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Impaction and Sedimentation Deposition of Fibers in Airways

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Theoretical impaction and sedimentation deposition of fibers in a model airway have been obtained based upon Jeffery's theory of particle motion. The corresponding expressions for the equivalent diameter of fibers have also been derived. The results are compared with experimental data and other formulas available in the literature for glass fibers. It is shown that for the flow condition existing in the airways, the equivalent diameters of fibers for both impaction and sedimentation are very close to the values obtained when the fibers are oriented parallel to the flow.

Introduction

The deposition of fibrous particles in the lung has been an important subject of investigation for many years because of the frequent occurrence of lung diseases associated with prolonged exposure to fibers. The elongated shape of fibers not only promotes the interceptional deposition of these particles along the airways, but it also affects the deposition processes by mechanisms such as impaction, sedimentation and diffusion, due to the periodic motion of the fibers.

One of the simple effective approaches to dealing with the dynamic behavior of fibrous particles is the use of the equivalent diameter of such particles. If this value is substituted for particle size in an expression giving collection efficiency for spherical particles, the collection efficiency of fibrous particles can be obtained.

There have been considerable efforts in the past to determine the equivalent diameter of fibers for sedimentation. Through the use of a horizontal elutriator with a divergent cross section, Timbrell$^{(1)}$ obtained an empirical relationship for glass fibers between the equivalent diameter d_{es} and the geometrical diameter of the fiber d_f in the form

$$\frac{d_{es}}{d_f} = 66\left(\frac{\beta}{2+4\beta}\right)^{2.2} \tag{1}$$

where β is the aspect ratio. In Equation (1), the effect of mass density of the glass fiber (2.53 g/cm^3) has been taken into consideration.

A different mathematical expression for d_{es}, proposed by Stober,$^{(2)}$ was based upon theoretical considerations. It gives

$$\frac{d_{es}}{d_f} = \left(\frac{\rho}{\rho_o}\right)^{1/2} (k_1+k_2)\,(\ln\beta)^{1/2} \tag{2}$$

where ρ is the mass density of the fiber in g/cm^3, $\rho_o = 1$ g/cm^3, and k_1 and k_2 are constants. In principle, the values of k_1 and k_2 depend upon the initial orientation of the fiber, as well as the flow field and dimension of the measuring device. For glass fibers, the best fit to the experimental data gives $k_1 = 0.7$ and $k_2 = 0.91$.

The equivalent diameter of fibers for impaction does not necessarily follow the relationship obtained from sedimentation experiments. A recent study by Burke and Esmen$^{(3)}$ has demonstrated that the aspect ratio of fibers plays a much more important role in impactional deposition than was found in sedimentation. Using a cascade impactor, they obtained a relationship for impaction equivalent diameter for glass fibers in the form

$$\frac{d_{ei}}{d_f} = \left(\frac{\rho}{\rho}\right)^{1/2} (0.71+0.91\ln\beta)^{1/2}[1+0.013(\ln\beta)^3]. \tag{3}$$

The geometry and flow field that is encountered in the lung deposition problem is considerably different than that in an elutriator or a cascade impactor. It is not clear whether the expressions for the equivalent diameter given by Equations (1)-(3) can be used directly for calculating deposition in the lung. In this paper, theoretical studies are made to determine deposition efficiencies in a model airway for impaction and for sedimentation, and to compare the results with those predicted by Equations (1)-(3).

Motion of a Fiber in a Shear Flow

The motion of a fiber in an airway can be determined under simplified assumptions. If the fiber is considered to be a

