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**N° O3a-6**

**PROPERTIES OF NANOPARTICLES AFFECTING SIMULATION OF FIBROUS GAS FILTER PERFORMANCE**

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Computational Fluid Dynamics (CFD) software now widely available allows detailed simulation of the flow of gases through fibrous filter media. When the pattern of gas velocity vectors in the interstices between fibers has been established, a simulated particle of any desired size can be “injected” into the entering gas stream, and its path under the influence of aerodynamic drag, Brownian motion, electrostatic forces and thermal gradients traced, until the particle either collides with a fiber, or passes through the entire filter medium. Successive simulated injection of many particles at random locations in the entering stream allows an average probability of capture to be calculated. If the particles can be assumed to adhere permanently to fibers after a collision, the average thus determined will represent the capture probability, or “efficiency” for that particle type and size of particle.

Many particle properties must be available as parameters for the equations defining aerodynamic drag, electrical and thermal mobility, and Brownian velocity. Particle morphology, size, density, Knudsen Number, charge, and dielectric constant are examples of influential properties. These properties have been characterized and measured in many studies for micrometer-scale particles, but less so for nanoparticles.

A particle which collides with a fiber does not necessarily remain permanently attached to that fiber. Under some conditions, a particle will bounce off the fiber, re-entering the gas stream with some velocity and direction dependent its shape, its velocity and angle of approach to the fiber surface, and the elastic properties of the particle-fiber combination. If the particle does not bounce, it may still be bound to the fiber surface weakly enough to be removed by the gas flow past the fiber, or by vibration. A particle retained on the fiber surface becomes a potential object for collisions by later arrivals of its own kind. Indeed, the formation of fiber-like chains of captured particles – dendrites – has been observed in filter media. Thus both particle-fiber and particle-particle bounce and adhesion properties are needed for a complete simulation of particle filtration. This is especially important in simulating the “loading” of filter media, which can enable prediction of the rise in pressure drop across a filter medium when some distribution of aerosol particles is fed to it over an extended period of time.

Accurate values for all properties affecting particle dynamics are needed, not only for predicting particle capture in actual service, but also to validate models for media geometries and computational procedures used in CFD.

We present a survey of existing literature on the properties influencing the effects listed above, with emphasis on nanoparticles where available. In some cases, effects which are significant for particles with micrometer dimensions are trivial for nanoparticles; in some cases, the reverse is true. We discuss the reliability of extrapolation of property values from micrometer-scale studies to nanoparticles, where nanoparticle data are not available.