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Dynamic Shape Factor of Nonspherical Aerosol Particles in the Diffusion Regime

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Diffusional losses of monodisperse polysterene spheres and doublets from laminar aerosol flows and stagnant aerosols in cylindrical tubes were measured. The losses of spheres were used to determine their diameter (range 69–120 nm) and the volume equivalent diameter of their doublets. The losses of the doublets were used to determine their dynamic shape factor which for randomly oriented doublets was established to be 1.127 ± 0.085 for Knudsen numbers between 1.1 and 2.0.

INTRODUCTION

Several definitions of a dynamic shape factor have been used in the aerosol literature: Megaw and Wells (1971), Maltoni et al. (1973), van de Vate et al. (1980), Kasper (1982), and Zeller (1985). The most widely used definition is that of Fuchs (1964) which, in the diffusion controlled thermodynamic particle size range, is given by

$$\kappa = \frac{F(v)}{F_{ve}(v)} = \frac{D_{ve}}{D}, \tag{1}$$

where $F(v)$ is the fluid drag force acting on an irregularly shaped aerosol particle moving through a viscous fluid with velocity v, and $F_{ve}(v)$ is the drag force acting on a sphere having the same volume and velocity as the nonspherical particle. D is the diffusion coefficient of the nonspherical particle and D_{ve} that of its volume equivalent sphere.

For nonspherical particles that are large enough to consider their surrounding fluid a viscous continuum, the drag force depends on their shape and orientation. This is usually accounted for by the dynamic shape factor κ_0, which depends on particle orientation. For diffusable nonspherical particles the drag force further depends on fluid slip which, for aggregates of uniform spheres, is expressed by the empirical relation:

$$\kappa = \kappa_0 + f Kn, \tag{2}$$

where Kn is the Knudsen number of the spheres and f is a constant. Another approach has been used by introducing the slip equivalent sphere of a nonspherical particle with diameter d_s (Dahneke, 1973) and, for aggregates of uniform spheres of diameter d, an adjusted sphere factor ψ

$$\psi = d_s/d \tag{3}$$

was introduced by Allen and Raabe (1985). ψ is a measure of the shape dependence of the slip factor for the aggregates. This approach yields

$$\kappa = \kappa_0 \frac{C(d_{ve})}{C(\psi d)} \tag{4}$$

where C is the slip correction factor and d_{ve} the diameter of the volume equivalent sphere

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of an aggregate of uniform spheres (see Appendix).

It was the purpose of the work described in this paper to determine the dynamic shape factor for randomly oriented doublets and to estimate their adjusted sphere factor. In a previous study by Heyder and Scheuch (1985), the dynamic shape factor of doublets was evaluated by measuring diffusional losses of these particles from laminar aerosol flows through a diffusion battery consisting of a bundle of cylindrical tubes. It remained, however, uncertain whether or not these doublets were randomly oriented. Therefore, in this paper diffusional losses of doublets in long cylindrical tubes from stagnant aerosols were also studied. In this case the doublets are randomly oriented so that their dynamic shape factor for random orientation could be evaluated. In addition a comparison of the shape factor obtained from studies with laminar aerosol flows and stagnant aerosols allows an estimation of the orientation of doublets in laminar flow fields.

MATERIALS AND METHODS

General Methods

Diffusion losses of particles or deposition DE from a stagnant aerosol initially uniformly distributed in a long cylinder are described by Buchwald (1911).

$$DE = 1-4 \sum_{\nu=1}^{\infty} \beta_\nu^{-2} \exp\left[-\beta_\nu^2 \mu\right], \tag{5}$$

where

$$\mu = \frac{Dt}{R^2} \tag{6}$$

is a diffusion parameter relating the radius R of the cylinder to the distance $\sqrt{Dt}$ over which aerosol particles with a diffusion coefficient D are transported by diffusion in time t. β_ν is defined as the νth zero of the zero-order Bessel function.

These losses can be estimated by measuring the declining particle number concentration c in the tube

$$DE = 1 - c/c_0, \tag{7}$$

where c_0 is the initial particle number concentration at time zero.

