CHAPTER 4

STOCHASTIC MODEL FOR CONVECTIVE DIFFUSIONAL DEPOSITION OF AEROSOLS ON A DUST LOADED FIBER

The success or failure of any simulation study depends on the sufficiency of the mathematical model being used to depict the real physical process. This study was aimed at the effects of polydispersity of the particle sizea on collection efficiency of a single cylindrical fiber for the case in which the dominant transport mechanism is convective diffusion. A realistic and general dynamic model is desirable. The word "model" here includes a set of assumptions and the corresponding equations required to describe a system (or process), involving (1) the application of the conservation laws of mass and of energy and (2) appropriate expressions to account for the transfer of mass and energy across the boundary of the system. In Section 4.1 a brief discussion of the basic theory of aerosol filtration is presented for convective diffusional deposition. An introduction to particle size distribution is given in Section 4.2 and the present model is explained in Section 4.3.

4.1 Basic Theory of Aerosol Deposition on a Filter Fiber

Particles are deposited on a filter fiber from the gas layer adjacent to the fiber; therefore, to calculte particle deposition, the flow field in the proximity of the fiber surface should be known in detail. It can be said that the development of the theory of gas filtration on fibrous filters was determined by the achievements of the theory of gas flow around a cylinder.

Theories of arosol filtration and their historical developments in the study of aerosols can be found in the literature. (Fuchs, N.A., 1964; Davies, C.N., 1966, 1973; etc.) and no attempt will be made to review all of them. The only attempt made here is to introduce only that was necessary to grasp and construct the present model. Because of the complex structure of a fibrous filter and, consequently, the complex pattern of the flow, simplified filter models with known flow field were use for theorical studies.

One widely used flow field around a cylinder was derived by Kuwabara (1959). Since his flow field describes the velocity field in a random array of parallel fibers, it is quite realistic in representing the actual flow field.

4.1.1 Kuwabara Flow Field

Kuwabara (1959) solved the Navier-Stokes equations for viscous flow transverse to a set of parallel cylinders which are randomly arranged. His method assumed that each cylinder, or fiber, of radius R_f was surrounded by an imaginary coaxial cylindricall cell of radius R_c (Figure 4.1). If there are n parallel fibers per unit volume of filter the volume fraction or packing density, α, is

