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Novel methodology for estimation of mass and surface area of aggregated particles deposited in the human respiratory tract

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The particle mass and surface area is believed to be crucial parameters for the health effects of inhaling non-soluble air-borne particles. Often the deposited dose and particulate surface area are estimated from particle number concentrations measured by DMA techniques. For spherical particles such estimations are good. For non-spherical particles, however, the estimations can deviate from the real deposited surface area or mass by an order of magnitude. Aggregated or agglomerated particles require additional information about both particle shape and particle effective densities.

The aim of this work is to describe and apply a methodology for assessing surface area and mass of aggregated/agglomerated particles based on number size distributions measured by DMA-techniques. The method is applied in three studies: estimating the deposition in the human respiratory tract of diesel soot, deposition of gold aggregates in protein solutions and direct onto cell cultures (Savi et al., 2008).

The principle of the method used to estimate the surface area size distribution is shown in Figure 1. As input (i) the mass of the individual aggregates of a certain mobility diameter $m_{agg}(d_{me})$, (ii) the primary particle size (d_p), and (iii) number size distribution ($dN_{agg}/d\log d_{me}$) are needed. For mass determination of individual aggregates the novel DMA-Aerosol Particle Mass Analyzer (DMA-APM McMurry et al., 2002) is used. The mass size distribution of the aerosol is estimated by combining the results of the DMA-APM system and the number size distribution. For estimation of surface area the size of the primary particles is also needed, here estimated from TEM images.

From $m_{agg}(d_{me})$ and d_p the number of primary particles of the individual aggregates of a certain size ($N_p(d_{me})$) is calculated (assuming a density of the primary particles of $\rho_p=1.8 \text{ g/cm}^3$ for soot and 19.3 for gold) according to $N_p(d_{me}) = m_{agg}(d_{me}) / (\rho_p \cdot \pi \cdot d_p / 6)$.

By combining $N_p(d_{me})$ and the particle number size distribution, the distribution of the total number of primary particles of all aggregates of a certain d_{me} is

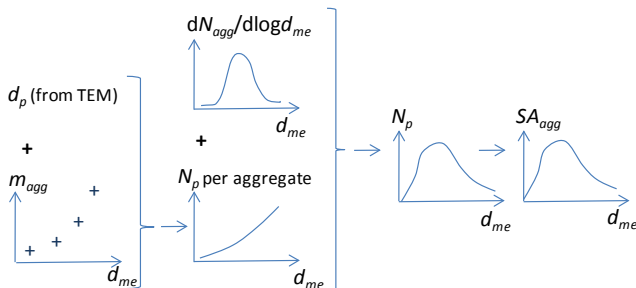


Figure 1. Principle of the methodology.

estimated, and thereafter the total surface area of all aggregates of a certain d_{me} ($SA(d_{me})$). Knowing the size resolved fraction of particles deposited (measured or modeled) in the lung, into the protein solution or onto the cell cultures, the total deposited dose and surface area is determined.

The method was applied in the three studies. All showed that when estimating mass from size distributions measured by an SMPS assuming spherical particles, gave 4-6 times higher doses than if the measured particle mass was used. Surface area was not as sensitive for aggregation state and the aggregates had a larger surface area than if assuming spherical particles, by typically 2-3 times. The contact area between primary particles in the aggregate is assumed to be infinitesimal. According to TEM images the true contact area is larger and the real surface area will probably lie between the two extremes; spherical particles and agglomerates.

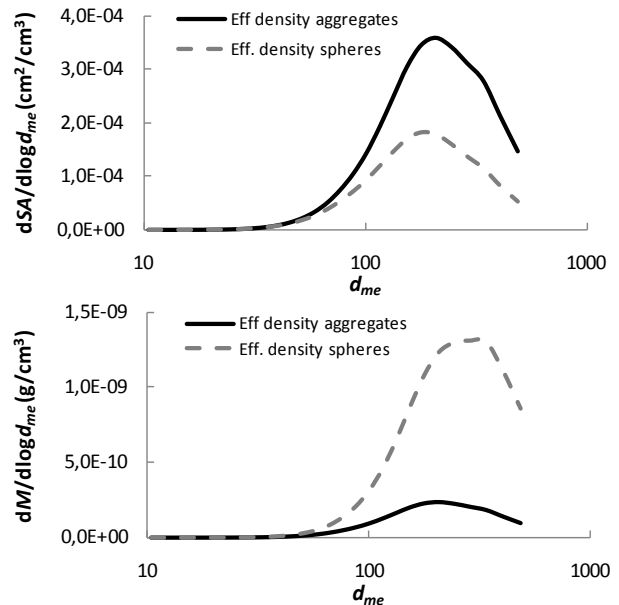


Figure 2. Distributions of surface area (SA) and mass (m) assuming either spherical or aggregated particles.

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Savi, M., et al., (2008) Environ. Sci. Technol., 42, 5667–5674.

McMurry P.H., et al. (2002), Aerosol Science and Technology 36: 227–238.