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Effect of the necking phenomenon on the optical properties of soot particles

Krzysztof Skorupski*, Janusz Mroczka

Wroclaw University of Technology, Chair of Electronic and Photonic Metrology, Boleslawa Prusa 53/55, 50-317 Wroclaw, Poland

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ABSTRACT

Fractal-like aggregates are commonly modeled as assemblies of spheres positioned in point contact only. The necking phenomenon is usually neglected. Such an approach has some advantages, e.g. faster light scattering simulation programs can be used, however, it may result in many additional errors and inaccuracies. In our study we try to approximate them and select the most suitable connection model. In our work we focus on the impact of the necking phenomenon on the optical properties of two and five monodisperse soot particles. The results show that small connections can be neglected. Different connection types (the cylindrical, the linear and the quadratic connector) can be used interchangeably, therefore, we recommend the most basic one (i.e. the cylindrical connector). Additionally, when particles are not positioned in point contact (they tend to overlap) this phenomenon should not be omitted due to its impact on the resulting scattering cross sections.

1. Introduction

Small particles tend to aggregate and create large structures that may reveal some general fractal-like properties [1,2]. This process is considered as a universal, independent of particle material and shape, phenomenon [3]. In most studies aggregates are represented as assemblies of spheres positioned in point contact only. Common phenomena like overlapping or necking are neglected what may result in additional errors and inaccuracies [4,5]. Nevertheless, real fractal-like aggregates are much more complex and specific connections between primary particles, e.g. due to the sintering process, always exist [6]. The goal of our research was to investigate the impact of different connections on the optical properties of such structures. To highlight this effect, only aggregates composed of two $N_p=2$ and five $N_p=5$ soot particles were considered. In our study we were focused on the absorption cross section C_{abs} which is, in this case, the main component of the extinction cross section defined by the following equation:

$$C_{ext}=C_{abs}+C_{sca}, \tag{1}$$

where C_{sca} denotes the scattering cross section. Our results can be used to approximate the relative error that persists when no connectors are implemented or to improve the modeling process, which is necessary for understanding many physical phenomena [7]. The simulations were performed with the DDScat code, which is capable of simulating the amount of the light scattered by any shape [8,9].

2. Methodology

The first step of our study was to create four different connector types, which are specified as follows.

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* Corresponding author.
E-mail addresses: krzysztof.skorupski@pwr.wroc.pl (K. Skorupski), janusz.mroczka@pwr.wroc.pl (J. Mroczka).

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2.1. *Cylindrical connector*

It can be visualized as a cylinder positioned between the particle centers, as presented in Fig. 1. To keep the same volume of the structure V the reduction of the particle radius r_p can be compensated by the growth of the neck. The dimensionless parameter Y_{con} denotes the radius of this cylinder in the following manner:

$$r_{con} = Y_{con} \cdot r_p. \tag{2}$$

It varies from $Y_{con} = 0$ (the connection does not exist) to $Y_{con} = 1$ (the radius of the cylinder r_{con} is equal to the particle radius r_p).

2.2. *Linear connector*

The next connector type is based on the following linear function:

$$y = |ax| + b, \tag{3a}$$

$$x \in [-l/2; l/2], \quad y \in [0; r_p], \tag{3b}$$

in which a and b are parameters dependent on Y_{con}. The particle centers are aligned along the X-axis, i.e. $(-l/2, 0)$ and $(l/2, 0)$, and the center of the coordinate system (0,0) is positioned in the same point as the geometric center of the connector. The value of y for the $x=0$ condition is determined by the parameter Y_{con} in the following manner:

$$y_{(x=0)} = Y_{con} \cdot r_p \tag{4}$$

and the boundary points are defined as follows:

$$y_{(|x|=l/2)} = r_p. \tag{5}$$

After calculating a and b the resulting curve is rotated around the X-axis to create a three-dimensional shape. The main idea of this connector is presented in Fig. 2. This type of connection is slightly more realistic than the previous one, especially when large values of Y_{con} are used. However, it is also more difficult to implement.

2.3. *Quadratic connector*

The most complex connector is based on the following quadratic function:

$$y = ax^2 + b, \tag{6a}$$

$$x \in [-l/2; l/2], \quad y \in [0; r_p]. \tag{6b}$$

The generation algorithm is very similar to the previous one. The quadratic connector is comparable to the linear connector, but its greatest advantage is that the bending point in $y_{(x=0)}$ does not exist. Therefore, it is more similar to real structures (see Fig. 3). Note that every proposed connection type looks alike when $Y_{con} = 1$ or $Y_{con} = 0$ (providing that the particles are positioned in point contact only).

2.4. *Overlap factor*

It is one of the most common connection types, which was studied, for example, by Brasil et al. [4], Oh and Sorensen [5] and Mishchenko and Videen [10]. It is a well-known fact that the overlap factor C_{ov} has an undeniable impact on the morphological parameters of fractal-like aggregates. Because in our work such complex structures are not investigated, detailed study with discussion on this topic can be found elsewhere [4,5,11].

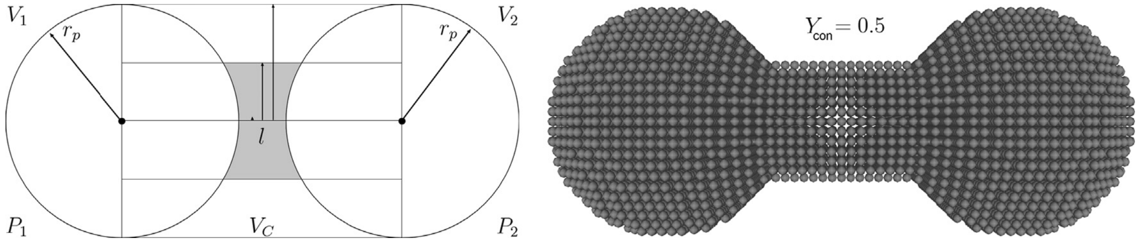

Fig. 1. The picture presents two monodisperse particles, denoted as P_1 and P_2 respectively, and a cylindrical connector. l is the distance between particle centers, r_p describes their radius and V_1, V_2 represent their volume. Y_{con} is a dimensionless parameter which defines the size of the connector. V_c denotes the volume of the total intersection area (colored in gray). The shape on the right depicts two particles and a single connector ($Y_{con} = 0.5$) decomposed into an array of dipoles.

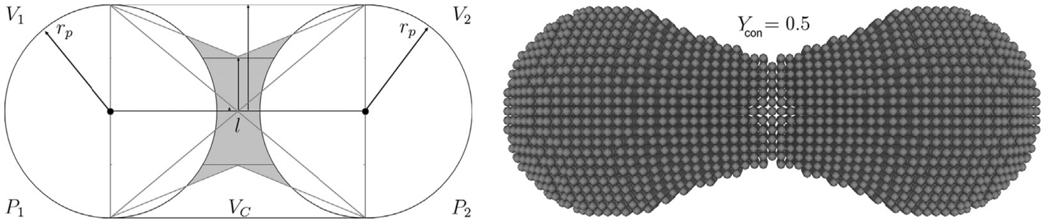

Fig. 2. The picture presents two monodisperse particles, denoted as P_1 and P_2 respectively, and a linear connector. l is the distance between particle centers, r_p describes their radius and V_1, V_2 represent their volume. Y_{con} is a dimensionless parameter which defines the size of the connector. V_c denotes the volume of the total intersection area (colored in gray). The shape on the right depicts two particles and a single connector ($Y_{con} = 0.5$) decomposed into an array of dipoles.