Aerosol Dynamics Modeling and Computational Fluid Dynamics of a Laser-Driven Nanoparticle Synthesis Reactor

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A frequent by-product of silicon CVD is the formation of powder from gas-phase particle nucleation. In most cases, gas-phase nucleation is viewed as an undesirable phenomenon, which limits film growth rate and causes contamination[1]. Intentional silicon nanoparticle synthesis is also of great interest, due to the photoluminescence properties of these silicon nanoparticles that are not present in bulk silicon.

In order to understand particle formation, the general dynamic equation (GDE), which represents a population balance on the particles, for simultaneous nucleation, growth and coagulation is solved. An efficient and reasonably accurate method is the method of moments (MOM)[2], which has been used extensively due to its relative ease of implementation and low computational cost. One of the major limitations of the MOM is that a prior knowledge of the shape of the size distribution is necessary and it is thus unable to capture the evolution of size distribution during the early stages of particle formation. The quadrature method of moments (QMOM) avoids this complication by approximating the integral moments by an n-point Gaussian quadrature[3]. The sectional method approximates the continuous size distribution by a finite number of sections or bins within which the particle size distribution remains constant[4,5]. A relatively simple method for coagulation is implemented here, which makes the computation easier without loss in accuracy.

Simulations using the three methods described above were carried out for a 1-D plug flow reactor model. Particle size distributions were plotted as shown in Figure 1. Size distributions using the MOM and sectional method were compared.

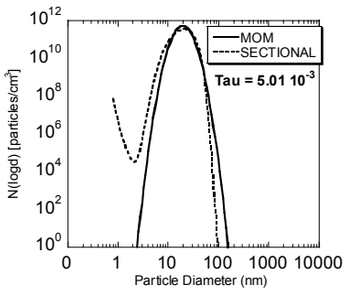

Fig 1: Comparing particle size distribution

At the early stages of particle formation, both nucleation and coagulation modes are captured by the sectional method as observed by other groups. The three methods that were used to solve the GDE are now compared with respect to some characteristics aerosol properties (particle concentration, volume fraction and particle diameter). Particle concentration predicted by all three methods is almost identical as shown in Figure 2.

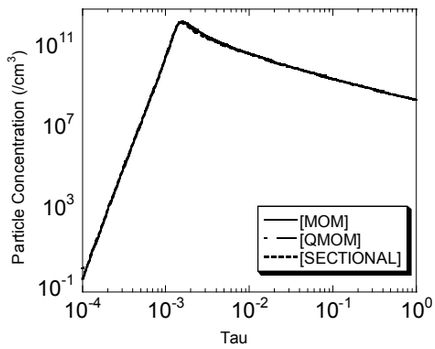

Fig 2: Particle concentration versus residence time for the three methods used to solve GDE.

FIDAP, a commercial fluid dynamics package was used for the detailed 3-D reactor modeling in order to simulate reactor conditions in our laboratory.

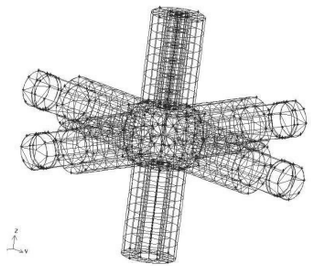

Figure 3: Using GAMBIT for creating and meshing the geometry. 11480 nodes were used for all simulations

Figure 3 shows the reactor geometry and the computational mess used in these simulations. Preliminary results from the CFD simulations are promising and show that the reaction zone is centered in the middle as was observed in our experiments.

An aerosol dynamics model was successfully implemented using MOM, QMOM and sectional method. All three methods predicted the same particle concentration, volume fraction and particle diameter. Work is in progress to get detailed temperature and velocity distributions for the actual reactor and couple that to the aerosol dynamics model to gain a more complete understanding of the evolution of particle size distributions with changing reactor conditions.

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