NANO HIGHLIGHT

Nano Carbon Particles in the Atmosphere: Formation and Transformation

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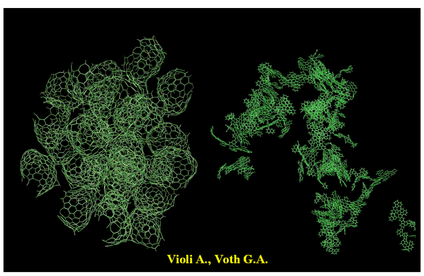
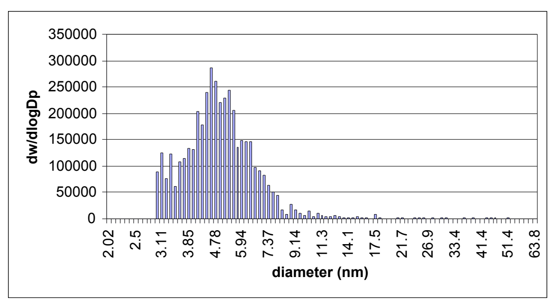
The University of Utah has an interdisciplinary team specializing in combustion, computational chemistry, aerosol dynamics and analytical chemistry to address the problem associated with the emission of carbonaceous nanoparticles from diesels. The project integrates experimental studies and theoretical simulation, in multi-level time and particle size scales, specifically addressing the following needs:

- Development of theoretical and experimental methodologies to describe the formation of heavier hydrocarbons and particle inception;
- modeling and measuring the particle size distribution; and,
- modeling of soot optical properties and free electrons as it ages.

This year's work has focused on particle inception and agglomeration, optical properties, and experimental work on young soot. As a first step, the nanoparticles inception is predicted with the atomistic combined Kinetic Monte Carlo/Molecular Dynamics code. These nanoparticles are mapped onto coarse-grained particles while preserving their unique topology (see below) by a multi-scale course-graining methodology. These coarse-grained units then interact and aggregate into much larger structures. Fig. 1 (left) shows an example of the simulation, for two different agglomeration geometries. Round particles (left) tend to cluster, while "flaky" particles behave differently and tend to subcluster. These simulations, combined with experimental results, will begin to help validate the agglomeration kinetics of soot particles.



An inverse diffusion flame (IDF) to investigate "young" soot has been built. In the IDF, air is fed in the middle, surrounded by fuel, and a nitrogen shroud. As soot is formed, it passes through nitrogen into the cooler region, quenching reactions. This differs from the premixed burner, where soot is formed and then diffuses through an oxygen region where the soot further reacts. The resulting particle size distribution is below 10 nm from the IDF flame, as seen in Fig. 2 (right), and as compared to 30-55 nm for a premixed burner. These particle size distributions were obtained from a nano-Scanning Mobility Particle Sizer (nano-SMPS), purchased with the funds from this grant. The nano-SMPS allows us to obtain particle size distributions down to 3 nanometers.



As we begin our collaborations with ANL, we will switch to a diffusion burner and further explore through Small Angle X-Ray Scattering (SAXS) the particle geometry and size. In addition, we will begin data exchange with Naples, where both the experimental and modeling PIs have now visited. Naples will give us information regarding particle geometry, size, and optical properties.