To calculate diffusional losses of particles from laminar aerosol flows through long cylinders several formulas have been proposed: Davies (1946, 1973), Gormley and Kennedy (1949), Thomas (1967), Tan and Hsu (1971), Ingham (1975), and Soderholm (1979). In Table 1 computed values of aerosol deposition, DE, from these formulas are compared. In this paper the empirical formula

$$\begin{aligned} DE = 1 &- 0.819\exp(-14.63(\mu/4)) \\ &- 0.0976\exp(-89.22(\mu/4)) \\ &- 0.0325\exp(-228(\mu/4)) \\ &- 0.0509\exp\left(-125.9(\mu/4)^{2/3}\right) \end{aligned} \tag{8}$$

proposed by Ingham (1975) was used. In this case the time t, available for diffusional particle transport is the mean residence time of the aerosols in the cylinder.

The losses of aerosol particles in the tube can be estimated by measuring the particle number concentration of an aerosol entering the cylinder c_0, and leaving the cylinder c.

In Figure 1 deposition values computed from Eqs. (5) and (8) are plotted as a function of the diffusion parameter μ. It can be seen that for the same μ value and, therefore, the same mean residence time of an aerosol in a cylinder, particle losses from a stagnant aerosol are higher than those from a laminar aerosol flow.

By measuring diffusional losses of spheres, their diffusion coefficients can be calculated by means of Eqs. (5) and (8). And, hence, their diameters, d, can be determined with

$$D = \frac{C(d)}{3\pi\eta d}, \tag{9}$$

where η is the viscosity of the air.

These diameters can be used to calculate the volume equivalent diameters, d_{ve} and diffusion coefficients, D_{ve}, for doublets consisting of two uniform spheres.

TABLE 1. Predicted Diffusional Losses of Spherical Aerosol Particles from Laminar Aerosol Flows through Cylindrical Tubes

μ	Davies (1946)	Gormley and Kennedy (1949)		Thomas (1967)	Tan & Hsu (1971)	Ingham (1975)	Soderholm (1979)	
0.0002	0.9344	(0.9477)	0.9915	0.9945	0.9906	0.9906	(0.9628)	0.9915
0.0004	0.9331	(0.9463)	0.9866	0.9894	0.9862	0.9851	(0.9293)	0.9866
0.0006	0.9319	(0.9449)	0.9825	0.9849	0.9823	0.9806	(0.9594)	0.9825
0.0008	0.9307	(0.9435)	0.9789	0.9807	0.9788	0.9766	(0.9577)	0.9789
0.001	0.9295	(0.9422)	0.9756	0.9768	0.9755	0.9730	(0.9560)	0.9756
0.002	0.9235	(0.9354)	0.9617	0.9610	0.9617	0.9584	(0.9478)	0.9617
0.004	0.9117	(0.9223)	0.9403	0.9391	0.9403	0.9367	(0.9323)	0.9403
0.006	0.9004	(0.9097)	0.9227	0.9220	0.9227	0.9195	(0.9178)	0.9227
0.008	0.8895	(0.8977)	0.9073	0.9070	0.9073	0.9045	(0.9042)	0.9073
0.01	0.8789	(0.8861)	0.8934	0.8932	0.8934	0.8911	(0.8913)	0.8934
0.02	0.8303	(0.8341)	0.8360	0.8359	0.8362	0.8354	(0.8359)	0.8361
0.04	0.7498	0.7509	(0.7505)	0.7508	0.7511	0.7511	0.7511	(0.7506)
0.06	0.6840	0.6844	(0.6832)	0.6842	0.6843	0.6843	0.6844	(0.6833)
0.08	0.6279	0.6281	(0.6261)	0.6279	0.6280	0.6280	0.6280	(0.6261)
0.1	0.5787	0.5787	(0.5758)	0.5787	0.5787	0.5788	0.5788	(0.5759)
0.2	0.3952	0.3953	(0.3838)	0.3953	0.3952	0.3952	0.3953	(0.3839)
0.4	0.1896	0.1897	(0.1402)	0.1897	0.1897	0.1896	0.1897	(0.1404)
0.6	0.0912	0.0913	—	0.0913	0.0912	0.0912	0.0913	—
0.8	0.0439	0.0439	—	0.0439	0.0439	0.0439	0.0439	—
1.0	0.0211	0.0211	—	0.0211	0.0211	0.0211	0.0211	—

Gormley and Kennedy as well as Soderholm proposed two equations. The values in brackets indicate the range of the diffusion parameter μ in which the equations are not valid.