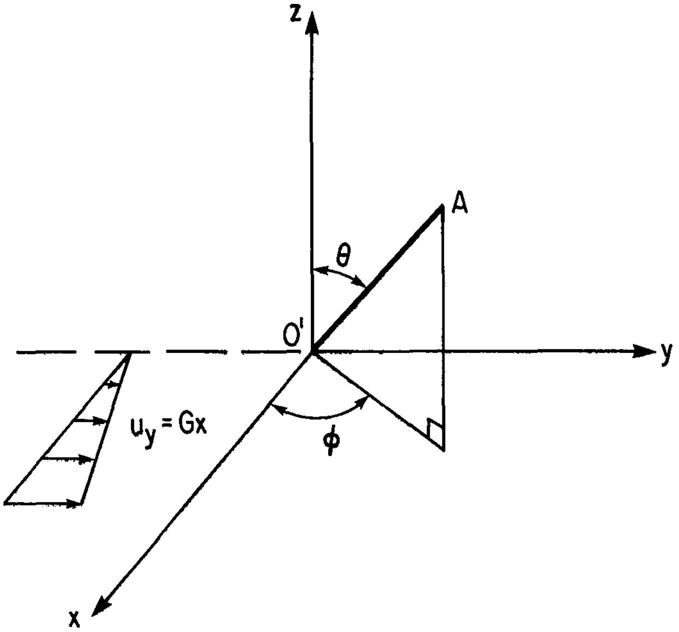

Figure 1—Coordinate System for the Motion of a Fiber.

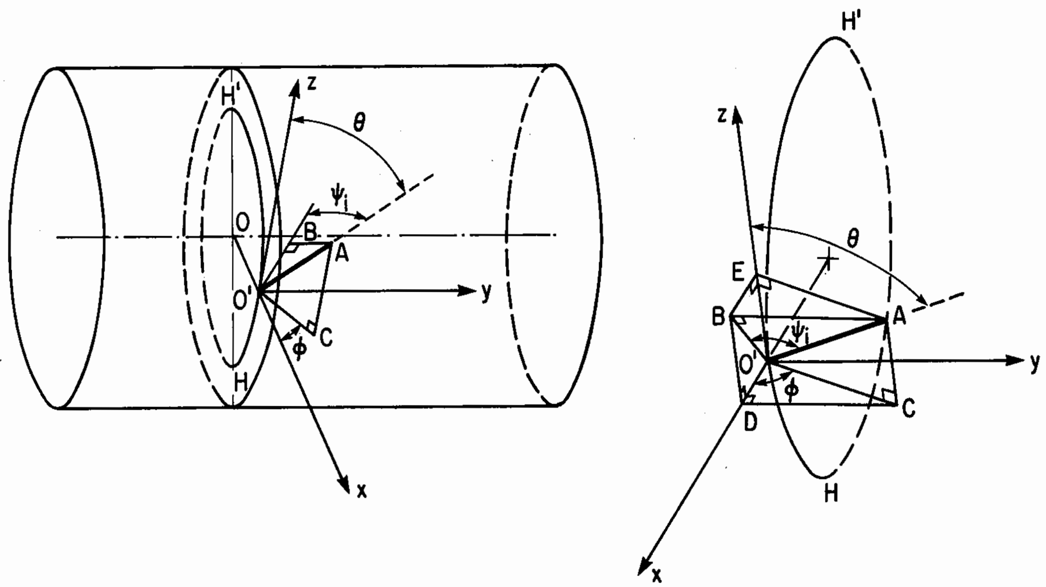

Figure 2—Geometrical Description of Impaction Angle ψ_i.

prolate ellipsoid and the flow in the airway is laminar with a constant average velocity gradient G, then the position and the orientation of the fiber can be determined at any instant of time by using Jeffery's theory.(4) For a parabolic flow, the average velocity gradient G was found to be (5)

$$G = \frac{8U}{3R} \tag{4}$$

where U is the average velocity and R is the radius of the airway.

Consider a prolate ellipsoid with its center at the origin of a Cartesian coordinate system xyz and its orientation specified by the angles θ and ϕ as shown in Figure 1. Assuming a fluid velocity of u_y=Gx in the y direction and zero velocity in the x and z directions, Jeffery(4) obtained the following equations to determine θ and ϕ:

$$\frac{d\theta}{dt} = \frac{G}{\ell_f^2+d_f^2}(\ell_f^2-d_f^2) \sin\theta \sin\phi \cos\theta \cos\phi \tag{5}$$

$$\frac{d\phi}{dt} = \frac{G}{\ell_f^2+d_f^2}(\ell_f^2 \cos^2\phi + d_f^2 \sin^2\phi) \tag{6}$$

where ℓ_f and d_f are, respectively, the length of the major and minor axes of the ellipsoid.

