020516 Quiz 7 Nanopowders

1) A self-preserving size distribution has been proposed for many particle growth models using the Smoluchowski equation.

a) **What** does the term "self-preserving distribution" mean?

b) **What** is the relationship between the terms "self-preserving distribution" and "similarity solution"?

c) **What** steps were given in class to determine if a similarity solution is possible for a given form of the Smoluchowski equation and the collision kernel?

d) **What** are the advantages of finding a similarity solution from a numerical solution to the integro differential equation that results from a manipulation of the Smoluchowski equation using a similarity distribution?

e) **Explain** why one would want to know the time to reach a self-preserving distribution?

f) **How** would this vary with the standard deviation of the initial distribution?

2)

a) **What** is a mass-fractal aggregate?

b) **What** advantages might a mass fractal aggregate have over dispersed nanoparticles?

c) **What** disadvantages does an aggregate of this type have compared to dispersed nanoparticles?

d) In addition to the mass fractal dimension **what else** is needed to distinguish a Brownian aggregate from a plate?

e) **Why** have different values for the mass-fractal dimension been obtained from diffusion limited aggregate simulations obtained from different computer programs (even those from the same lab)? **Give** some typical values that have been obtained.

Answers: 020516 Quiz 7 Nanopowders

1) a) During particle growth the particle size distribution, as obtained from the Smoluchowski equation, leads to a function with a maximum and a similar shape that increases in peak position with time but retains some features associated with the shape of the distribution curve. By normalizing the distribution function a general function can be determined for the self-preserving distribution associated with the collision kernel used in the Smoluchowski equation and the assumptions made concerning particles growth. The ability to determine this general function for the distribution indicates that the distribution is self-preserving.

b) A self-preserving distribution often has a similarity solution, that is a unitless function that describes all distributions which occur while the particles are in the self-preserving regime. By considering the average volume at a given time and the total number of particles in the system, the entire distribution can be calculated from the similarity solution.

c) First, the collision kernel must be shown to be a homogeneous function of the particle volume, that is $\beta(\alpha v_i, \alpha v_j) = \alpha^{\lambda}\beta(v_i, v_j)$, where λ is the order of the equation in particle volume. Second, the Smoluchowski equatio must be able to be transformed into an ordinary interodifferential equation. This equation must meet the boundary conditions that are known for the particle growth problem. The equation then must be solved numerically for the similarity solution. The similarity solution can be used to calculate particle size distributions generically.

d) The advantage is that a general solution can be applied to a wide variety of problems. For a given solution the same similarity solution might be applied to pyrolytic growth of silica (fumed silica) or plasma or arc growth of gold nano-particles or the particle size distribution in an industrial effluent. Since there are only a few main categories of particle growth conditions a single similarity solution can have broad implications.

e) The time to reach the SPD is important since it governs the applicability and importance of the SPD to a given problem of calculating the particle size distribution. Prior to the SPD calculation of the particle size distribution would involve numerical solutions of integrodifferential equations for each value of time for instance. In the SPD all distributions can be calculated directly from the similarity solution.

f) The further the standard deviation is from the SPD standard deviation, the longer it will take to reach the SPD. The SPD is reached faster for distributions with a smaller standard deviation than that of the SPD.

2) a) A mass-fractal aggregate is a ramified structure composed of primary particles, that are generally close to monodisperse, and which are bonded into an open branched structure. The mass, N, of a mass-fractal structure is related to the size, R, between the primary particle size and the aggregate size by the mass fractal dimension, d_f,