Soot modelling - describing the dynamics of organic nanoparticles

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Abstract

The organic nano-particles are produced in vast quantities two prominent examples are soot emissions of internal combustion engines and carbon black. In order to produce a product with specified properties or to avoid soot emissions industry one is interested in numerical models that can predict the formation and growth of soot particles. In this paper present a detailed soot model, which is validated by spatially, resolved measurements of the soot particle size distribution function (PSDF) in a laminar premixed ethylene-argon-oxygen flame using a Scanning Mobility Particle Sizer. The emphasis of the study was to follow the evolution of the PSDF from the onset of particle inception to particle mass growth. It was found that the PSDF becomes bimodal at a larger height above the burner surface, and remains bimodal throughout the flame. Numerical simulation using a soot kinetic model proposed previously and a stochastic approach to solve aerosol dynamics equations again showed a bimodal PSDF. Further analysis revealed that bimodality is intrinsic to an aerosol process involving particle-particle coagulation and particle nucleation dominated by monomer dimerization. The numerical method will be discussed in detail and the extension to high-pressure flames will be discussed.