020502 Quiz 5 Nanoparticles

1) (30 pts) For Brownian particles or atoms how is the diffusion coefficient, D, related to the friction factor (friction coefficient), f?
   For a particle traveling at a speed c with a friction coefficient f, what is the drag force due to friction?
   What is f in the continuum range? (Define the terms)
   What is f in the free molecular range? (Define the terms)

2) (10pts) Is D for an ellipsoidal particle larger or smaller than D for a sphere of the same volume, D_0?
   Why?

3) (30pts) For a ramified mass-fractal aggregate, what is D for the continuum range?
   What is D for the free molecular range?
   What is the basis for these two equations?
   Keeping in mind that $1 \le d_f \le 3$ which is expected to have a larger value?

4) (30pts) The kinetic theory of gasses gives $l_p = 1/(\pi\sqrt{2}\ \text{mass}\ d^2)$ for the persistence of velocity for a gas molecule.
   How does this compare with l_{pa} for a nano-particle in the continuum range and in the free molecular range?
   Give an equation for l_{pa} in these two ranges.
   Sketch log l_{pa} verus log particle size for nano to micron scale particles.

Answers: 020502 Quiz 5 Nanoparticles

1) $D = \frac{kT}{f}$

$F_{drag} = -fc$

Continuum: $f = 3\pi\eta d_p$, where η is the gas viscosity.

Free Molecular: $f = \frac{2}{3} d_p^2 \rho \left(\frac{2\pi kT}{m}\right)^{\frac{1}{2}} \left[1 + \frac{\pi\alpha}{8}\right]$ where ρ is the gas density, m is the gas molecular mass from kinetic theory and α is the accommodation coefficient that describes the probability of a gas molecule contributing its kT energy to the nanoparticle.

2) D for an ellipsoidal particle is generally larger since the particle can present a lower drag profile on average.

3) For the continuum range the aggregate is treated as a large sphere of size $d_{agg} \sim N_{agg}^{1/df}$. Then Stokes law can be used, $f = 3\pi\eta d_{agg} \sim 3\pi\eta\, N_{agg}^{1/df} = f_1\, d_{agg}/d_1$. Using the Einstein equation we have, $D \sim D_1/N_{agg}^{1/df} = (d_1/\, d_{agg})\, D_1$.
For the free molecular range the aggregate is treated as a Rousian string of primary particles that contribute individually, so, $f = 3\pi\eta 3\pi\eta d_{agg}/d_1 D \sim D_1/N_{agg} = (d_1/\, d_{agg})^{df}\, D_1$.
The free molecular aggregate will have a higher diffusion coefficient.

4) Nanoparticles, using turbulent flow theory, have a persistence of velocity of, $l_{pa} = \frac{(mkT)^{\frac{1}{2}}}{f}$.

For the continuum regime this yields $l_{pa} = \frac{(mkT)^{\frac{1}{2}}}{f} = \frac{d_p^{1/2}(\rho kT)^{1/2}}{3\pi\eta}$. This increases with the square root of the particle size while the gas persistence of velocity decrease with the square of particle size. For the free molecular range, f scales with d_p^2, so l_{pa} scales with $d_p^{-1/2}$ which follows the same trend as low molecular weight gasses but has a weaker dependence on d_p.

The sketch shows l_{pa} decreasing until about 0.1 micron then increasing in the continuum regime. The minimum is at about 7nm.