020523 Quiz 8 Nanoparticles

1)

a) **How do you account** for reaction limited aggregation in a computer simulation?

b) **What** is the effect on the mass-fractal dimension of the resulting aggregates compared to DLA values?

c) **Explain** the following sentence from the notes:
"While the velocity depends on a Rouse like model, the aggregate cross section is viewed from a non-draining hydrodynamic perspective" pertaining to mass fractal aggregates in the free moleculare regime.

d) **What is** the collision kernel for mass fractal aggregates in the free molecular regime?

e) **What is** the collision kernel for mass fractal aggregates in the continuum regime?

2)

a) In the Agashe presentation, **what does** the VLS method mean?

b) In the Abhijit presentation, **what advantage** was mentioned for nanoparticles in photocatalysis?

c) For Ernie's presentation, **what is** the paramagnetic limit?

d) For Jennifer's presentation, **what advantage** is there to nano- hydroxyapatite in bone polymer composites compared to micron size hydroxyapatite?

e) For Brian, **what advantages** are there for carbon nanotubes over an activated carbon with primary particles on the order of 10 nm?

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1) a) Sticking probability introduces reaction limited growth.

b) For cluster-cluster aggregation in DLA the mass fractal dimension is for example, 1.8, while for reaction limited growth it is about 2.1.

c) Rouse like model means contributions from each primary particle are summed so the drag used to calculate the velocity is the sum of the drag from all the particles, i.e. N times the drag for one particle. The non draining hydrodynamic perspective means the mass fractal is treated as if it were a sphere with a radius of R = $N^{1/df}$. There are the components of the collision kernel for free molecular range for instance.

d) $\beta\left(v_i, v_j\right) = \left(\frac{6kT}{\rho}\right)^{1/2} \left(\frac{3}{4\pi}\right)^{\lambda} a_{p0}^{2-6/d_f} \left(v_i^{1/d_f} + v_j^{1/d_f}\right)^2 \left(\frac{1}{v_i} + \frac{1}{v_j}\right)^{1/2}$ Free Molecular Regime

e) $\beta\left(v_i, v_j\right) = \frac{2kT}{3\mu}\left(v_i^{1/d_f} + v_j^{1/d_f}\right)^2 \left(\frac{1}{v_i^{1/d_f} + v_j^{1/d_f}}\right)^{1/2}$

2)
a) VLS means vapor-liquid-solid growth path, i.e. condensation of a vapor to a liquid from which nano particles grow.

b) Small size leads to high surface area was mentioned. There are other features that enhance catalytic activity such as shift of electron band gaps.

c) "This scaling runs into limits though as the paramagnetic limit is approached. In simple terms the paramagnetic limit is reached as the magnetic energy stored becomes close to the thermal energy of the atoms, making it impossible to store magnetic states [3,4,5]. The relationship between the magnetic energy density per particle (K_uV, where K_u is the magnetic anisotropy energy density, and V is the grain volume) and the thermal energy (k_BT, where k_b is Boltzmann's constant, and T is temperature in Kelvin) needs to exceed 40 for stability for great than 10 years [5]. Analyzing the relationship K_uV/k_BT, one can quickly see that while Boltzmann's constant is fixed, as is the operating temperature for all intents and purposes, the magnetic anisotropy energy density and the volume can both be increased. The problem arises though that the volume must be decreased to increase storage capacity of hard drives, unless one wants hard drives that are as big as the original RAMAC drive. Therefore, to maintain a K_uV/k_BT ratio greater than 40, the magnetic anisotropy energy density must be increased. The problem with increasing K_u is that the critical coercive field, H_{CR} scales linearly with K_u [5]. This increase in H_{CR} means that the energy required to write to the disk increases, as it takes more to reverse the fields in each grain."

d) Advantage is that it apparently is easier to disperse nano-particles in a uniform manner.

e) Advantages are many, CNT's have higher surface area, hydrogen can be stored inside the tube an outside, CNT's can hold catalysts that activate hydrogen storage, there are other advantages that he mentioned.