Nascent Soot Formation by Agglomeration & Surface Growth

Numerical investigation of nascent soot structure and size distribution

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Abstract

Nascent soot particles of mobility size 1 – 10 nm have been observed in a wide range of combustion sources, from laminar diffusion and premixed flames to diesel engines. There are major concerns about the adverse effects of nascent soot particles due to their small size and high specific surface area. For example, the fraction of soot particles that deposit in the human lung is increasing for lower mobility sizes. Furthermore, the reactivity of nascent soot particles correlates with their high surface area, inducing the condensation of toxic volatile and semi-volatile species on their surface. Thus, a better understanding of nascent soot growth is required for identification of process parameters that determine particle size and morphology.

Here, Discrete Element Model (DEM) simulations are used to investigate nascent soot particle growth after nucleation accounting for simultaneous surface growth and agglomeration in the absence of soot oxidation. The model is validated with theoretical expressions for full coalescence with surface growth. Nascent soot growth by agglomeration with or without acetylene molecule reaction (pyrolysis) is compared to that by full coalescence. Neglecting the non-spherical or fractal-like nature of soot underestimates its mobility size and polydispersity up to 40 and 25%, respectively. The DEM-obtained size distributions of soot growing by agglomeration with surface growth are in good agreement with microscopy measurements of a benchmark ethylene flame, indicating that surface growth narrows down soot size distributions at low heights above the burner, consistent with literature. The evolution of nascent soot structure from spheres to aggregates quantified by mass fractal dimension and mass-mobility exponent is in excellent agreement with microscopy and mass-mobility experiments. Surface growth chemically bonds the constituent primary particles of aggregates while the effect of soot volume fraction on nascent soot morphology is elucidated. Based on the aggregate projected area, a scaling law is derived for determining the number and the size of the nascent soot primary particles from mass-mobility measurements.