$$\alpha = n\pi R_f^2 \qquad (4.1.1)$$

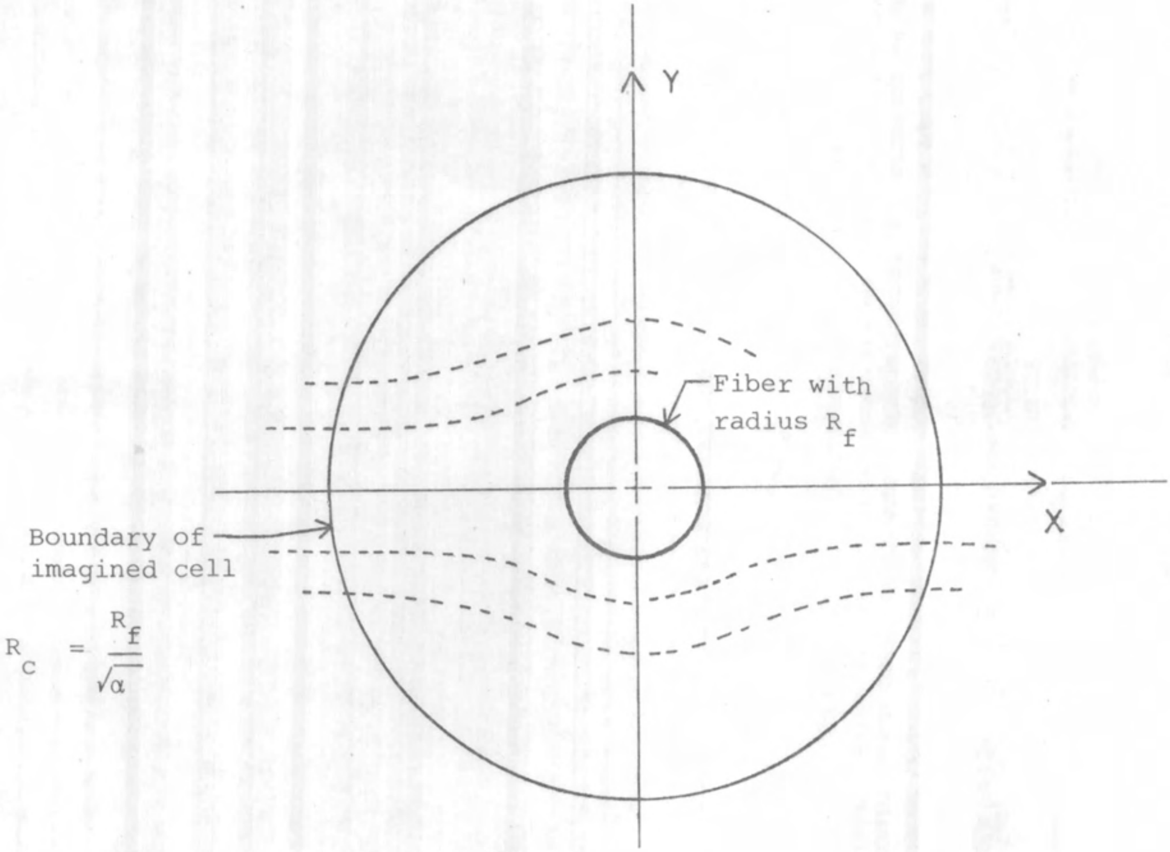

Figure 4.1 Cross section of Kuwabara's cell

and R_c in adjusted so that

$$n\pi R_c^{\ 2} = 1 \qquad (4.1.2)$$

thus

$$R_c = \frac{R_f}{\sqrt{\alpha}} \qquad (4.1.3)$$

$$= \frac{1}{\sqrt{\alpha}} \quad \text{for } R_f = 1$$

The boundary conditions used by Kuwabara were zero velocity on the surface of a fiber and zero vorticity on the surface of the cell, R_c. Kuwabara flow field was investigated experimentally by Kirsch and Fuchs (1967). They found that the experimental velocities agreed closely with the values obtained from Kuwabara's equations.

The stream function, ψ, obtained by Kuwabara expressed in dimensionless form is

$$\psi = \frac{Y}{2K}\left[(1 - \frac{\alpha}{2})\frac{1}{X^2 + Y^2} - (1 - \alpha) + \ln(X^2 + Y^2) - \frac{\alpha}{2}(X^2 + Y^2)\right] \qquad (4.1.4)$$

where K is a a hydrodynamic factor defined as

$$K = -\tfrac{1}{2}\ln\alpha + \alpha - \frac{\alpha^2}{4} - \frac{3}{4} \qquad (4.1.5)$$

and

$$X = x/R_f, \quad Y = y/R_f, \quad Z = z/R_f. \qquad (4.1.6)$$

The corresponding dimensionless velocity components are

$$U_x = \frac{\partial\psi}{\partial Y}, \quad U_y = -\frac{\partial\psi}{\partial X}, \quad U_z = 0 \qquad (4.1.7)$$

4.1.2 Single Fiber Representation of a Fibrous Filter

A filter consists of a mass of fibers which usually are randomly oriented and placed perpendicular to the direction of flow. Suppose a filter of unit cross flow lies across the direction of flow and the total length of all fibers in unit thickness is L. The packing density, α, of a filter with a fiber radius R_f is

$$\alpha = \pi R_f^2 L \qquad (4.1.8)$$

If the filter consists of fiber i of length L_i and radius R_{fi}, and so on,

$$\alpha = \pi \sum_i R_{fi}^2 L_i \qquad (4.1.9)$$

The collection efficiency of a fiber is usually defined as the ratio of the number (of mass) of particles striking it to the number (or mass) that would strike it if the streamlines were not diverted by the presence of the fiber. If a fiber of radius R_f removes all particles of radius r_p contained in layer of thickness 2y (see Figure 4.2), the collection effiency η is

$$\eta = \frac{Y}{R_f} \qquad (4.1.10)$$

The change in aerosol concentration across a fibrous mat of thickness dx is given by