By measuring the diffusional losses of doublets, their diffusion coefficients can be determined by means of Eqs. (5) and (8). Finally, the dynamic shape factors, κ, of the doublets can be calculated by means of Eq. (1) and the adjusted sphere factor by means of Eqs. (4) or (A6) with κ_0 evaluated by a regression analysis with Eq. (2).

Aerosols

Aerosols with monodisperse fractions of spheres (singlets) and agglomerates of spheres (doublets,...) were produced by nebulization of commercially available polystyrene latices with a nebulizer described by Gebhart et al. (1980). Charge equilibrium of the particles was obtained by exposing the aerosols to a bipolar ion gas.

Methods to Study Diffusional Losses

A high resolution laser aerosol size spectrometer (Heyder et al., 1972) was used to measure the particle number concentration of singlets and doublets. To study the diffusional losses of the aerosol particles from laminar flows through cylindrical tubes a diffusion battery previously described by Heyder and Scheuch (1985) was used. A bundle of 27 parallel brass tubes with 2 mm inner diameter and a length of 98 cm was placed in an outer brass tube of 22 mm diameter. The interstitial areas were sealed, to ensure that the aerosols could only flow through the 27 tubes of the battery. An aerosol mixer was connected at the inlet of the outer tube in order to obtain uniform particle number concentration across the face of the battery. To measure number concentrations of singlets and doublets small fractions of aerosols entering and leaving the battery were alternatively sampled by the laser spectrometer through two identical sampling lines. The residence time of the aerosol in the battery was varied by varying the aerosol flow rate between 0.5 and 5

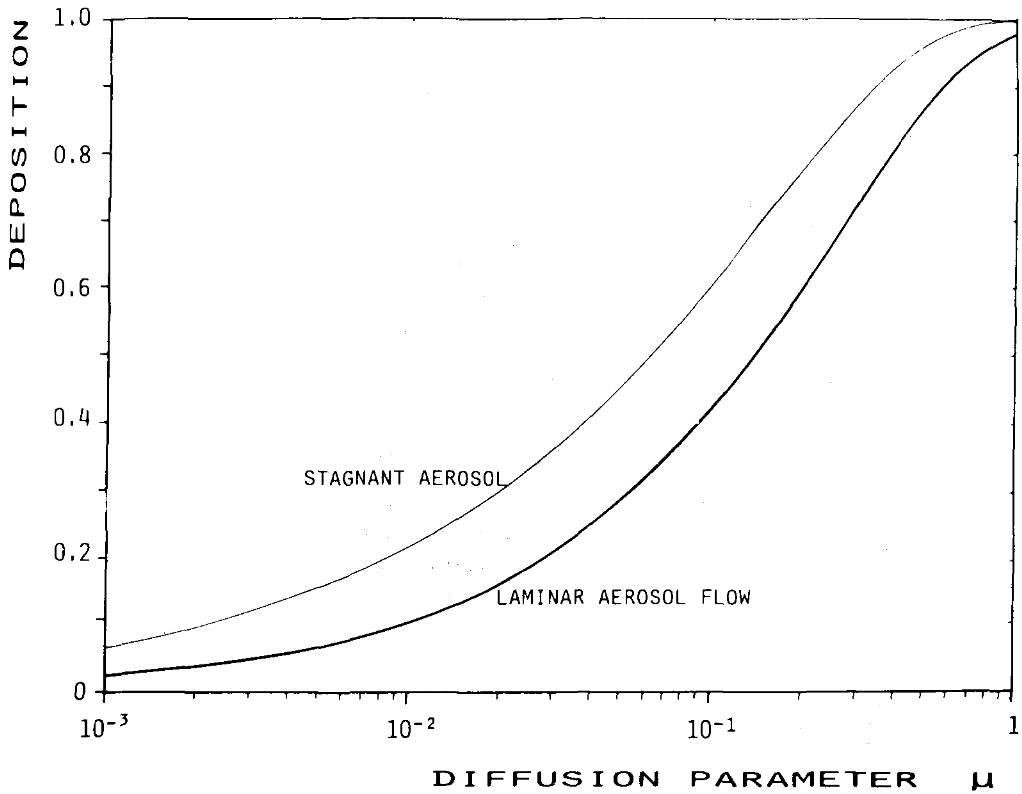
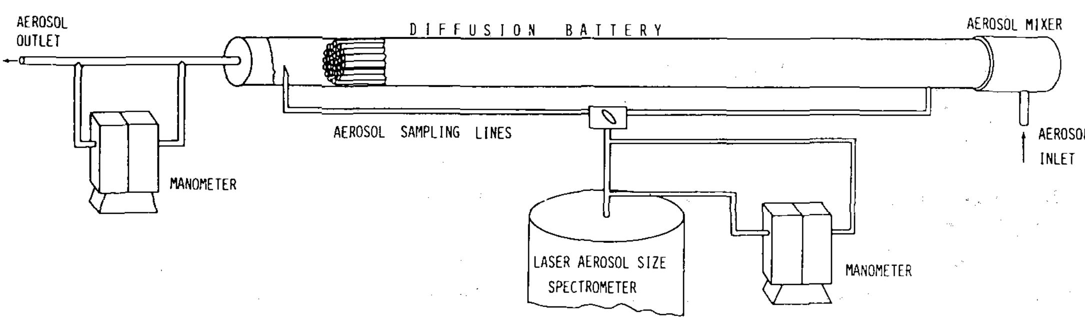


