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Nascent Soot Formation by Agglomeration & Surface Growth

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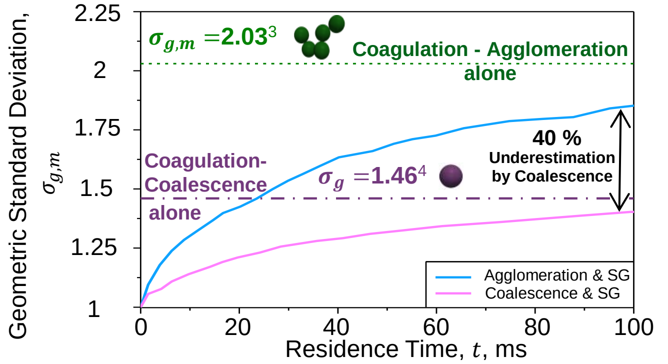
Motivation

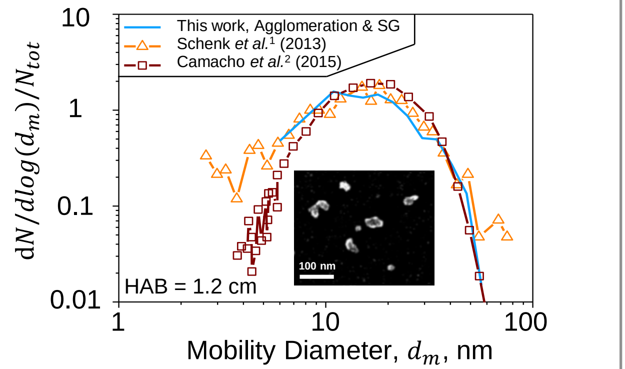
Major concerns have been raised about the adverse effects of nascent soot, since microscopy[1] and mass-mobility measurements[2] have proved the existence of ultrafine aggregates. So, their impact on climate, health and nanomaterials manufacturing needs to be determined accurately. Here, nascent soot dynamics in an ethylene flame with equivalence ratio $\varphi = 2.07$ are investigated by a Discrete Element Model (DEM) for agglomeration & surface growth.

Dynamics of Nascent Soot Polydispersity



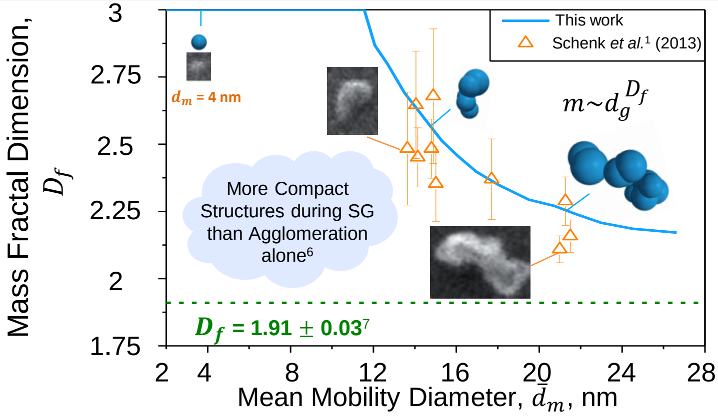
Evolution of $\sigma_{g,m}$ of soot particles growing by coagulation in the presence or in the absence of surface growth (SG). Narrower size distributions are attained by SG.[5]

Soot Size Distribution by Combustion of Ethylene

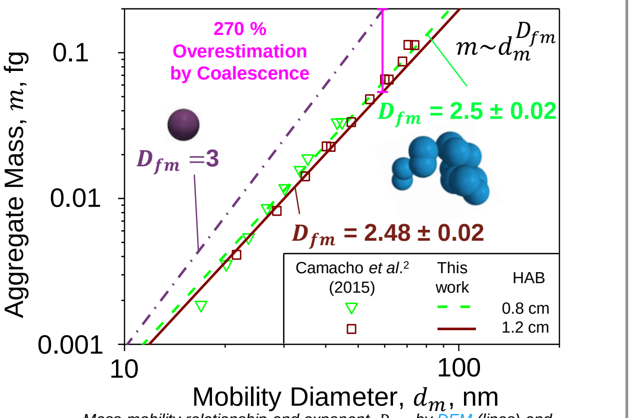


Normalized soot size distributions by DEM (line), microscopy[1] (triangles, inset) and mobility size measurements[2] (squares) at 1.2 cm Height Above the Burner (HAB).

Evolution of Soot Morphology (D_f, D_{fm})

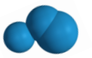
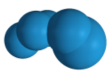
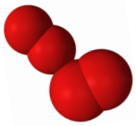
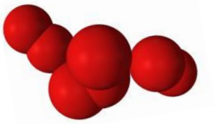


Evolution of Mass Fractal Dimension, D_f, of soot particles obtained by DEM (line) and microscopy[1] (symbols, insets).

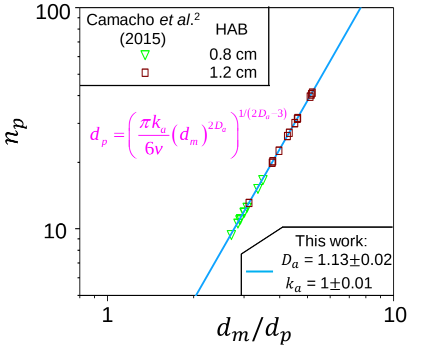


Mass-mobility relationship and exponent, D_{fm}, by DEM (lines) and mass-mobility measurements[2] (symbols) at two HABs.

Number of Primary Particles in Nascent Soot Aggregates: $n_p = k_a \left({}^{d_m}/_{d_p} \right)^{2D_a}$

$f_{v,max}$ \ t	10 ms	20 ms	30 ms
10^{-8}	D_a = 1.14 k_a = 1 	D_a = 1.12 k_a = 1 	D_a = 1.13 k_a = 1 
10^{-7}	D_a = 1.13 k_a = 1 	D_a = 1.14 k_a = 1 	D_a = 1.13 k_a = 1.02 

Evolution of DEM-derived soot aggregate morphology along with projected area exponent, D_a, and prefactor, k_a, for different maximum soot volume fractions, $f_{v,max}$.



Estimation of n_p from combined mass-mobility measurements,[2] a scaling law[8] and the DEM-derived D_a and k_a.

References

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Conclusions

1. Surface growth contributes to the attainment of narrower distributions during coagulation by coalescence or agglomeration in the free molecular regime, consistent with literature.[4]
2. Neglecting the fractal morphology of nascent soot leads to underprediction of its polydispersity up to 40% and overprediction of its mass up to 270 %.
3. Nascent soot forms compact but not spherical structures ($D_f, D_{fm} \neq 3$). Surface growth delays the attainment of the asymptotic $D_f = 1.91$ of pure agglomeration in the free molecular regime.
4. Good agreement between DEM and experimental data on soot size distributions & structure was found.
5. The D_a and k_a of nascent soot are independent of $f_{v,max}$ and can be used in tandem with mass-mobility measurements to determine d_p and n_p.