$$-\frac{dn}{dx} = n\eta\, L2R_f/(1-\alpha) \qquad (4.1.11)$$

where n is the number concentration of aerosol particles

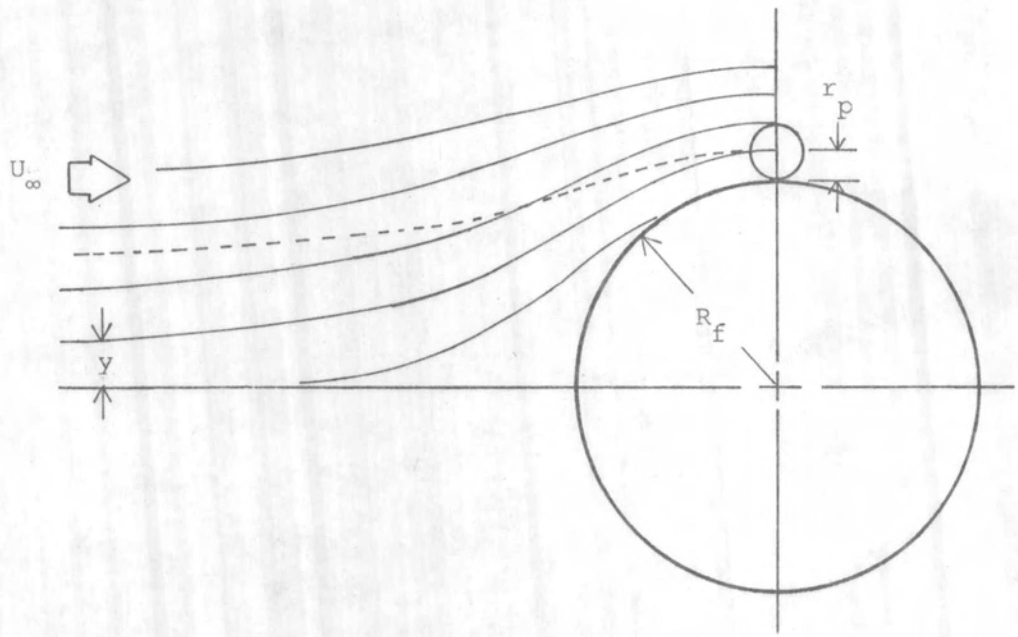

Figure 4.2 Streamlines near a cylindrical fiber lying transverse to flow, and the definition of single fiber efficiency

Integration over the thickness, h, of the filter gives

$$\frac{n}{n_o} = \exp\left[-2\eta\ LR_f\ h/(1-\alpha)\right] \tag{4.1.12}$$

n being the concentration of particles penetrating through the filter and n_0, the concentration of particles entering the filter.

For cylindrical fibers of constant radius, L can be eliminated.

From
$$L = \frac{\alpha}{\pi R_f^2} \tag{4.1.8}$$

then

$$\frac{n}{n_o} = \exp\left[-2\eta\ \alpha\ h/\pi R_f(1-\alpha)\right] \tag{4.1.13}$$

Single fiber efficiency can be found via an experimental or theoretical investigation. One would expect that the theoretical values would be higher than experimental ones. The reason is that the spatial distribution of fibers in a real filter is non-uniform; some fiber might clump together, some screen one another and not all lie transverse to air flow.

4.1.3 Filtration Mechanisms

Filtration under the condition of viscous flow which holds in high efficiency fibrous filters is governed mainly by Brownian motion, intertia, direct interception, sedimentary settling, electrostatic deposition etc.

Deposition by interception is shown in Figure 4.2. This mechanism is directly related to the size of the particle. The particle is intercepted once it approches the surface of the fiber to a distance equal to its radius.

A massive particle approching the fiber will not exactly follow the streamline of the air flow but, because of inertia, will trace out a more direct path as indicated by the dotted line. The deviation will be greater, the more massive the particle and the higher the velocity of approach

When a particle is very small, in the submicron size region (0.5 - 1 micron or less), the main deposition mechanism is Brownian diffusion caused by collisions with the molecules of fluid medium.

Sedimentary settling and electrostatic deposition are, respectively, due to gravitational forces and Coulomb's induction forces between charged particles and fibers. The following discussion, will be restricted to the subject of our interest, namely, convective Brownian diffusion.

Owing to Brownian motion the trajectory of a fine particle does not coincide with the streamline of the air : the particle may diffuse a way from the streamline to deposit on the fiber. As the particle size decreases, the intensity of the Brownian motion increases, and so does, in consequence, the efficiency of diffusional deposition.

