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Calculation of the Mass Absorption Cross Sections for carbonaceous nanonanoparticles modeling soot

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It is now well recognized that the optical properties of soot depend widely on their location in the atmosphere, on their geometrical properties and on their aging conditions. However, a direct relation between the optical properties of these atmospheric carbonaceous particles and their atomic structure is still lacking.
In this study, we use an atomistic model [1, 2] to calculate the mass specific absorption cross section coefficient (MAC) of carbonaceous particles of nanometer size in the optical and near-UV domain. The carbonaceous particles are built numerically to reproduce most of the structural characteristics of typical soot nanoparticles emitted in the Troposphere from combustion sources. Our model is based on the PDI (point dipole interaction) approach, which is similar to the discrete-dipole-approximation (DDA) method. It uses the knowledge of the atomic positions and polarizabilities of the atoms inside the nanoparticles to study the influence of these atomistic characteristics on the optical properties of the nanoparticles.
The results indicate that the atomistic composition of the soot nanoparticle may have a sufficiently strong impact on the MAC curves to allow qualitative detection of differences between nanoparticles by using UV-visible spectroscopic measurements. However, MAC measurements could give quantitative information on the atomic details of the nanoparticles only if they are performed in a well-suited wavelength range,i.e. at wavelengths typically between 200 and 350 nm [3].
In addition, because soot is not solely made of independent particles but rather made of aggregates of nanoparticles, we also developed an (approximate) multi-step method that allowed us to extend our simulations to the characterization of the optical properties of soot aggregates. Relation between optical properties and characteristics of the aggregates such as their fractal dimension are thus discussed within this atomistic framework.

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