models representing fly ash particles were built via the random midpoint algorithm, in which overall shapes including sphere, Gaussian random sphere, cube, oblate and prolate spheroids were considered. Focusing on fly ash composed of clay minerals, which can be generated in coal combustion processes, we considered a relative refractive index of $m = 1.5 + 0.005i$ and applied the discrete dipole approximation method to calculate the radiative properties of porous fly ash particles with a size parameter from 2 to 15 at the wavelength of 633 nm. Effects of porosity and pore size were analyzed. Meanwhile, approximations by the equivalent mass sphere (EMS) and the equivalent volume sphere (EVS) based on the effective medium approximation were examined. Generally, the angular patterns of the Muller matrix elements get smoother with increasing porosity and pore size, which tend to be insensitive to the particle external shape for a porosity as large as 50%. The scattered intensity increases with increasing pore size in a wide scattering angle range. Larger porosity leads to larger positive linear polarization for unpolarized incident light in the side scattering directions. With increasing porosity, the depolarization-related term S_{22}/S_{11} decreases for spherical particle but increases for non-spherical ones. In addition, smaller pore size leads to larger asymmetry parameter and single-scattering albedo. The EMS and EVS models predict the radiative properties of porous particles with distinct errors especially for non-spherical particle overall shape. The EVS model only works well for porous spherical particle with pore size parameters smaller than 0.46.

1. Introduction

Fly ash, one of the primary atmospheric pollutants, is generated from coal combustion in power plant, incineration of municipal solid waste, off gas releasing of vehicle, etc. Fly ash has significant impact on the global climate through the radiative process, poses a threat to aviation, and is the hazardous source of respiratory diseases [1–4]. Therefore, it is of great importance to detect fly ash particles and, if possible, to identify it from different sources by means of remote sensing method, which is principally based on the electromagnetic scattering by these particles. In order to interpret the information from remote sensing measurement, it is necessary to investigate the radiative properties of porous fly ash particles, which depend on the size, shape and composition [5].

Depending on the generating conditions and sources, the overall shape of the fly ash particles can vary to a large degree, it can be nearly spherical, cubic, or randomly shaped. Moreover, fly ash particles usually possess internal porous structures which also vary in porosity and relative size. For example, porous fly ash particles generated from combustion of coal [6–8], oil fuel [9] and municipal solid waste [10] usually have large porosity, whereas porous mineral particles often show a small porosity. Porous fly ash particles generated from combustion of solid material usually have a large particle size and relative small pore size, while particles generated from oil fuel combustion [9] exhibit small particle size and relative large pore size. Regarding the particle external shape, it has been realized that porous structure plays a significant role in determining the scattering signals of particle [11–16]. Therefore, in the retrieving of fly ash particle sources, its porosity, pore size as well as its size and shape can provide useful information, which can be reflected through their impacts on the radiative properties of fly ash particles.

Thanks to the development of electromagnetic numerical tools including the T-matrix method [17], the superposition T-matrix method [18,19], the discrete dipole approximation (DDA) [20], the finite difference time domain (FDTD) method [21] and so forth, the