The efficiency pertaining to a given mechanism is generally a function of the parameters describing it. A characteristic parameter that determines diffusional deposition is the Peclet number

$Pe = U_\infty D_f/D$, where D is the diffusion coefficient. Other parameters which are common to all deposition mechanisms are the density of the particle ρ_p, air viscosity μ, and the interception paramenter $R = r_p/R_f$. The capture of small particles whose inertial effect is negligible by a single fiber, has received considerable attention. The first stage efficiency or clean fiber efficiency is obtained for different cases by many researches. Their results are published elsewhere (Fuchs, 1964; Devies, 1966, 1973; Emi et al., 1973; Kirsch et al., 1978; Crawford, 1980 and Ingham, 1981) and they are not restated here. However it is interestiong to summarize the results for a simple case of diffusional deposition based on the Kuwabara flow field which has the advantage that there is no need to correct for the interference effect between fibers. The case is the convective diffusional deposition of inertia-less particles on a single cylindrical fiber placed transverse to air flow. The diffusion equation in cylindrical coordinates is

$$v_r \frac{\partial n}{\partial r} + v_\theta \frac{\partial n}{\partial \theta} = D \frac{\partial^2 n}{\partial r^2} + \frac{1}{r}\frac{\partial n}{\partial r} + \frac{1}{r^2}\frac{\partial^2 n}{\partial \theta^2} \qquad (4.1.14)$$

Here n is the concentration of aerosols; v_r and v_θ are the tangential and radial components of the velocity of air stream, given by the Kuwabara expression; and, D is the diffusion coeffieient of the aerosol particles.

The collection effieiency of the cylinder is

$$\eta_D = \frac{2\, D(R_f + r_p) \left(\frac{\partial n}{\partial r}\right)_{r = R_f + r_p} d\theta.}{2\, v\, R\, n_0} \qquad (4.1.15)$$

In order to obtain $(\partial n/\partial r)_{r = R_f + r_p}$ it is necessary to solve equation (4.1.14), which cannot be done analytically. Stechina and Fuchs (1966) have given the solution to the simplified equation that leaves out the term $\frac{1}{r^2} \frac{\partial^2 n}{\partial \theta^2}$. The boundary conditions are

$$n = 0 \text{ at } r = R_f + r_p, \; n = n_0 \text{ at } r = \sigma.$$

Here σ is the mass transfer boundary layer thickness, at which the concentration of aerosols fall from n_0 to zero on the surface of the fiber. The approximate value of σ is deduced from equation (4.1.4). That is,

$$\frac{\sigma}{R} = \frac{¶^2 K}{(1-\alpha)} \left[\frac{1}{2Pe}\right]^{\frac{1}{3}} \qquad (4.1.16)$$

Davies (1973) gave the range of σ for Pe range between 100 and 10,000. In most cases, σ is usually small and K is near to unity. Therefore

$$0.32 > \frac{\alpha}{R} > 0.0.7$$

and it decreases as particle size and Peclet number increase.

The collection effieiency of a single fiber is obtained by solving equation (4.1.14) and equation (4.1.15). The result is then written in the form

$$\eta_D = 2.9K^{-\frac{1}{3}} \, Pe^{-\frac{2}{3}} + 0.624 \, Pe^{-1} \qquad (4.1.17)$$

4.2 Particle Size Distribution

In specifying the size distribution of aerosols and in solving theoretical and applied aerosol problems, it is convenient to use a mathematic expression with a mininum number of parameters to characterize the distribution. Yet it is desirable that such an expression should be applicable to the largest possible number of aerodisperse systems so that in going from one system to another only the values of the parameters would change.

By employing a sufficiently large number of parameters it would be possible to represent by a single mathematical expression all the distributions encountered in practice. However the choice of parameters would require a large volume of work and it would be difficult to assign intelligent physical meaning to them; for this reason expressions with many parameters are rarely used in practice. As a rule, mathemetical expressions with only two parameters are widely used, one parameter defining the mean particle size and the other a measure of the dispersion of particle size.

Because of its desirable mathematical properties, the standard deviation, σ is almost exclusively used as the measure of dispersion. The standard deviation is the root mean square deviation about the mean value. Its derivation and application in significance testing and setting confidence levels can be found in most texbooks on statistics.