FIGURE 1. Predicted diffusional deposition of spherical aerosol particles in a cylindrical tube as a function of the diffusion parameter μ.

$cm^3\ s^{-1}$ through the battery. This flow rate and that through the battery and the laser spectrometer were evaluated from pressure drops measured with commercially available capacitance manometers (Setra model 239). The entire experimental setup is shown in Figure 2.

In Figure 3 a schematic drawing of the experimental setup for studying diffusional particle losses from stagnant aerosols in a

FIGURE 2. Setup for studying diffusional particle losses from laminar aerosol flows through cylindrical tubes.



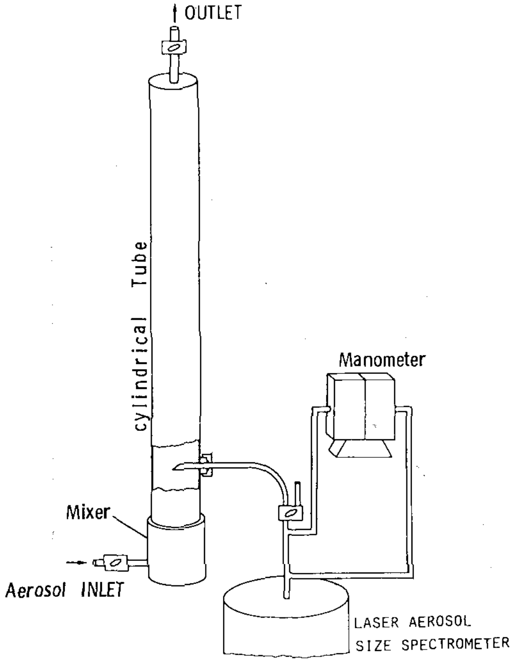


FIGURE 3. Setup for studying diffusional particle losses from stagnant aerosols in a cylindrical tube.

cylindrical tube is shown. The brass tube had a volume of 415 cm^3 with an inner diameter of 14 mm and a length of 270 cm. Its vertical position excluded particle losses by sedimentation. The aerosols entered the tube through a mixer to ensure uniform spatial number concentrations. Fractions of the aerosols were sampled in regular intervals between 50 and 180 minutes from the center of the otherwise closed cylindrical tube by the laser spectrometer.

RESULTS AND DISCUSSION

Various polystyrene latices were used to generate aerosols. The modal diameters of the monodisperse fractions of spherical aerosol particles determined with the laser aerosol size spectrometer were 69, 84, 116, and 120 nm.

Experimentally determined deposition of these fractions in cylindrical tubes from laminar aerosol flows through the diffusion battery and from stagnant aerosols in a tube is shown in Figure 4 as a function of the diffusion parameter, μ. The diffusion parameter was calculated for each experiment by means of Eq. (6). Close agreement was found between predicted and measured deposition values except for those values determined for the stagnant aerosol at small values of diffusion parameter. This slight discrepancy is due to the nonuniform decrease in particle number concentration across the tube. The concentration decreases more rapidly close to the walls than in the center of the tube. Therefore, sampling the particles from the center overestimates the average particle number concentration in the tube and underestimates particle deposition and results, consequently, in an overestimation of the particle diameter. This phenomenon becomes less effective with increasing time available for diffusion and, therefore, vanishes for large values of the diffusion parameter.