Assuming that initially the fiber has an orientation θ_o and ϕ_o, Equations (5) and (6) can be solved to yield

$$\tan\phi = \beta \tan\left(\frac{2\pi t}{T} + C_1\right) \tag{7}$$

$$\tan\phi = \frac{C_2}{(\beta^2\cos^2\phi+\sin^2\phi)} \tag{8}$$

where C_1 and C_2 are two constants related to θ_o and ϕ_o such that

$$C_1 = \tan^{-1}\left(\frac{\tan\phi_o}{\beta}\right) \tag{9}$$

$$C_2 = \tan\theta_o(\beta^2\cos^2\phi_o+\sin^2\phi_o)^{1/2} \tag{10}$$

and T is the orbit period defined by

$$T = \frac{2\pi(\ell_f^2+d_f^2)}{\ell_f d_f G}. \tag{11}$$

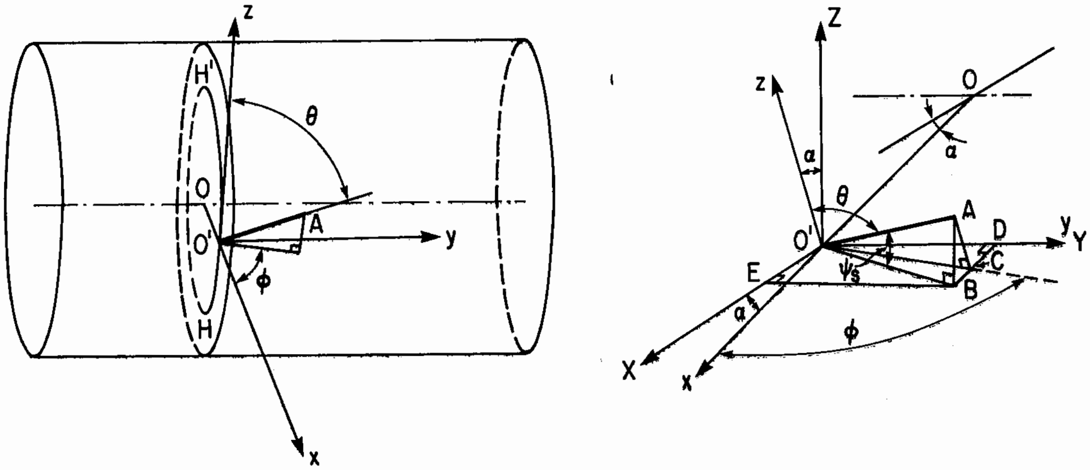

Figure 3—Geometrical Description of Sedimentation Angle ψ_s.

Equation (7) describes a periodic motion of the fiber about the z axis with period T. This motion has been confirmed experimentally by Goldsmith and Mason.(6)

In order to use the results of Equations (7) and (8) for determination of the collection efficiencies of fibers, we consider a horizontal tube of radius R and length L in which there is a parabolic flow with an average velocity gradient G in the radial direction. A fiber with an orientation θ_0 and ϕ_0 enters the airway at t=0. The orientation of the fiber will change with respect to the tube as it travels downstream due to the presence of the velocity gradient G. Two particular angles are of importance in connection with the calculation of collection efficiencies. One is the angle between the major axis of the fiber and the cross section of the tube, and the other is the angle between the major axis of the fiber and the horizontal plane. We shall call the first angle the impaction angle ψ_i, and the second angle the sedimentation angle ψ_s. These two angles can be calculated as follows: Let 0′ be the center of a fiber and $\overline{0'A}$ be its half length as shown in Figure 2. The projection of $\overline{0'A}$ on the xy plane is $\overline{0'B}$. Therefore, angle ψ_i is equal to

$$\psi_i = \cos^{-1}\left(\frac{\overline{0'B}}{\overline{0'A}}\right) \qquad (12)$$

From Figure 2, we have

$$\overline{0'B} = (\overline{0'D}^2 + \overline{0'E}^2)^{1/2} \qquad (13)$$

where $\overline{0'D}$ and $\overline{0'E}$ are the components of the fiber in the z and x directions respectively. In terms of θ and ϕ, we may write

$$\overline{0'D} = \overline{0'C}\cos\phi = \frac{\ell_f}{2}\sin\theta\cos\phi \qquad (14)$$

and

$$\overline{0'E} = \overline{0'A}\cos\theta = \frac{\ell_f}{2}\cos\theta; \qquad (15)$$

hence,

$$\overline{0'B} = \left(\frac{\ell_f^2}{4}\sin^2\theta\cos^2\phi + \frac{\ell_f^2}{4}\cos^2\theta\right)^{1/2} = \frac{\ell_f}{2}(1-\sin^2\theta\sin^2\phi)^{1/2}. \qquad (16)$$