Many fine-particle systems, whether formed by comminution of a bulk material or grown by accretion, have particle size distributions that obey the log-normal distribution function. When the frequency of occurence of a particle size is plotted against particle sizes, a skewed particle size distribution is obtained, as illustrated in Figure 4.3 (a). The majority of dispersion and condensation aerosols possess such asymmetrical distributions, the steeper slope corresponding to the size of small diameter. However, when the same distribution is replotted against the logarithm of the particle size, the asymmetrical or skewed curve is often transformed into a symmetrical bell-shaped normal distribution, as in Figure 4.3 (b). This transformation is of utmost importance because in this form the distribution is amenable to all the statistical procedure developed for the normal or Gaussian distribution.

In this case, the distribution is called log-normal and is expressed by

$$f(d)\,d(d) = \frac{1}{d \ln \sigma_g \sqrt{2\pi}} \exp\left[-\frac{(\ln d - \ln d_g)^2}{2(\ln \sigma_g)^2}\right] d(d) \qquad (4.2.1)$$

Here $\log d_g = \frac{1}{N} \sum_i^N \log d_i$, and consequently

$d_g = (\prod_i^N d_i)^{1/N}$ is the geometrical mean of the particle diameter.

$(\ln \sigma_g)^2 = \frac{\sum_i^N (\ln di/d_g)^2}{N}$ is the varience of the logarithm of particle sizes. σ_g, is called the standard geometric deviation. N is the total number of particles in the collection.

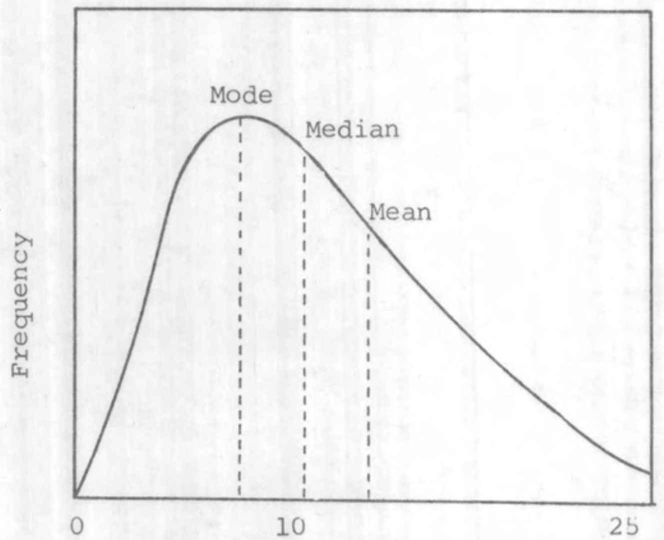

Figure 4.3 (a) Skewed particle size distribution of some typical dust

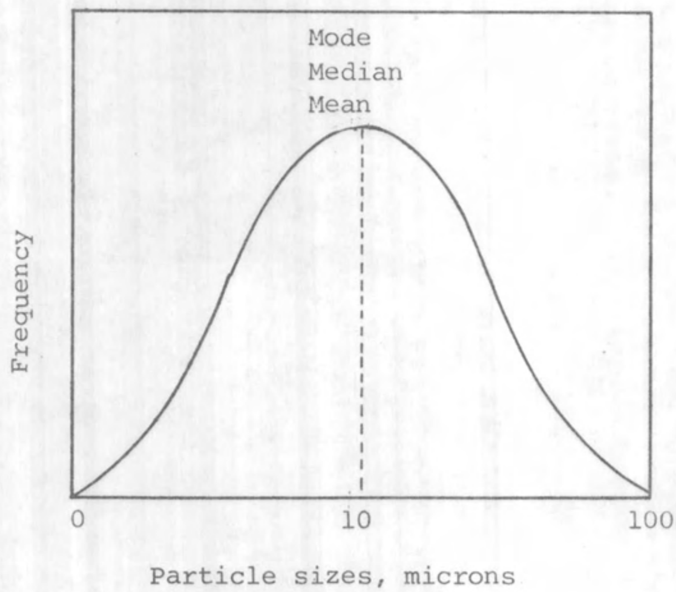

Figure 4.3 (b) Particle size distribution of (a). Plotted against logarithm of particle size

