From fuels to nanoparticle formation: how combustion environment affects the chemical and physical processes in flames

Angela Violi

Departments of Mechanical Engineering, Chemical Engineering and Biomedical Engineering
University of Michigan

http://www.umich.edu/~avioli

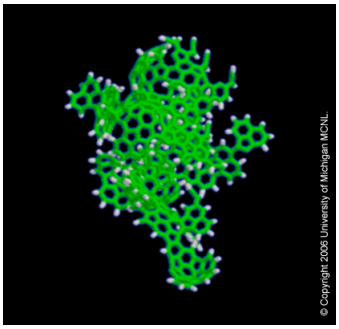
Abstract

Mechanisms of soot formation have been studied for quite some time, and there is general consensus that polycyclic aromatic hydrocarbons (PAH) are key intermediates: their growth leads to nucleation of particles and the latter continue to add mass via surface growth. Even though we are now able to predict the rate of soot formation to some degree of accuracy due to the development of detailed soot models, key uncertainties remain. Particularly, the mechanisms of soot nucleation and mass growth remain phenomenological. The majority of models of soot formation invoke irreversible dimerization of pyrene molecules as the initial nucleation step for the condensed. PAH dimers collide with PAH molecules forming PAH trimers or with other dimers forming PAH tetramers, and so on, all while individual PAH species keep increasing in size via molecular chemical growth reactions. Yet from thermodynamic considerations the condensed-phase PAH would evaporate at the flame temperature, rather than vapor-phase PAH condensing into particles.

In this work we report on recent results obtained in Violi group using computer simulations to study the formation of nanoparticles from different fuels, demonstrating the need to study the growth process using atomistic simulations. In particular, we will report on chemical and physical surrogates for jet fuels, combustion chemistry of gas-phase species and a unique computational tool that describe the formation of nanoparticles using atomistic simulations.

Molecular Dynamics simulations are used to provide molecular-level insight into the relationship between fuels, nanoparticle morphology, composition, and mechanisms of growth.

The multiscale computational method used to study these phenomena provide a connection between the various time scales in the high molecular mass compound growth problem, together with an unprecedented opportunity for the understanding of how the environment affects the formation and growth of nanoparticles.



The figure on the right shows the structure of a carbonaceous nanoparticle produced in high temperature regimes using multiscale simulations.