miniDiSC application note #9: mass and surface area calculation

As of software version 1.2, the miniDiSC java tool can calculate particle mass and particle surface area concentrations in addition to the previously available measurements of number, average diameter and lung-deposited surface area. This application note explains how this is done, and what the limitations are.

The miniDiSC data inversion relies on the assumption that the particle size distribution is lognormal with a geometric standard deviation of 1.9. The new surface area and mass concentration calculation also relies on this assumption. Naively, one might try to calculate particle mass per volume as (wrong!):

$$m = \rho \cdot N \cdot \frac{\pi}{6} d^3$$

Where *N* and *d* are the particle number concentration and the average particle diameter reported by the miniDiSC, and ρ the particle density. This is incorrect, as the larger particles contribute much more to the total mass. Luckily, for lognormal particle size distributions, analytical expressions exist to calculate the diameter of average mass (or any other moment), i.e. that size of particle whose mass multiplied by the total number of particles gives the total mass. These expressions are known as the Hatch-Choate equations (see e.g. Hinds, Aerosol Technology). The diameter of average d^x is given by

$$d_{\bar{x}} = d \exp(\frac{x}{2} ln^2 \sigma)$$

Where *d* is the geometric mean diameter, and σ the geometric standard deviation of the lognormal particle size distribution. Using *x* = 2 for surface area and *x* = 3 for mass, one arrives at the equations

$$S = N \cdot \pi d^2 \exp(2 \cdot ln^2 \sigma)$$

$$m = \rho \cdot N \cdot \frac{\pi}{6} d^3 \exp(4.5 \cdot ln^2 \sigma)$$

Which are the equations that the java tool uses to calculate surface area concentration *S* and mass concentration *m*, using a density of ρ = 1200 kg/m^3.