Nascent and Mature Soot Morphology Dynamics

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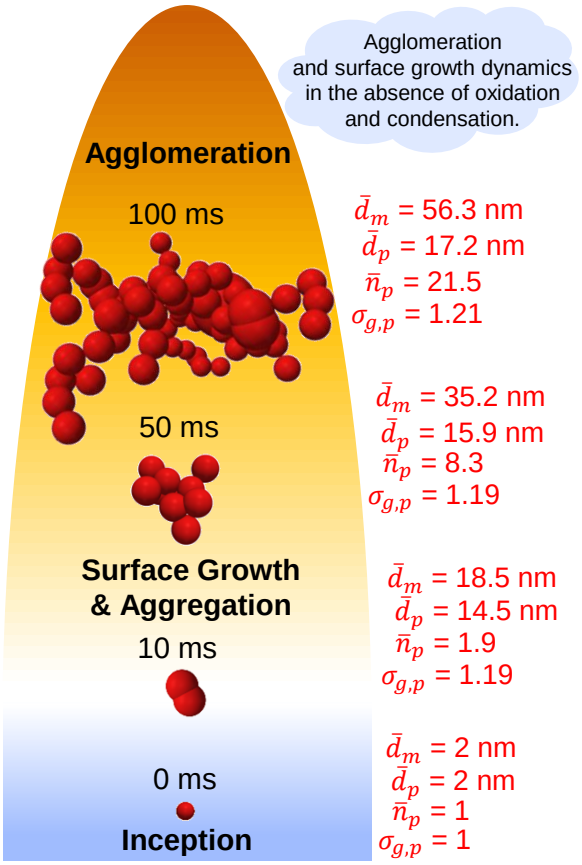
Motivation

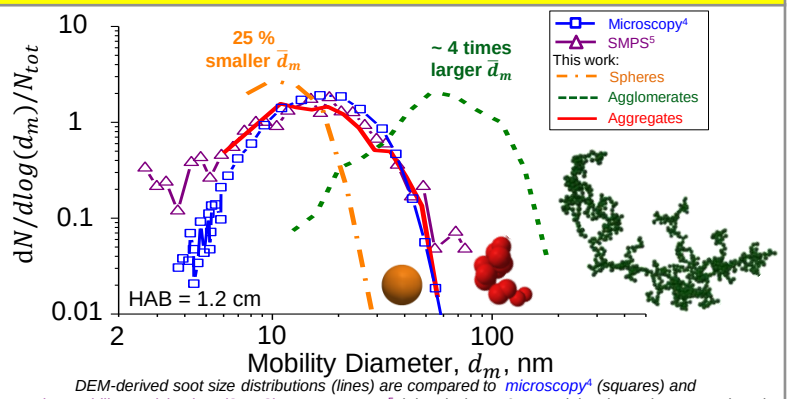
Soot impact on health and environment strongly depends on its mobility size, d_m, and effective density, ρ_{eff}.[1] Current scaling laws for d_m and ρ_{eff} based on clusters of primary particles in point contact (agglomerates) neglect their chemical bonding (aggregation) and polydispersity, deviating significantly from measurements.[1] Here, new relationships are derived by investigating soot aggregate dynamics with a Discrete Element Model (DEM) for agglomeration & surface growth.[2]

Evolution of Nascent to Mature Soot [2]