Experimentally determined deposition in cylindrical tubes of the doublet fractions of the polystyrene aerosols is shown in Figure 5. The diffusion parameter was calculated for the experimental conditions by

$$\mu = D_{ve}t/R^2. \qquad (10)$$

A comparison with deposition predicted for spheres by Eqs. (5) and (8) shows that deposition of doublets is less than that predicted using their volume equivalent spheres (Figure 5) and consequently, the true diffusion coefficient must be smaller than that for the volume equivalent sphere of a doublet.

The dynamic shape factors, κ, calculated by means of equation (1) are listed in Table 2. Based on 108 measurements, $\kappa = 1.127 \pm 0.085$ was established as the mean value of the dynamic shape factor for Knudsen numbers between 1.1 and 2. Since doublets are randomly oriented in stagnant aerosol, the close agreement of the dynamic shape factors evaluated for laminar aerosol flows and stagnant aerosols indicates that the doublets

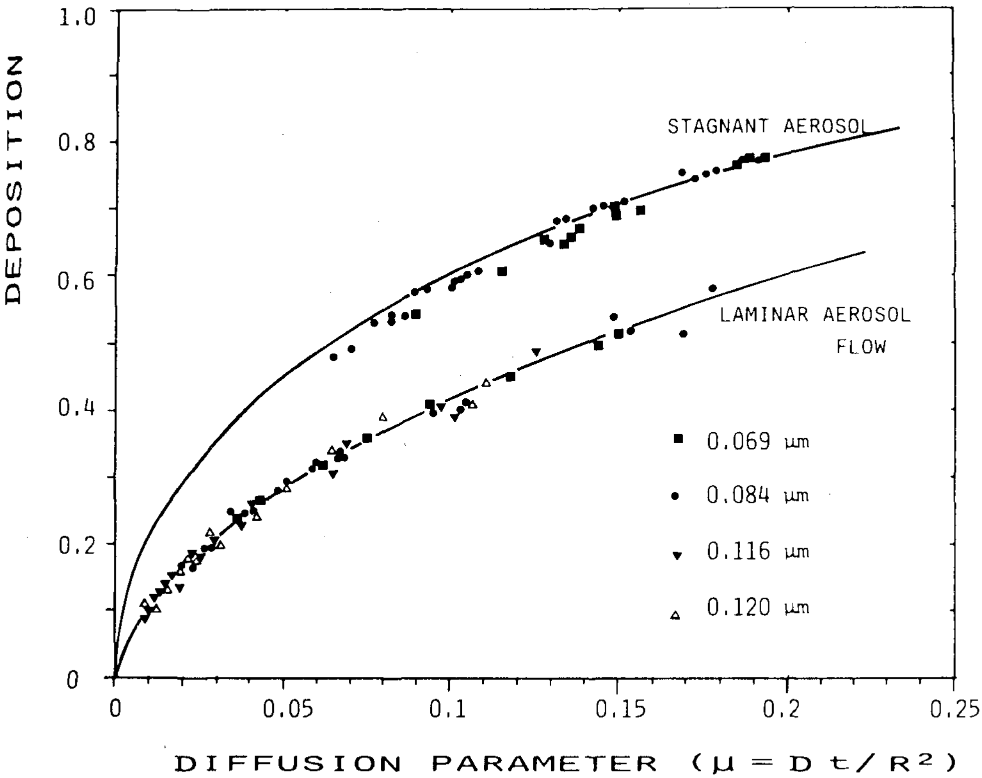


FIGURE 4. Measured and predicted deposition of spherical aerosol particles in cylindrical tubes as a function of the diffusion parameter μ.

FIGURE 5. Measured and predicted deposition of doublets in cylindrical tubes as a function of the diffusion parameter μ.

