The physical properties of carbon nanoparticles such as soot, carbon black, etc. depend on the nanostructure of the particles, especially aggregate structure. Development of predictive tools which estimate the mean properties and the aggregate shape can be of great help to better understand their formation and to custom-build specific grades of material. The number of carbon nanoparticle numerical models that can predict the aggregate structure is limited. Therefore, this work seeks the implementation of a recently developed aerosol dynamic model into a plug flow reactor code to simulate the carbon nanoparticle synthesis in flow reactors and predict the aggregate structure.

The aerosol dynamics model used in this study is based on the formation of polycyclic aromatic hydrocarbons (PAHs) and includes reversible particle inception, reversible surface PAH addition, hydrogen abstraction carbon addition (HACA), and particle aggregation. The modeling results are validated with experimental particle size distribution (PSD) and the aggregate structure generated from ethylene in a laminar flow reactor. Two chemical kinetic mechanisms which describe the formation and growth of PAHs are used for comparison purposes. The combination of both chemical kinetic mechanisms with the aerosol dynamics model predict PSD profiles reasonably well. The model's capability of predicting the number of primary particles per aggregate is promising.