Substituting Equation (16) into Equation (12) yields

$$\psi_i = \cos^{-1}[(1-\sin^2\theta\sin^2\phi)^{1/2}]. \qquad (17)$$

The sedimentation angle ψ_s is shown in Figure 3. Let $\overline{0'B}$ be the projection of $\overline{0'A}$ in the horizontal plane. Then

$$\psi_s = \cos^{-1}\left(\frac{\overline{0'B}}{\overline{0'A}}\right) \qquad (18)$$

In the xyz coordinate system, the components of $\overline{0'B}$ along the x,y and z direction are given by

$$x_b = \frac{\ell_f}{2}\sin\theta\cos\phi \qquad (19a)$$

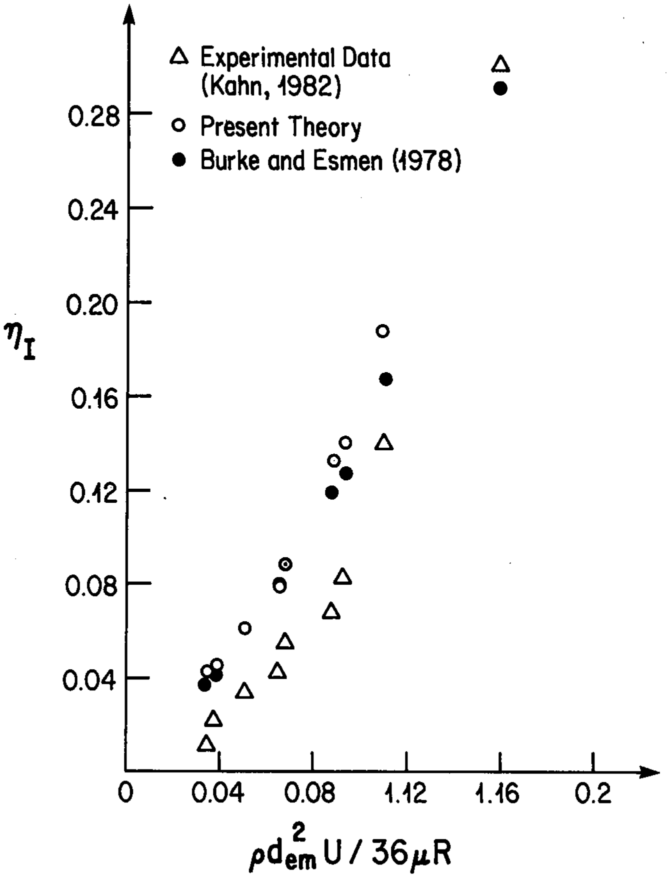

Figure 4—Comparison between Theoretical and Experimental Impaction Deposition of Glass Fibers at the Carina of Excised Calf Lungs. Particle Size: 10.9x50μm.