To find the probability that the diameter of a log-normal aerosol assumes a value between a and b ($0 \leqslant a \leqslant b$), we write

$$P\,(a \leqslant d \leqslant b) \;=\; \frac{1}{d\,\ln\sigma_g\sqrt{2\pi}}\;\exp\left[-\frac{(\ln d - \ln d_g)^2}{2(\ln\sigma_g)^2}\right] d(d) \qquad (4.2.2)$$

Changing variables by letting $x = \ln d$, $\bar{x} = \ln d_g$, $\sigma_g = \ln\sigma_g$ and, hence $d\,x = d^{-1}\,d(d)$, we obtain

$$P\,(a \leqslant d \leqslant b) \;=\; \frac{1}{\sqrt{2\pi}\,\sigma}\;\exp\left[-\frac{(x-\bar{x})^2}{2\,\sigma^2}\right] d\,x \qquad (4.2.3)$$

It can be seen that this probabiligy is equivalent to that of a normal random variable with $\bar{x} = \ln d_g = \ln d_i$ and $\sigma^2 = (\ln\sigma_g)^2 = (\ln d - \ln d_g)^2$.

Two parameters, namely, the geometric mean particle size. d_g, and the geometric standard deviation, σ_g, completely specify a log-normal particle size distribution. The geometric standard deviation, σ_g is identical for all methods of specifying the particle size distribution, whether by particle number, surface, mass or any other quantity of the form $K\,d^n$ where d is the particle diameter and K is a parameter common to all particles. The geometric mean diameter, d_g, is equal to the median or central value of the distribution.

Two samples having identical d_g and σ_g values can be said to be drawn from the same total population and they exhibit properties characteristic of the total population. These two values should be determined and reported as part of any aerosol or powder study. Obedience to the log-normal distribution function can be verified because the values of d_g and σ_g are easily obtained by plotting the cumulative frequency data on logarithmic probability graph paper. If the particle size distribution obeys the log-normal distribution function, a straight line will be obtained on the log-probability graph shown in Figure 4.4. The value of d_g is equal to the 50 % value of the distribution, and σ_g is equal to the ratio of the 84.1 % value divided by the 50 % value.

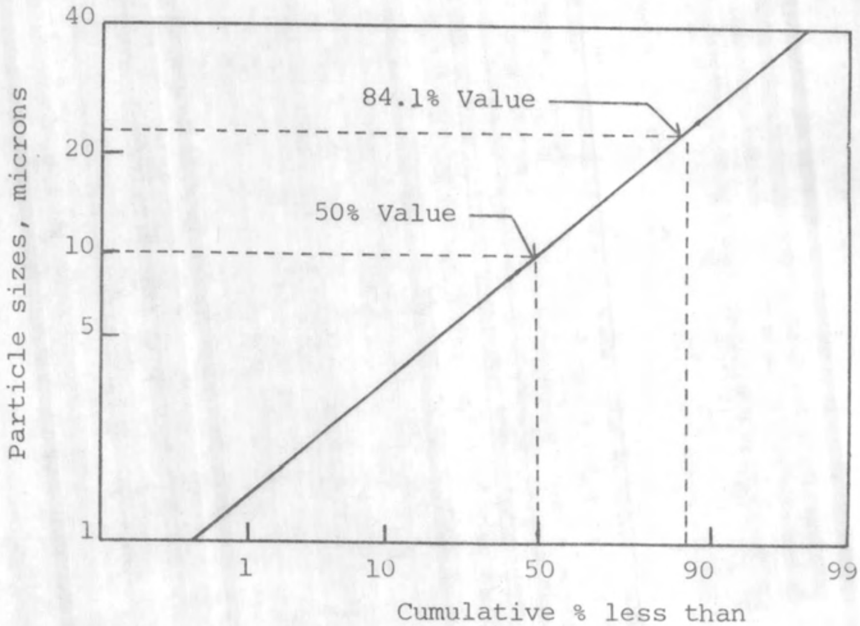

Figure 4.4 Cumulative log-probability curve for particle size distribution of Figure 4.3

4.3 Stochastic Model for Convective Diffusional Deposition of Polydisperse Aerosols on a Dust Loaded Fiber

The present model is an extension of the model presented by Kanaoka et al. (1981), which was originally a stochastic model to simulate the convective diffusional deposition of polydisperse aerosols via Monte Carlo method.

