Effects of overlapping in the evaluation of volume and surface area of complex soot aggregates in flames

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The release of ultrafine soot particles to the atmosphere can cause detrimental effects on the environment for example by influencing the formation of clouds and/or by changing the radiative properties of the atmosphere [1]. In most numerical works, soot particles are typically considered either spherical in some numerical simulations or fractal aggregates in advanced codes that neglect the overlapping between primary particles. These approximations lead to significant deviations in the surface area and volume of soot particles, which in turn can cause large uncertainties in modeling soot physicochemical processes depending on particle sizes, such as collision rates and surface reaction rates (both surface growth and oxidation).

Fractal-like aggregates representative of flame-made soot (fractal dimension 1.78, prefactor 1.30, and 2-1000 number of spherical monodisperse primary particles) are generated by using a recently developed sequential algorithm called FracVAL [2]. Subsequently, primary particles are enlarged uniformly to induce a desired level of overlap in the 0-90% range. The volume and surface area of these aggregates are then calculated using the accurate but expensive (in CPU time) SBL library [3]. Based on these calculations, different equations to approximate their volume and surface area are proposed. In addition, a new method to estimate the population average overlapping coefficient is introduced. This requires the total number of collisions to be known at all times. As a test case, the method is implemented to predict the total surface area and volume of soot aggregates in an ethylene (C/O=0.94) laminar premixed flame [4].

The proposed equations extend the works of [4,5] to determine total soot volume and surface area in time. Current expressions are accurate for aggregates of any size relevant to soot particles produced in flames at atmospheric pressure. Under the test case conditions (premixed flame), neglecting primary particle overlapping leads to a maximum overestimation of soot particle total volume and surface area of 91 and 218%, respectively. The proposed approach exhibits a maximum error of 0.6% for total volume and 5.75% for total surface area. This method only requires the total number of collisions in time, the surface growth rate (the rate of change in primary particle diameter), and the number of primary particles per aggregate. All of these parameters are readily available in most population balance simulations making its implementation in existing codes straightforward. The proposed method can also be used in future Monte Carlo or Langevin Dynamics discrete element simulations to potentially reduce the CPU time associated with the evaluation of aggregate volume and surface area.

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