Network analysis for the formation of aromatics in a co-flow flame

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An important step in predicting the growth of soot nanoparticles is understanding how gas phase variations affect the formation of their aromatic precursors. Once formed, these aromatic structures begin to assemble into nanoparticles and, regardless of the clustering process, the molecular properties of the aromatic precursors play an important role.

In this work, we report on a detailed study of the spatial evolution of molecular structures of polycyclic aromatic compounds (PACs) and their corresponding formation pathways. To this end, we employed the SNapS2 kinetic Monte Carlo software to simulate the chemical evolution of PACs along multiple streamlines. The results show that growth only occurs along streamlines that traverse regions of high acetylene concentrations in the center of the flame. The PACs predicted in various conditions show diverse chemical properties, including aliphatic chains, five-membered, and heteroaromatic rings. PACs in streamlines close to the flame wings begin growing immediately due to the high temperature and large amounts of radical species, while PACs originating along inner streamlines do not appreciably grow until they pass through an area characterized by high radical concentrations. Using graph theory and network analysis, we investigated the complex reaction network generated by SNapS2 and determined that the growth pathways of many PACs center around a few stable structures that also promote oxygen addition reactions due to their morphology and long lifetimes.

These pathways play a significant role along streamlines near the centerline, compared to the flame wings, which show more variety due to the highly reactive environment encountered during early growth. The results of this study provide insights on the reaction pathways that determine the properties of PACs at different flame locations as well as information on the chemical characteristics of the formed PACs, with emphasis on oxygenated structures.