Analysis of Nascent Soot Particles from Acetylene Pyrolysis: A Molecular Modeling Perspective

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Abstract:

Soot or black carbons are combustion-generated carbonaceous nanoparticles formed during incomplete combustion of hydrocarbon fuels. Due to the complexity of hydrocarbon combustion systems, there exists a considerable knowledge gap in the fundamental processes and properties of soot as they form and evolve during combustion. This study uses reactive molecular dynamics (RMD) simulations with reactive force field (ReaxFF) potentials to address this knowledge gap. The focus of the current work is the formation and evolution of soot during acetylene pyrolysis at different temperatures. One thousand acetylene molecules are allowed to collide and react at four different temperatures from 1350 K to 1800 K. The analysis provides insights into physicochemical aspects of soot formation as well as the maturation of incipient soot particles at different temperatures. The chemical evolution of the acetylene systems points to a boundary between gas-phase and potential particle-phase indicated by a steady decrease of smaller hydrocarbons, followed by a spike in C6-C10 molecules and the eventual formation of a cluster with more than 30 carbon atoms, which morphs into a soot particle. Once a soot particle is formed, we focus on the evolution and interdependence of features such as the number of carbon atoms, number of aromatic rings, mass, C/H ratio, the radius of gyration, fractal dimension, surface area, volume, fringe spacing distribution, and density. The soot particles, irrespective of process temperature, become more spherical and more compact with time, while the C/H ratio converges to a value around 2.5. Qualitative correlations of various degrees are also observed between some of these morphological features. This ongoing study is expected to provide important insights into the pathways of soot formation and help develop more accurate engineering-scale models for soot formation in combustion simulations.