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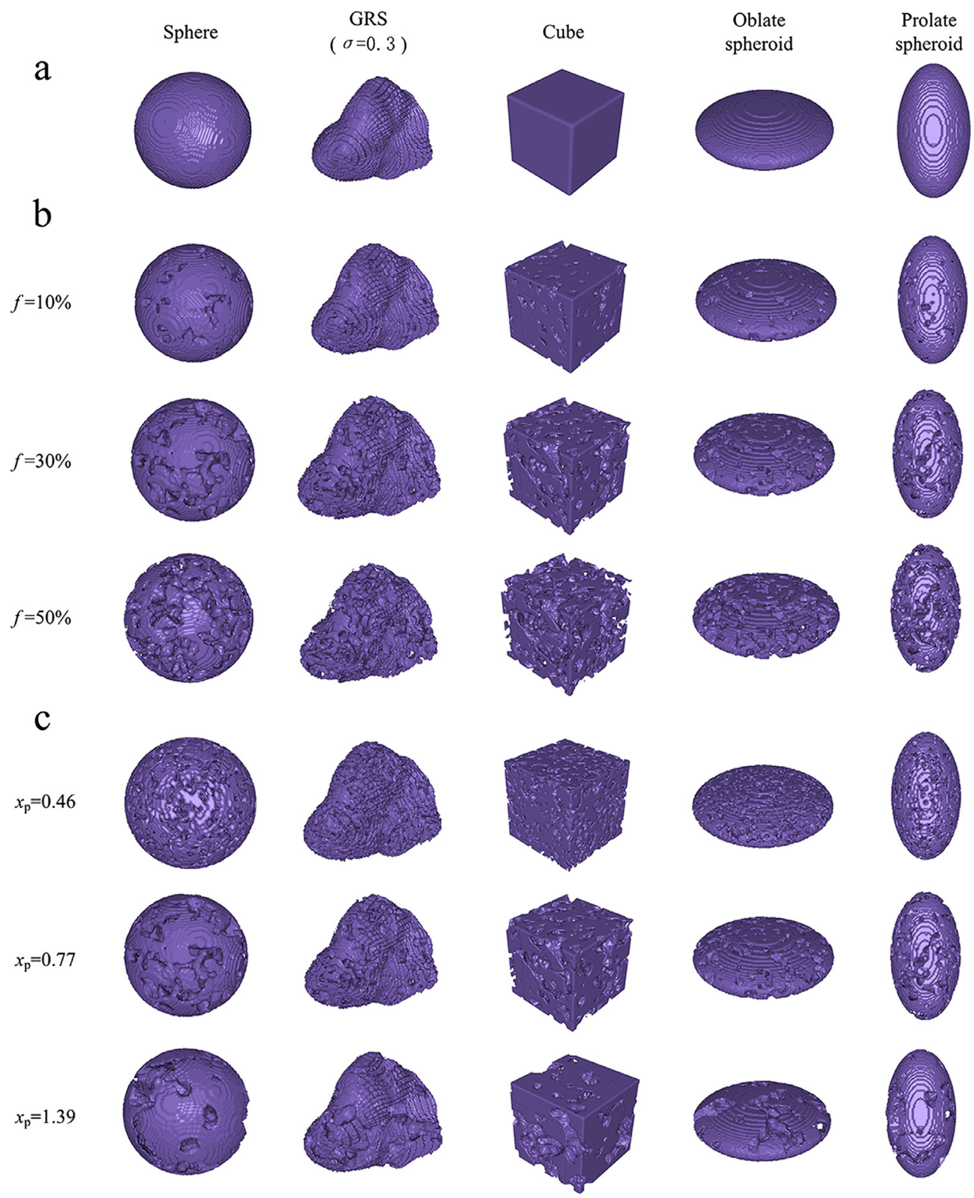

Fig. 1. Porous model particles with different porosities and pore sizes: (a) compact particles, (b) porous particles with pore size $x_p = 0.77$ but for different porosity f, (c) porous particles with porosity $f = 30\%$ but for different pore size x_p. The external particle shapes from left to right are the sphere, GRS ($\sigma = 0.3$), cube, oblate spheroid, and prolate spheroid, respectively.

radiative properties of particle with complex structures can now be studied. Lumme et al. [11] and Vilaplana et al. [12] studied the radiative properties of porous particles by the DDA method, in which the models were constructed by moving the dipole stochastically. They found that the porosity smoothens the phase function and promotes scattering intensity in the backward hemisphere. Zubko et al. [13] used the DDA method to calculate polarization characteristic of porous debris generated by inserting dipoles randomly in space, and they found that the porosity produces Rayleigh-like positive linear polarization. Wheeler et al. [14] proposed an ordered macro-porous model by using a face-centered cubic lattice arrangement to simulate the ceria porous particles, which was able to reproduce the feature of regular porous structures. However, such periodic modular structure cannot be used to represent the fly ash with arbitrary porous structure. Lindqvist et al. [15,16] constructed a vividly optical model of vesicular volcanic ash particle by adding some Gaussian random sphere shaped holes and studied its radiative properties based on the DDA method. The results indicated that the porosity tends to promote the positive polarization, lead to larger asymmetry parameter and single-scattering albedo. Many useful conclusions about the porous effect on the radiative properties of particles have been drawn by the above works. However, detailed studies of the porous effect regarding the porosity, pore size and the overall particle shapes still lacks, for which suitable model particles should be established that can vividly describe the variation in the porosity and pore size.

Therefore, the aim of this paper is to give a more detailed study of the porous effect on the radiative properties of such particles. Specially, we focus on compact fly ash particles composed of clay minerals, which can be generated in coal combustion process. Porous model particles of various porosity and pore size are built over typical shapes including sphere, cube, spheroid and Gaussian random spheres. The radiative properties are calculated by the DDA method. The effects of porosity and pore size on the radiative properties are analyzed. Moreover, the results are used as refer-