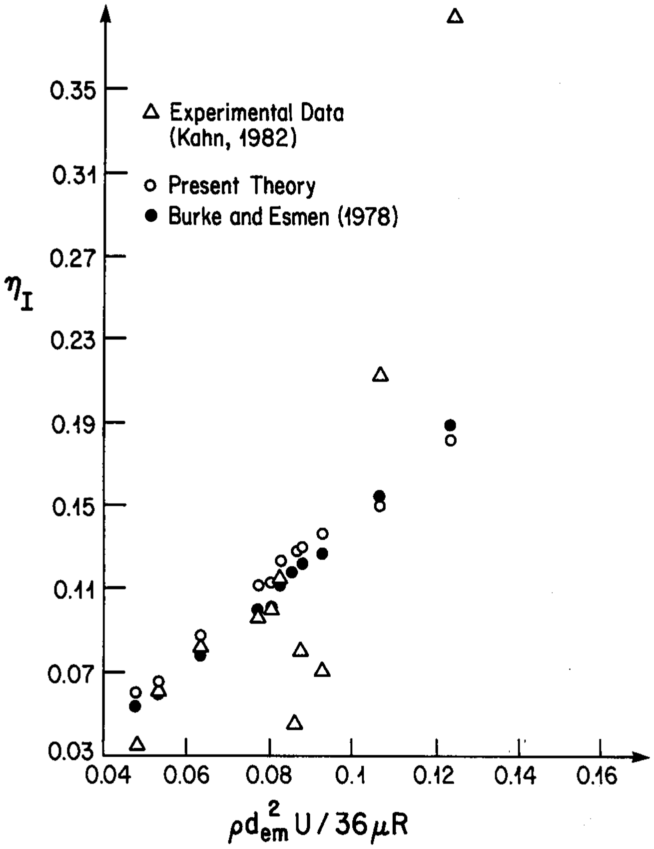

Figure 5—Comparison between Theoretical and Experimental Impaction Deposition of Glass Fibers at the Carina of Excised Calf Lungs. Particle Size: 9.1x50μm.

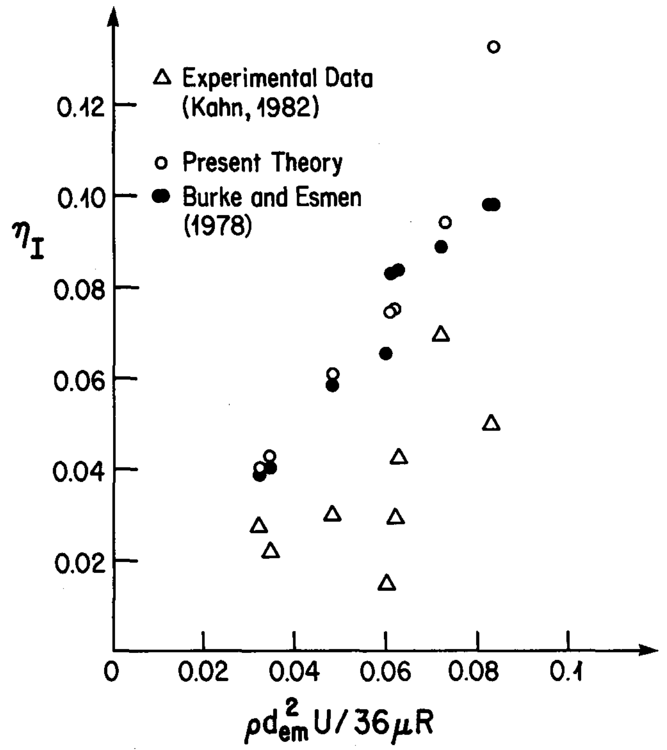

Figure 6—Comparison between Theoretical and Experimental Impaction Deposition of Glass Fibers at the Carina of Excised Calf Lungs. Particle Size: 6.4x48μm.

$$y_b = \frac{\ell_f}{2} \sin\theta \sin\phi \tag{19b}$$

$$z_b = \frac{\ell_f}{2} \cos\theta. \tag{19c}$$

Let XYZ be another coordinate system with the Y axis along the airway axis and the Z axis in the vertical direction. It is then easily seen from Figure 3 that the XYZ coordinate system has an angle of rotation α with respect to the xyz coordinate system about the y axis. In the new coordinate system, $\overline{0'B}$ has the components

$$X_b = x_b \cos\alpha + y_b \sin\alpha \tag{20a}$$

$$Y_b = y_b \tag{20b}$$

$$Z_b = z_b \cos\alpha - x_b \sin\alpha\ . \tag{20c}$$

Then the projected length of the fiber $\overline{0'B}$ can be written as

$$\overline{0'B} = (X_b^2 + Y_b^2)^{1/2}. \tag{21}$$

Using Equations (19)-(21), we obtained from Equation (18)

$$\psi_s = \cos^{-1}\{[\sin\theta\cos\phi\cos\alpha + \cos\theta\sin\alpha)^2 + (\sin\theta\sin\phi)^2]^{1/2}\}. \tag{22}$$

When the fiber is oriented at angles ψ_i and ψ_s, the drag force per unit velocity on the fiber in the direction of the flow f_i and that in vertical direction f_s will equal, respectively,

$$f_i = 3\pi\mu d_{em} C_i \tag{23}$$

$$f_s = 3\pi\mu d_{em} C_s \tag{24}$$

where $d_{em} = d_f\beta^{1/3}$ is the mass equivalent diameter of the fiber and C_i and C_s are given by

$$C_i = \frac{2\beta^{2/3}}{3}\left(\frac{\sin^2\psi_i}{\ell n\,(2\beta)-0.5} + \frac{2\cos^2\psi_i}{\ell n\,(2\beta)+0.5}\right) \tag{25}$$

$$C_s = \frac{2\beta^{2/3}}{3}\left(\frac{\sin^2\psi_s}{\ell n\,(2\beta)-0.5} + \frac{2\cos^2\psi_s}{\ell n\,(2\beta)+0.5}\right) \tag{26}$$

In Equations (23) and (24), we have neglected the Cunningham correction drag force because we consider only large particles.

