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An Algorithm for Soot Aggregate Restructuring[1] DIVJYOT SINGH, OGOCHUKWU ENEKWIZU, ALEXEI KHALIZOV, New Jersey Inst of Tech — Soot aggregates, derived from the incomplete combustion of fossil fuels and biomass burning, are ubiquitous in the atmosphere and adversely impact air quality and global climate. The fractal-like structure of soot aggregates undergoes significant restructuring due to interaction with condensable trace-gas chemicals during atmospheric aging. This morphological change affects the properties of soot aggregates including their light scattering and absorption, surface chemistry, cloud nucleation efficiency and atmospheric lifetime. In this study, we develop an algorithm to simulate the condensation-induced restructuring of soot aggregates. The restructuring algorithm accounts for adhesion forces between soot monomers, capillary forces due to coating trapped in junctions between monomers, and viscous dissipation forces. We test our restructuring algorithm on an ensemble of initially fractal aggregates and track the morphological evolution of the aggregate backbone. We also compare our predictions of final aggregate morphology against compact aggregates generated directly via traditional Diffusion Limited Cluster Aggregation (DLCA) methods. The results of our findings will provide a framework that facilitates predictions of morphologically dependent soot properties.

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