Abstract

Light scattering studies of small particulate matter provides significant contribution towards atmospheric aerosol monitoring, aerosol generation processes, climate modelling, remote sensing, nanoscience, medical applications and most importantly astrophysical dust characterization. Laboratory modelling and simulation of interstellar dust particles and atmospheric aerosols using analogue sample is an efficient technique to measure the optical and radiative properties of such particles. Laser based light scattering studies are of utmost importance mainly for inaccessible particles.

This PhD work has been performed for a better understanding of the light scattering properties of irregularly shaped particles. The study was centred on elastic scattering behaviour, where the scattered radiation has the same frequency as the incident one and the particle sizes are comparable or slightly greater than the incident wavelength (Mie scattering).

A laboratory light scattering setup has been used to experimentally measure the light scattering parameters namely the phase function $F_{11}(\theta)$ and the degree of linear polarization, $-F_{12}(\theta)/F_{11}(\theta)$ in the Optoelectronics and Photonics Research Laboratory, Tezpur University, India. The setup consists of a laser source, a controlled sample holder with flexible particle sprayer systems, silicon photodiode, data acquisition system and associated instrumentation. The setup is capable of measuring the scattered light intensities and polarization within an angular range of 10° to 170° in steps of 1° and 5° respectively. Three lasers of wavelengths 543.5 nm, 594.5 nm and 632.8 nm are alternately used according to the requirement of the experiment.

A computational technique has been developed based on four different software packages to calculate the light scattering properties of irregularly shaped dust particles. The computational tool consists of a volumetric geometry design software available in the public domain – BLENDER3D. It was used to generate models of arbitrarily shaped Gaussian particles to be used as target geometries. A software called DDSCATCONVERT was employed to convert the target geometries into dipole arrays. The primary software DDSCAT7.3 was used to compute the scattering efficiencies and cross sections (scattering, absorption, polarization and extinction), asymmetry parameters, single scattering albedos and elements of the Mueller matrix. An indigenously developed code in Matlab platform was employed to facilitate the automatic averaging over a wide range of shape and size distributions using the Discrete Dipole Approximation (DDA) generated computational results. Realistic models of irregular, shape and size dispersed dust particles are generated

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with the visual evidences found in scanning electron microscopy (SEM) images and their light scattering properties are computed using DDA. In order to model the particles (considering surface smoothness, surface roughness and aggregation or their combined effects) that gives the best fit to observed results, a number of variable parameters were used in the simulation.

The light scattering properties of graphite particles with a size distribution ranging from 0.5 to 5.0 μm were studied and the effects of particle shape and surface roughness on the size averaged and normalized values of scattering parameters are found at 543.5 nm and 632.8 nm incident wavelengths are observed.

The light scattering properties of Fayalite (Fe_2Si0_4), the iron end-member of the olivine group are studied to simulate the silicate dust particles found in the interstellar medium. The findings are important keeping in mind the fact that it is the rarest studied species of silicate dust, due to limited availability in the earth's crust. Simulations with a particle size distribution of 0.3 to 4 μm, validates the realistic computational models of irregular particles based on real analogue samples taking into account surface roughness and porosity, by varying shape deformations and number of dipoles respectively.

Silica microparticles are studied as an atmospheric aerosol analogue and due its importance as a drug delivery agent. Laboratory simulations with a size distribution of 0.35 to 4 μm was employed which provided important clues about modelling approaches for detection and characterization of highly irregular unknown scatterers. An efficient way of particle detection and size distribution measurements, and its applicability to remote sensing, atmospheric, astrophysical, medical applications was demonstrated. It can be also applied in finding potential health hazards in the form of inhalable and respirable silica particles.

A mixture of graphite and fayalite dust as interstellar dust aggregates were studied simulated using two computational models for a particle size distribution range of 0.3μm to 5μm. An efficient model has been developed and demonstrated to represent dust aggregates with two or three constituent elements. Effects of changing the percentage composition, number of dipoles, and the number orientation directions in DDA computations were successfully revealed. It was established that the accuracy of dust models could be improved by increasing the number of physical variables in the calculations of scattering properties.