Consider the motion of a fine particle that, besides moving orderly under the influence of an external force or the motion of a fluid, is also moving randomly due to Brownian effect. The ordered motion or forced convection of a particle can be described by a Kuwabara stream function which was explained in the preceding section. Due to its stochastic nature, the Brownian motion is, on the other hand, governed by a probability function.

For a fine particle of radius r_p, the motion along an air stream of velocity u is given by rewriting Langevin's equation, as

$$\frac{d\,v}{dt} = -\beta(v - u) + A(t) \qquad (4.3.1)$$

where

v is the velocity of the aerosol particle,

u is the velocity of the fluid stream,

$\beta(v - u)$ is a dynamical friction experienced by the particle,

and

A(t) is a fluctuating force which is characteristic of the Brownian motion.

For a relative short time period Δt during which the fluid velocity u remains essentially constant, we have

$$\frac{dw}{dt} = -\beta w + A(t) \qquad (4.3.2)$$

where $w = v - u$ is the particle velocity relative to u. By assuming that A(t) is essentially independent of the fluid velocity u, the transition probability of the particle from point r_0 to point r in time Δt is (Chandrasekhar, 1943)

$$W(r, \Delta t; r_0) = \frac{1}{(4\pi D\Delta t)^{\frac{3}{2}}} \exp(-|r - r_0|^2/4D\Delta t)dV \qquad (4.3.3)$$

$$(t >> \tau)$$

where D = KTB is the diffusion coefficient, dV is an element of volume, k is the Boltzmann constant, T is the absolute temperature, and B is the mobility of particles.

Note that $W(r, \Delta t; r_0)$ is an independent of the initial velocity w_0.

The mean square displacement in one coordinate, $(x - x_0)^2$, of the particle in time Δt is obtained by noting that

$$W(x, \Delta t; x_0) = \frac{1}{(4\pi D\Delta t)^{\frac{1}{2}}} \exp(-|x - x_0|^2/4D\Delta t)dx \qquad (4.3.4)$$

By means of the substitution $(x - x_0)/\sqrt{4Dt} = \zeta$, we find

$$(x - x_0)^2 = \frac{1}{(4\pi D\Delta t)^{\frac{1}{2}}} \int_{-\infty}^{\infty} (x - x_0)^2 \exp(-|x - x_0|^2/4D\Delta t)dx$$

$$= \frac{4 D\Delta t}{\pi^{\frac{1}{2}}} \int_{-\infty}^{\infty} \zeta^2 \exp |(-\zeta)^2| d\zeta = 2D\Delta t \qquad (4.3.5)$$

Though the mean square displacement in space, $\overline{|r - r_0|^2}$, can similarly be determined with the aid of equation (4.3.3), it can readily be found by remembering that

$$\overline{(x - x_0)^2} = \overline{(y - y_0)^2} = \overline{(z - z_0)^2} = 2D\Delta t \ .$$

Thus

$$\begin{aligned}\overline{|r - r_0|^2} &= \overline{(x - x_0)^2 + (y - Y_0)^2 + (z - z_0)^2} \\ &= \overline{(x - x_0)^2} + \overline{(y - Y_0)^2} + \overline{(z - z_0)^2} \\ &= 6D\Delta t \qquad (4.3.6)\end{aligned}$$

When the particle is moving in an ordered manner at a constant velocity u on top of its random motion, the transition probability is simply

$$W(r,\Delta t;r_o) = \frac{1}{(4\P D\Delta t)}^{\frac{3}{2}} \exp\left(-|r-r_o-u\Delta t|^2/4D\Delta t\right) \qquad (4.3.7)$$

Likewise the one-dimensional transition probabity for the present case is

$$W(x,\Delta t;x_o) = \frac{1}{(4\P D\Delta t)}^{\frac{1}{2}} \exp\left(-|x-x_o-u_x\Delta t|^2/4D\Delta t\right) \qquad (4.3.8)$$

For a sufficient small period of time, Δt, the air velocity u_x remains essentially constant. By setting $(x - x_0 - u_x t)/\sqrt{4Dt} = \zeta$, we have

$$\begin{aligned}\overline{|x-x_o|^2} &= \frac{1}{(4\P D\Delta t)}^{\frac{1}{2}} (x-x_o)^2 \exp\left(-|x-x_o-u_x\Delta t|^2/4D\Delta t\right) dx \\ &= \frac{1}{\sqrt{\P}} (u_x\Delta t+\zeta(4D\Delta t)^2 \exp(-\zeta^2)d\zeta \\ &= \frac{1}{\sqrt{\P}} (u_x^2\Delta t^2\sqrt{\P} + 4D\Delta t \frac{\sqrt{\P}}{2}) \\ &= u_x^2\Delta t^2+2D\Delta t \qquad (4.3.9)\end{aligned}$$

