# Soot Primary Particle Size by Agglomeration & Surface Growth

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### Abstract

Soot impact on health and environment strongly depends on its primary particle size and effective density. Scaling laws based on clusters of primary particles in point contact (agglomerates) or chemically bonded (aggregates) have been used in tandem with mass-mobility measurements to obtain effective density and even primary particle size, as an alternative to off-line microscopy.

Here, such relationships are derived by investigating soot dynamics after inception by a Discrete Element Model (DEM) of agglomeration and surface growth by the Hydrogen Abstraction Carbon Addition mechanism. The initial hydrogen atom molar fraction is varied to attain different maximum soot volume fractions, $f_{v,max}$. For high soot volume fractions, more acetylene molecules react on the surface of soot primary particles increasing rapidly their mass and size. The soot mobility size distribution narrows down and its self-preserving geometric standard deviation, $\sigma_{g,m}$, decreases from 2.03 to 1.8. The evolution of soot morphology from nascent to mature soot is quantified by the fractal dimension, $D_f$, and mass-mobility exponent, $D_{fm}$. An asymptotic $D_{fm} = 2.45 \pm 0.05$ is attained by agglomeration of chemically bonded dimers that form more compact structures than agglomerates consisting of primary particles in point contact. Further cluster-cluster agglomeration decreases $D_f$ and $D_{fm}$ down to the asymptotic value for large ramified agglomerates. The $D_f$ and $D_{fm}$ evolutions in terms of the normalized mobility diameter are in good agreement with microscopy and mass-mobility measurements of nascent and mature soot, respectively.

The correlation between the number of primary particles, the mobility and the primary particle diameters quantified by the projected area exponent, $D_a$, and prefactor, $k_a$, derived for mature soot is in better agreement with mass-mobility measurements of soot aggregates than prior models for agglomeration of monodisperse and polydisperse primary particles. A relationship for the soot effective density as function of the normalized mobility size is derived and compared to measurements from different combustion sources. The asymptotic $D_a$ and $k_a$ for mature soot aggregates are combined with a power law relationship to calculate the primary particle size of diesel and flame soot, achieving relative errors down to 0.2 and 1 %, respectively.