596c Carbonaceous Nanoparticles in Combustion: a Multiscale Perspective

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The process of combustion is the dominant pathway through which mankind continuously injects particulate matter into the atmosphere at the present time. These combustion-generated particles are present not only in a very large amount, but are produced, at the smallest scale, in the form of clusters with nanometric dimensions. Although the total mass of particulate emissions has been significantly reduced with improvement of combustion efficiency and emissions control systems, the very small nanoparticles are exceedingly difficult to control by the emission systems typically installed on vehicles. In addition, the current emissions regulations are mass-based and do not address the presence of nanoparticles. Predictive models of nanoparticle formation and oxidation that provide detailed chemical structures of the particles currently do not exist, a fact that greatly limits our ability to control this important chemical process. The objectives of this work are focused on gaining a clearer understanding of the chemical and physical processes occurring in the formation of carbon nanoparticles in combustion conditions and their fate in the environment. The primary focus is to provide a detailed multi-scale characterization of nanoparticle formation in combustion environments, through the use of novel simulation methodologies operating across disparate (spatial/temporal) regimes. The use of atomistic models, such as the Kinetic Monte Carlo technique and Molecular Dynamics simulation, allow us to follow the transformations that occur during nanoparticle formation in a chemically specific way, thereby providing information on both the chemical structure and the configuration of the nanoparticles and their agglomeration. The figure below shows a typical nanoparticle obtained through the use of the Atomistic Model for Particle Inception (AMPI) code in a benzene-oxygen laminar premixed flame. The capability of the AMPI code has been validated in different combustion conditions. Nanoparticles have been characterized in terms of chemical structure/components and relationships between structure and pathways, structure and properties, and structure and reactivity population of active sites have been addressed. This approach establishes a connection between the various time scales in the nanoparticle self-assembly problem, together with an unprecedented opportunity for the understanding of the atomistic interactions underlying carbonaceous nanoparticle structures and growth. Preliminary results will also be given from atomistic-scale simulations of the nanoparticles interacting with model cell membranes.