Process Design Tool for Gas-Phase Synthesis of Nanomaterials

Abstract:

Carbon nanotubes (CNTs) have attracted significant interest for their exceptional electrical, optical, and mechanical properties, making them promising for energy storage, photodetectors, and surface engineering. CNTs are commonly synthesized in flow reactors, where feedstock gases such as acetylene, ethylene, methane, and carbon monoxide thermally decompose on metallic nanoparticle (NP) catalysts such as nickel (Ni) and iron (Fe); the resulting carbon atoms saturate the NPs, leading to inception and growth of CNTs. Because this process spans many orders of magnitude in time and length scales, the first-principles design and optimization of CNT synthesis remain challenging.

This study develops CarbonX, an object-oriented numerical tool for simulating flow reactors and predicting the synthesis of single- and multi-walled CNTs and metallic NPs under different process conditions. CarbonX integrates four fully coupled submodules: a detailed gas kinetics module; a detailed surface kinetics module that accounts for catalyst activation, deactivation, and hydrogenation; a particle dynamics module for tracking the evolution of NP morphology during inception (nucleation), coagulation, and sintering; and a CNT dynamics module for predicting nanotube length, diameter, and wall number. Different surface kinetics models are adapted from substrate-based flow reactors in the literature and extended to floating-catalyst flow reactor conditions. Using CarbonX, comprehensive 2D parametric maps of NP and CNT characteristics can be generated over a broad range of process parameters, including the carbon feedstock inlet pressure, the reactor temperature-time history, and the initial size and inlet number concentration of NPs. Using a machine-learning submodule integrated into the package, the generated parametric maps are classified into distinct zones, each corresponding to the specific process conditions (e.g., temperature, pressure, and catalyst concentration) required for the formation of single- and multi-walled CNTs. The package submodules are comprehensively benchmarked against experimental measurements of NP size distributions and CNT growth kinetics from multiple flow reactor configurations. This study contributes to the field by connecting process parameters to NP and CNT product characteristics from first principles, facilitating the systematic control and fundamental understanding of aggregate/agglomerate structure and growth dynamics of particles from free-molecular to continuum regimes.

Bio:

Hossein Rahbar is a PhD candidate at the Energy and Particle Technology Laboratory (EPTL) at Carleton University. His research focuses on aerosol science, molecular dynamics, and nonlinear finite element analysis. Hossein has published findings from this research in the *Journal of Physical Chemistry C*, the *Journal of Aerosol Science*, and *Carbon*.