Impaction Deposition

Impaction deposition occurs when the flow changes direction at an airway bifurcation and the suspended particles in the air, due to their inertia, are not able to follow the new direction. As a result, the particles will hit the walls and will be captured. Using a bend model, Chan and Yu$^{(6)}$ have obtained the impaction efficiency at a bifurcation for spherical particles at small Stokes numbers in the following simple form

$$\eta_I = 0.768.\ St.\gamma \tag{27}$$

where η_I is the impaction efficiency, γ=L/8R is the bend angle, and St is the Stokes number defined by

$$St = \frac{\text{kinetic energy}}{\text{drag force x distance}} = \frac{\rho d_p^2 U}{36\mu R} \tag{28}$$

in which d_p is the diameter of the spherical particle; U is the average air velocity; μ is the air viscosity; R and L are the radius and length of the parent airway. In the lungs, since St is normally much less than one, Equation (27) has been found to predict deposition quite accurately.

To apply Equation (27) to fibrous particles, the Stokes number given by Equation (28) must be modified to account for the new kinetic energy and drag force on these particles. Consider an ensemble of fibers entering the airway with random orientation. Then from Equations (23), (25), and (28), the average Stokes number of the fiber system, neglecting the rotational kinetic energy, can be determined as

$$St_f = \frac{\rho d_{em}^2 U}{36\mu R\overline{C_i}} + \frac{\rho_f^2\beta^{2/3} U}{36\mu R\overline{C_i}} \tag{29}$$

where $\overline{C_i}$ is the ensemble average of C_i evaluated at $t=t_R=L/U$. Thus,

$$\overline{C_i} = \frac{1}{2\pi}\int_0^{\pi/2}\int_0^{2\pi} (C_i)_{t=t_R} \sin\theta_0 d\phi_0 d\theta_0. \tag{30}$$

If we define an equivalent diameter for impaction d_{ei} such that

$$St_f = \frac{\rho_0 d_{ei}^2 U}{36\mu R} \tag{31}$$

then from Equations (29) and (31), we obtain

$$\frac{d_{ei}}{d_f} = \left(\frac{\rho}{\rho_0\overline{C_i}}\right)^{1/2}\beta^{1/3}. \tag{32}$$

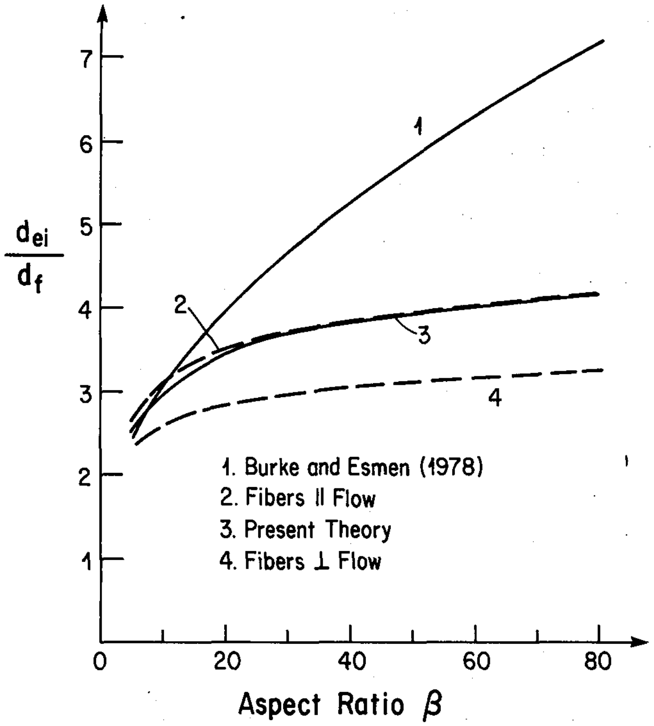

Figure 7—Equivalent Diameter of Glass Fibers for Impaction as a Function of Aspect Ratio.