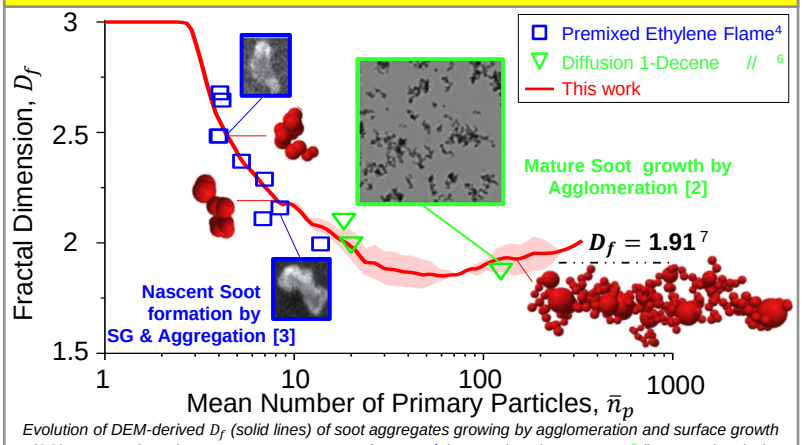
Evolution of soot mean mobility, $\bar{d}_m$, and primary particle diameter, $\bar{d}_p$, number of primary particles (PPs), $\bar{n}_p$ and standard deviation, $\sigma_{g,p}$.

Soot Size Distribution by Combustion of Ethylene [3]



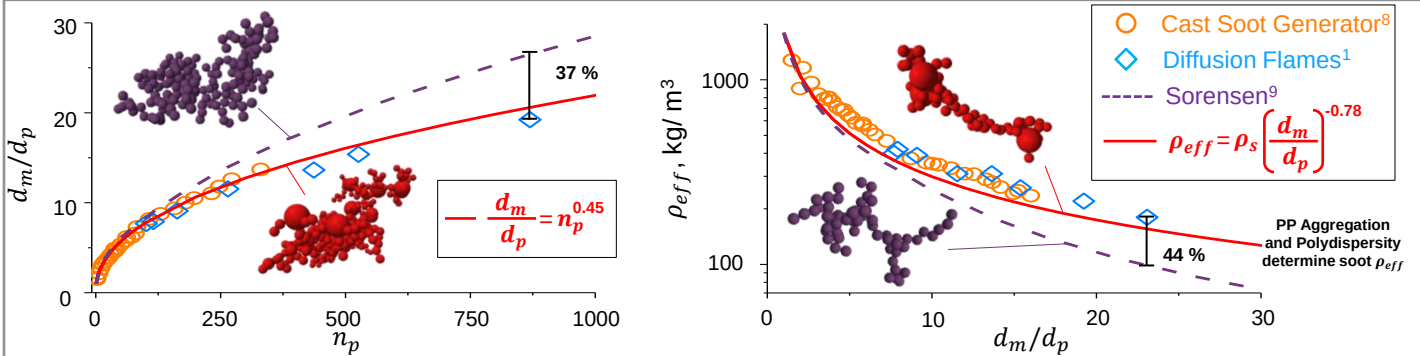
DEM-derived soot size distributions (lines) are compared to microscopy[4] (squares) and scanning mobility particle sizer (SMPS) measurements[5] (triangles) at 1.2 cm Height Above the Burner (HAB).

Morphology Dynamics of Nascent and Mature Soot [2]



Evolution of DEM-derived D_f (solid lines) of soot aggregates growing by agglomeration and surface growth (SG) compared to microscopy measurements of nascent[4] (squares) and mature soot[6] (inverse triangles).

Mature Soot Mobility Size and Effective Density Distributions [2]



The DEM-derived relationships (solid lines) between aggregate d_m/d_p and n_p or effective density, ρ_{eff}, compared to Sorensen's model for agglomerates[9] (broken lines) and mass-mobility measurements of mature soot aggregates from Cast soot generator[8] (circles) and diffusion flames[1] (diamonds).

References

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Conclusions

1. Excellent agreement between DEM and experimental data of nascent and mature soot structure and size distribution was found.
2. Neglecting the fractal morphology of nascent soot leads to underprediction of its mean mobility size up to 25 %.
3. Aggregation and SG form compact nascent soot aggregates, while the asymptotic mature soot morphology is attained by their subsequent agglomeration.
4. Neglecting primary particle aggregation and polydispersity leads up to 37 % overestimation of d_m and 44 % underestimation of ρ_{eff}.
5. The DEM-derived relationships for d_m and ρ_{eff} can be used to characterize soot aggregates formed by agglomeration and surface growth in the absence of oxidation and volatile condensation.