Modelling dynamic shape factors and lung deposition of small particle aggregates originating from combustion processes

R. Sturm and W. Hofmann

Department of Materials Engineering and Physics, Division of Physics and Biophysics, University of Salzburg, Hellbrunnerstrasse 34, A-5020 Salzburg, Austria

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Diesel exhaust particles and other soot particles originating from combustion processes are irregularly shaped particulate aggregates with diameters of several hundred nanometers. In the past, combustion particles have been increasingly emitted into the atmospheric air, enhancing their significance as a major public health hazard and contributing to the burden of pulmonary and cardiovascular diseases (Bayram et al., 2006).

For an appropriate simulation of non-spherical particle behaviour in the human respiratory tract, the concept of the dynamic shape factor and the aerodynamic diameter has been introduced by Stöber (1972) at the beginning of the 1970s. Dynamic shape factors adopt values >1 for prolate and oblate particle shapes (fibers, disks), whereas they may vary between 2 and 15 for particle clusters consisting of monodisperse spheres (Kasper, 1982). Especially high shape factors have a significant effect on the deposition of such clustered particles. The two main objectives of this study are: 1) to model dynamic shape factors of small particle aggregates, and 2) to apply these factors to inhaled particle deposition.

The dynamic shape factor $k$ of particulate clusters was computed according to the suggestions of Kasper (1982), where the parameter $k$ may be estimated according to the simple formula

$$k = \frac{d_{es}}{d_{ev}},$$

where $d_{es}$ denotes the diameter of the enveloping sphere and $d_{ev}$ the diameter of the equivalent volume sphere. Calculations of $k$ were carried out with a computer program allowing the variation of the number of monodisperse spheres defining the particulate cluster (Fig. 1). Computation of aerodynamic diameters $d_{ae}$ for the simulation of particle deposition in the human respiratory tract was based on the widely applied equation

$$d_{ae} = d_{ev} \cdot \sqrt[3]{\frac{\rho_p}{\rho_0} \cdot \frac{C_c(d_{es})}{C_c(d_{ev})}},$$

with $\rho_p$ and $\rho_0$, respectively, denoting the density of the cluster and unit density (1 g cm$^{-3}$), and $C_c(d_{es})$ and $C_c(d_{ev})$ representing the Cunningham slip correction factors of particles with $d_{es}$ and $d_{ev}$.

Particle deposition was calculated for light-work breathing conditions (ICRP, 1994), using the stochastic deposition model developed by Koblinger & Hofmann (1990). The diameter of the monodisperse spheres was assumed to be 10 nm, resulting in average cluster diameters of 71.2 (10 spheres) and 587.7 nm (100 spheres). Preliminary deposition results are summarized in Tab. 1.

Table 1. Relative deposition fractions (%) of cluster particles in different regions of the human respiratory tract.

<table>
<thead>
<tr>
<th>Lung region</th>
<th>10 spheres cl.</th>
<th>100 spheres cl.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extrathoracic</td>
<td>15.11</td>
<td>11.86</td>
</tr>
<tr>
<td>Bronchial</td>
<td>12.17</td>
<td>6.41</td>
</tr>
<tr>
<td>Bronchiolar</td>
<td>42.86</td>
<td>26.14</td>
</tr>
<tr>
<td>Alveolar</td>
<td>29.86</td>
<td>55.59</td>
</tr>
</tbody>
</table>

Table 1 demonstrates that particulate clusters containing 10 monodisperse spheres are preferably deposited in more proximal lung compartments under the given breathing conditions. Thereby, the uppermost airways serve as efficient filters prohibiting the total penetration of the clusters into deeper lung regions. In contrast, the larger clusters are deposited primarily in the more peripheral lung compartments, underlining their role as important carcinogen for alveolar tumors.


