

Supplement to “Importance of size representation and morphology in modelling optical properties of black carbon: comparison between laboratory measurements and model simulations”

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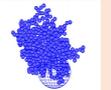
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1. Case study of intersecting spheres in MSTM code

He et al. (2015) studied various morphologies of black carbon aggregates with sulfuric acid (H₂SO₄) coating using the Geometric Optics Surface-wave (GOS) approach. In our manuscript, the case of ‘aggregate and sphere’ representation (Fig. 3f) matches morphologically to the case of BC aggregates partially embedded in a sulfuric acid (H₂SO₄) coating of the study by He et al. (2015). In order to test the results from the MSTM, the BC aggregates partially embedded in a sulfuric acid (H₂SO₄) coating were regenerated and their optical properties were calculated using MSTM. The specifications of the particles regenerated from the study of He et al. (2015) are summarized in Table S1. In the Fig. S1, the results from the MSTM for the particles in Table S1 are plotted over the figure copied from He et al. (2015). The results from the MSTM for the all the three cases of BC aggregates partially embedded in a sulfuric acid (H₂SO₄) coating closely match the GOS approach values. Therefore, the MSTM code was considered good enough for modeling the optical properties of aggregates with few intersecting spheres. It must be noted that if the number of intersecting spheres increase significantly, the difference between the MSTM and GOS approach might change.

Table S1. Details of the aggregates with spherical sulfuric acid coating modelled by He et al. (2015). In the case of the coated aggregate: values of mobility diameter of the core (BC D_p), number of primary particles (N_{pp}), radius of the primary particle (a_{pp}), and radius of the spherical coating. He et al. (2015) normalized each calculation with the results from their equivalent core-shell model. In the case of core-shell model: outer radius and inner radius.

Sphere embedded in aggregate	BC D_p (nm)	155	245	320
	N_{pp}	164	416	651
	a_{pp} (nm)	7.5	7.5	7.5
	D_f	2.1	2.1	2.1
	Coating sphere radius (nm)	3.5	55.5	65
	Image			
Core – shell model	Outer Radius (nm)	80.8	126.18	163.49
	Inner Radius (nm)	77.5	122.5	160

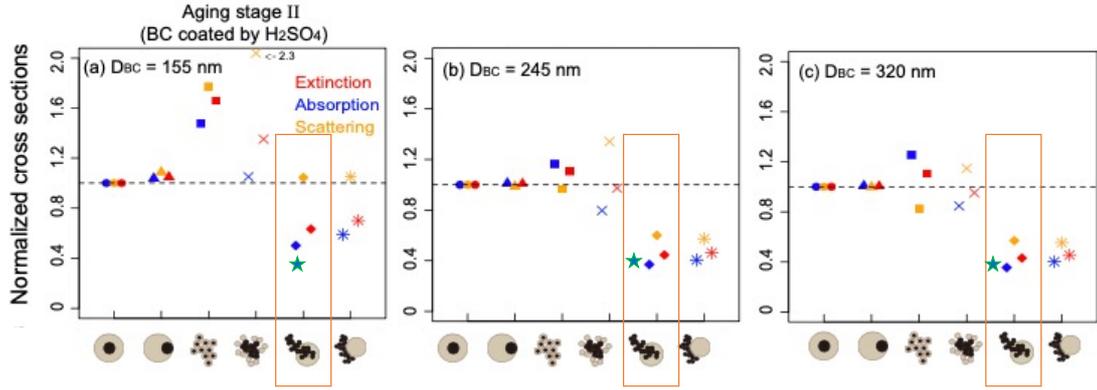


Figure S1. Comparison of the absorption results using MSTM for the three cases from He et al. (2015). The case for which the comparison is made is highlighted in a orange box. The blue star point represents the calculation using the MSTM code which should be compared to the blue diamond point of He et al. (2015). Adapted from He et al. (2015).

2. Optical properties of spherical and fractal bare BC particles using polydisperse method

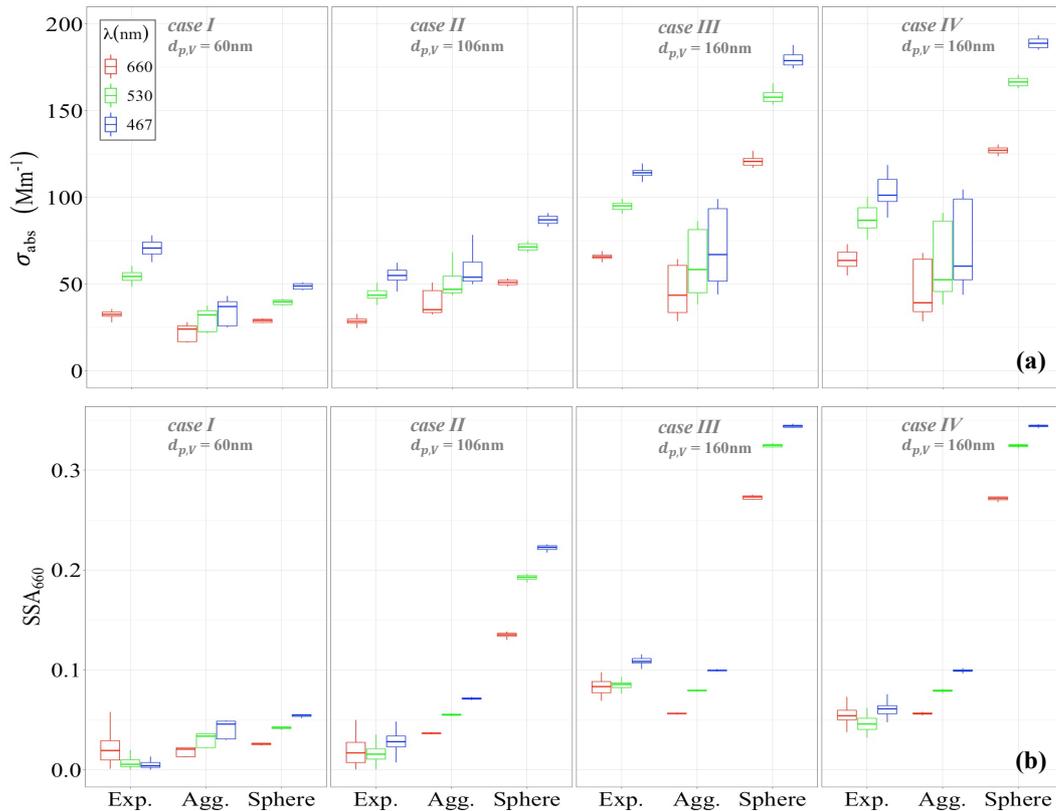


Figure S2. Modelled optical properties for three wavelengths in the visible range using the polydisperse method. Panels (a) and (b) shows the results of absorption coefficient σ_{abs} and single scattering albedo SSA_{660} , respectively, for the cases I – IV of E1 using the “aggregate” and “sphere” representation. For each case, the modelled optical property is compared to the experimentally measured values marked as “Exp.” on the X-axis.