For the limiting case for which fibers move in the airway with their axes along the direction of flow, $\psi_i = 90°$, Equation (32) reduces

$$\frac{d_{ei}}{d_f} = \frac{3}{2}\left[\frac{\rho}{\rho_0}\left(\ell n(2\beta)-\frac{1}{2}\right)\right]^{1/2} \qquad \textbf{(33)}$$

For fibers which move with their axes perpendicular to the flow $\psi_i = 0$, we have

$$\frac{d_{ei}}{d_f} = \frac{3}{4}\left[\frac{2\rho}{\rho_0}\left(\ell n(2\beta)+\frac{1}{2}\right)\right]^{1/2} \qquad \textbf{(34)}$$

Equations (33) and (34) were found previously by Harris.(5)

Figures 4 to 6 show the calculated impaction efficiency for glass fibers of three different sizes for which experimental data are available. These experiments were carried out by Kahn(8) at the carina of excised calf lungs. Kahn's reported values for the geometry and flow rate indicate that the flow is laminar and these values were used to obtain the theoretical results. For all cases, theory and experiment show reasonably good agreement, although the theoretical results are slightly higher. The discrepancy could be caused by the change in particle orientation due to the presence of secondary flow in the trachea. Also shown in Figures 4 to 6 are predicted depositions from Equation (3). For small values of β, it is seen that our theoretical results and Equation (3) agree with each other.

In Figure 7, a comparison is made on d_{ei} for glass fibers at various values of β. Our theoretical results were calculated at a third generation airway in Weibel's lung using Equation (32). The flow rate used in the calculation was 250 cm^3/sec, corresponding to the normal breathing condition. It is seen that the value of d_{ei} given by Burke and Esmen is much higher than Equation (32) except for very small values of β. It is also seen from Figure 7 that d_{ei} obtained from Equation (32) is very close to the value for the limiting case ψ_i=90° given by Equation (33), whereas the value for ψ_i=0 given by Equation (34) is much lower. Calculations for the large airways of other generations show similar results. Thus, for the evaluation of impaction deposition at a bifurcation, it is reasonable to assume that the fiber has an orientation parallel to the flow, according to the present theory.

Sedimentation Deposition

Airborne particles can also be deposited in the airways by gravitational settling. For spherical particles with a parabolic flow in a horizontal tube, the deposition efficiency has been obtained by Pich.(9) His result is

$$\eta s = \frac{2}{\pi}\left(2\epsilon(1-\epsilon^{2/3})^{1/2}-\epsilon^{1/3}(1-\epsilon^{2/3})^{1/2} + \sin^{-1}\epsilon^{1/3}\right) \qquad \textbf{(35)}$$

where

$$\epsilon = \frac{3Lu_g}{8UR} \qquad \textbf{(36)}$$

in which μg is the settling velocity of the particle, obtained by considering the balance between the particle weight and the drag force. It has the form

