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DEVELOPMENT OF A NUMERICAL MODEL TO SIMULATE CARBON BLACK SYNTHESIS AND PREDICT THE AGGREGATE STRUCTURE IN FLOW REACTORS

Ali Naseri[1], Murray J. Thomson[1*]

[1]*Mechanical and Industrial Engineering. University of Toronto, Toronto, Canada*

*Presenting author's e-mail: murray.thomson@utoronto.ca

Introduction

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.

Materials and Methods

The sectional 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[1]. The modeling results are validated with experimental particle size distribution (PSD)[2] and the aggregate structure generated from ethylene in a laminar flow reactor[2]. The two chemical kinetic mechanisms[3,4] 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 will be referred as Model 1 and Model 2 hereafter.

Results and Discussion

PSD profiles are usually measured using scanning mobility particle sizers (SMPSs). SMPS measures the mobility diameter and the count of particles. Figure 1 compares modeling results with the SMPS measurements at the end of a tube furnace measured for the inlet flow rate of 2 Nl/min[2]. Model 1 can capture the maximum diameter and Model 2 nicely captures the peak particle number concentration. This is the first step of the validation which shows the model can capture the general morphology of the particles.

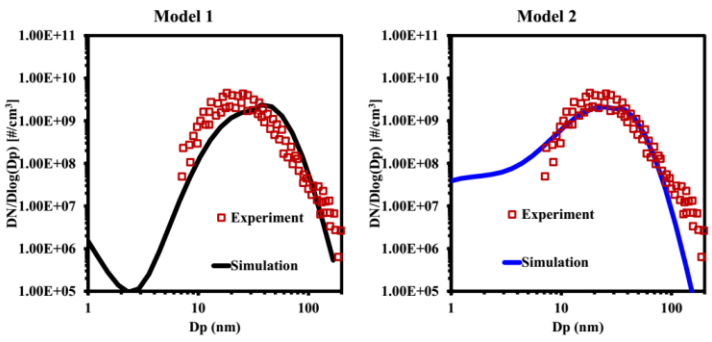

Figure 1. Particle size distribution

For the validation of the aggregation prediction, the SEM images of the particles by Dewa et al[2] were used. The number of primary particles per aggregate (n_P) and the primary particle diameter are summarized in Table 1 for the experment[2] and the simulations for three particles with mobility diameters of 30, 50, and 100 nm. There is a reasonably good agreement between the predicted and measured n_P, but the trends of the modelling and experimental results are opposite for the primary particle diameter. In a sectional model, the aggregation module considers the collision of different sections, i.e. primary particles with different diameters. However, the transfer of the particles between the sections takes place on a mass basis. To elaborate, the result of the collision of particles will be a lumped mass larger than the colliding particles. Then, this resulting mass will be transferred to a higher section. The amount of this mass divided by the section mass gives the total number of the particles transferred to this section. As a result, since everything happens on a mass basis, the history of the primary particle diameters is not tracked. This is an important simplifying assumption which reduces the computational cost and improves the convergence stability. Based on the modeling scheme we used, the primary particle diameter is a function of aggregate mass and n_P. Therefore, the primary particle diameter estimated for each section by the model is an average of all the contributing primary particles. That is the reason why the predicted primary particle trend contradicts the experimental data.

Table 1. Nanostructure study

	SEM images		Model 1		Model 2	
Mobility diameter [nm]	n_p	PP diameter [nm]	n_p	PP diameter [nm]	n_p	PP diameter [nm]
30	2	30	3	21	3	21
50	9	24	8	26	7	27
100	33	20	26	37	19	41

Conclusions

Models 1 and 2 predict the PSD profiles reasonably well. The model's capability of predicting the n_P is promising. CB manufacturers who use natural gas as their feedstock such as for thermal black can use this model to better understand their manufacturing process at least by considering the trends that can be derived from the model. For predicting the primary particle diameter size, new modeling techniques are required to capture the trends

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