The mean square displacement in space, $|r - r_0|^2$, is then

$$\overline{|r - r_0|^2} = |u|^2 \Delta t^2 + 6D\Delta t \qquad (4.3.10)$$

In this case, therefore, the mean square displacement is equal to the sum of squares of "ordered" displacements and of purely Brownian displacements.

For a stationary system the Brownian movement of a fine particle from time t to t + Δt may be simulated by the difference equation

$$r_i = r_{i-1} + \sigma n_{i-1} \quad (i = 1, 2, 3, ...) \qquad (4.3.11)$$

where r_i and r_{i-1} is the position vectors at time t + Δt and t, respectively. Here $n = n_x, n_y, n_z)$ is a standard mormal random vector with zero means ($\mu_x = \mu_y = \mu_z = 0$) and unit variences ($\sigma_x = \sigma_y = \sigma_z = 1$) whereas $\sigma = \sigma_x = \sigma_y = \sigma_z = \sqrt{2D\Delta t}$ is the magnitude of the average value of the Brownian displacement for the case u = o.

The subscript i refers to the next point of time, namely, the current time plus Δt.

For a nonstationary system, the same particle would have been carried an additional distance of u_{i-1} Δt along the fluid stream. Hence, if p is the position vector of the particle in a nonstationary system,

$$r_i = r_i + v_i \Delta t$$
$$\simeq r_{i-1} + u_{i-1} + (r_i - r_{i-1}) \qquad (4.3.12)$$

where $(r_i - r_{i-1}) \simeq \sigma n_{i-1}$. Next equation (4.3.12) is made dimensionless in terms of the following dimensionless variables :

$$P = P/(D_f/2) \tag{4.3.13}$$

$$U = u/U_\infty \tag{4.3.14}$$

$$\Delta\tau = \Delta t/(D_f/2U_\infty) \tag{4.3.15}$$

Thus, we have

$$P_i = P_{i-1} + U_{i-1}\,\Delta t + 2\sqrt{\frac{\Delta\tau}{Pe}}\;n_{i-1} \tag{4.3.16}$$

where $P = D_f U_\infty/D$ is the peclet number of the system.

In short, equation (4.3.16) can be used to simulate the sucessive movement of a fine particle in the vicinity of a single fiber of an air filter, provided U, ΔT, and Pe are specified. On the other hand, the velocity U of viscous flow across a random array of parallel fibers having packing density α is obtainable from equation (4.1.7)

To complete our model, a set of assumptions pertaining to the behavior of the system have been made :

1) Existence of dendrites on the fiber has little effect on the flow field around the fiber.

2) Spatial and time distribution of incoming particles are random microscopically.

3) The next particle will not enter Kuwabara's cell until the present one in it either deposits or passes through the cell.

The plausibility of the statement may be shown intuitively as follows. Let A be the area of the control surface, and c be the number concentration. For a time interval, Δt, the number of particles passing through the control surface, N, is

$$N = U_\infty A c \Delta t \qquad (4.3.17)$$

Since c is small value in the most aerosol systems, it is quite easy to select a sufficiently small Δt such that N is no more than one.

4) A particle is always retained once it comes within a distance of one particle radius r_p from a dendrite or the fiber surface. The exact position of deposition is the point where collision occurs. Here it should be pointed out that, although electrostatic forces are expected to have a dominant role in the formation of particle dendrites, chain-like structures can also be formed in the absence of electrostatic effects because no real particles are round and smooth. As a result, particle contacts are never single-point contacts, but rather j-point contacts, where $j \geqslant 3$. The adhesion forces at these j-point contacts "lock" the two particles rigidly. This phenomenon accounts for the rigidity of short chains of fine particles. These chains retain their shapes and orientations despite the distributed drag force acting on them. In any case electrostatic effects are not considered in the present model.

5) There is no re-entrainment or detachment of captured particles or dendrites from the fiber.

6) The inlet particle size distribution is governed by a log-normal distribution.