3-D tomographic morphology of soot aggregates from coal combustion and associated optical properties

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Soot aggregates constitute the major fraction of particulate matter emitted from anthropogenic sources. Freshly emitted soot particles have complex fractal-like structures. These complex morphologies can significantly influence particle microphysical and optical properties, thereby impacting the earth's radiative forcing. Accurate parameterization of aggregate morphology is a prerequisite for quantitatively evaluating soot spectral radiative properties.

Electron tomography is a powerful technique which can detect the detailed three-dimensional (3-D) structure of aggregates. However, a defect, namely the missing wedge, inherent to limited-angle projection images limits the accuracy of the final 3-D reconstruction. Here, we demonstrate a novel tomography technique for 3-D reconstruction of soot aggregates sampled from a coal-fired reactor in China. Compared to traditional weighted back projection and iterative reconstruction techniques, we incorporate total variation minimization to compensate for the missing wedge artefacts [1]. The reconstructed soot particle models precisely capture the detailed morphological information of the aggregates, for example, the exact shapes of primary particles and the necking between monomers. Next, we calculate the Fourier Transform of the density auto-correlation function of the voxels (also known as the particle structure factor) to accurately characterize the fractal morphology of the reconstructed particles. Our goal here is to validate the conventional viewpoint regarding combustion-generated fractal aggregates, formed via diffusion limited cluster-cluster aggregation, yielding a universal mass fractal dimension of 1.8 [2]. Finally, we conclude this work by applying the discrete-dipole approximation on reconstructed aggregate models to derive spectral optical properties including scattering and absorption cross-sections, and asymmetry and Stokes parameters.

References

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