$$u_g = \frac{\rho d_p^2 g}{18\mu}. \qquad \textbf{(37)}$$

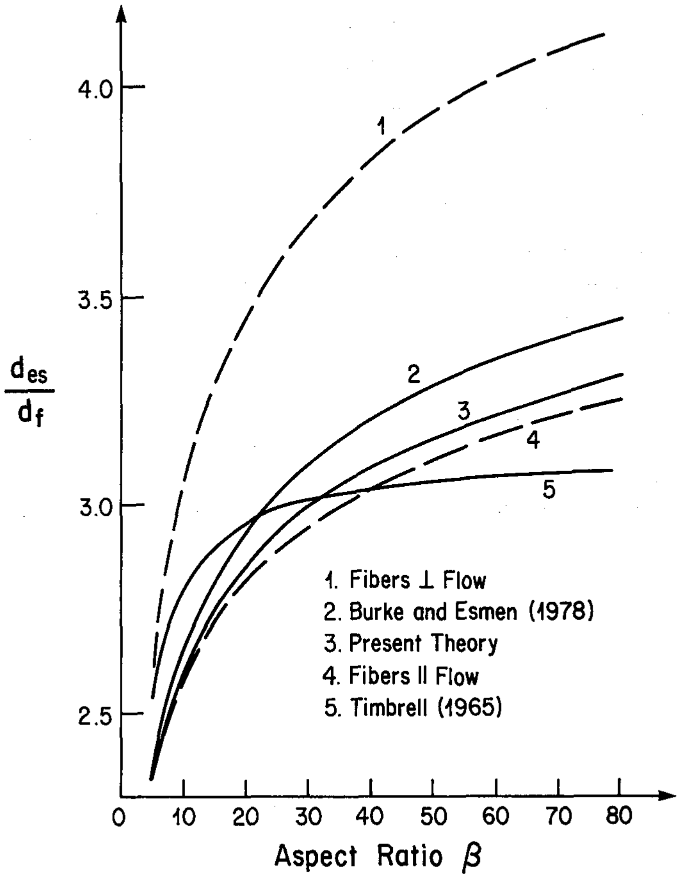

Figure 8—Equivalent Diameter of Glass Fibers for Sedimentation as a Function of Aspect Ratio.

To obtain an expression for deposition efficiency by sedimentation for fibrous particles, modifications to Equation (35) again need to be made so as to consider the drag force or settling velocity of these particles. Following the same approach used for impaction, consider an ensemble of fibrous particles which enter a horizontal tube with a random orientation. Over the time period of $t_R = L/U$, we may obtain an average settling velocity from Equation (24) for the ensemble of particles as follows

$$u_{gf} = \frac{\rho g d_{em}^2}{18\mu \overline{C_s}} = \frac{\rho g d_f^2 \beta^{2/3}}{18\mu \overline{C_s}} \tag{38}$$

where $\overline{C_s}$ is the ensemble and time average of C_s given by the expression

$$\overline{C_s} = \frac{1}{2\pi t_R} \int_{t=0}^{t_R} \int_{a=0}^{\pi/2} \int_{\theta_0=0}^{\pi/2} \int_{\phi_0=0}^{2\pi} C_s \sin\theta_0 d\phi_0 d\theta_0 d\alpha dt. \tag{39}$$

We define an equivalent diameter for sedimentation d_{es} such that

$$u_{gf} = \frac{\rho_0 g d_{es}^2}{18\mu}. \tag{40}$$

Then, from Equations (38) and (40), we find

$$\frac{d_{es}}{d_f} = \left(\frac{\rho}{\rho_0 \overline{C_s}}\right)^{1/2} \beta^{1/3} \tag{41}$$

For the limiting case for which fibers settle with their axes normal to the direction of fall,

$$\frac{d_{es}}{d_f} = \frac{3}{4} \left[\frac{2\rho}{\rho_0} \left(\ell n(2\beta) + \frac{1}{2} \right) \right]^{1/2} \tag{42}$$

and for fibers with their axes parallel to the direction of fall,

$$\frac{d_{es}}{d_f} = \frac{3}{2} \left[\frac{\rho}{\rho_0} \left(\ell n(2\beta) - \frac{1}{2} \right) \right]^{1/2} \tag{43}$$

Figure 8 shows a comparison of various d_{es} for glass fibers given by Equations (1), (2), (41), (42) and (43). The value of $\overline{C_s}$ in Equation (41) was calculated for a 19th generation airway of Weibel's lung at a total flow rate of 250 cm^3/sec. It is seen that the values of d_{es} given by Equations (1), (2), and (41) are all reasonably close to each other and they do not differ significantly from the value for the case of fibers parallel to the flow given by Equation (42). The diameter given by Equation (43) is much higher. In the calculation of deposition efficiency by sedimentation, we may therefore assume that fibers in an airway are parallel to the flow at all times.

Conclusions

Based upon Jeffery's theory of particle motion, we have derived expressions for the equivalent diameter of fibers for impaction and sedimentation in model airways. The application of the results to impaction deposition shows good agreement with experimental data for particles with small aspect ratio. For large aspect ratio, no experimental data are available and it is found that the equivalent diameter for impaction given by Burke and Esmen is significantly larger than our results.

For the calculation of sedimentation deposition in the lung, our theoretical equivalent diameter agrees reasonably well with the expressions proposed in the past. They are all close to the value for which fibers are oriented parallel to the flow.

Acknowledgment

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