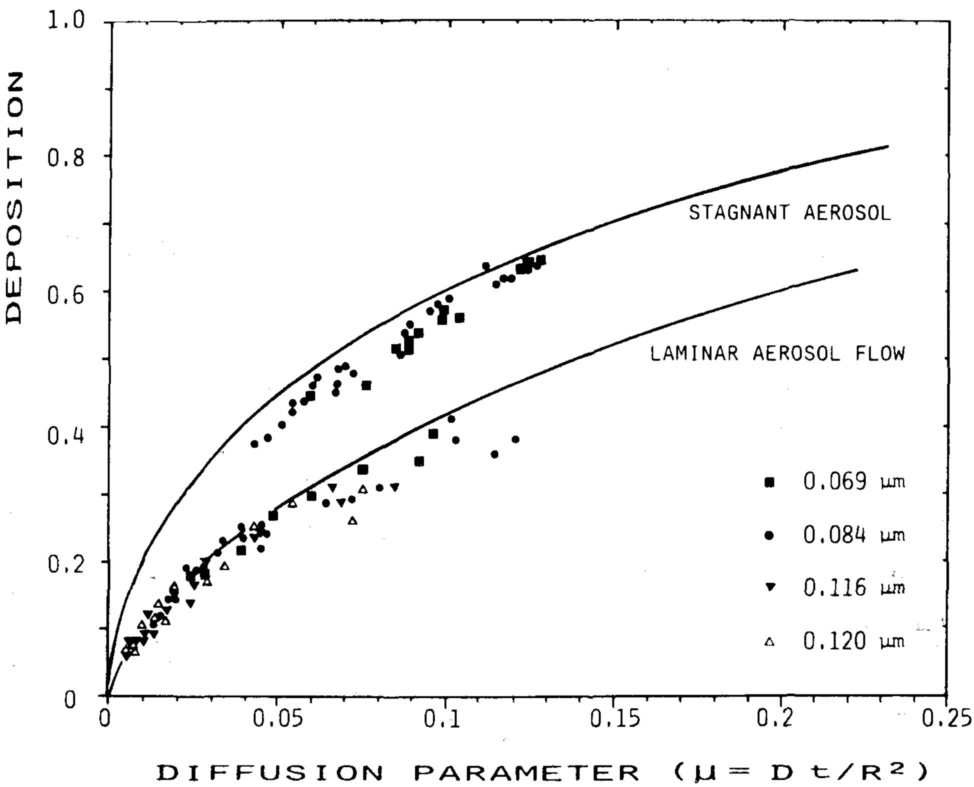


TABLE 2. Dynamic Shape Factors of Doublets Evaluated with the Diffusion Battery for Laminar Aerosol Flows and with the Diffusion Tube for Stagnant Aerosols

d (nm)	κ (DB) $\pm$SD	κ (DT) $\pm$SD
69	1.12 $\pm$0.09	1.14 $\pm$0.08
84	1.12 $\pm$0.10	1.14 $\pm$0.08
116	1.10 $\pm$0.09	—
120	1.14 $\pm$0.11	—

Abbreviations: DB, diffusion battery; DT, diffusion tube.

were also randomly oriented while carried through the diffusion battery. No flow dependency on the dynamic shape factor could be observed in the measured range of flow rate.

Using linear regression analysis to estimate κ_0 according to Eq. (2) yielded: $\kappa_0 = 1.101$. This value is in close agreement with values reported in the literature (Table 3).

If the mean value of $\kappa_0 = 1.100$ is used in Eq. (4) the adjusted sphere factor can be estimated to be $\psi = 1.32 \pm 0.11$ which is in close agreement with the value $\psi = 1.31 \pm 0.012$ reported by Cheng et al. (1987). However, a least square procedure to fit Eq. (4) yielded $\kappa_0 = 1.07$ and $\psi = 1.355$.

TABLE 3. Comparison of Dynamic Shape Factors for Randomly Oriented Doublets

Investigators	κ_0
Horvath (1974)	1.105
Hochrainer and Hänel (1975)	1.100
Horvath (1979)	1.099
Cheng et al. (1985)	1.098
Kasper et al. (1985)	1.100[a]
Cheng et al. (1987)	1.096
This work	1.101
Mean	1.100

[a]Calculated value.

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This work is dedicated to Professor Wolfgang Pohlit on the occasion of his 60th birthday.

APPENDIX

The drag force acting on the moving sphere with the slip equivalent diameter, d_s, of a doublet is given by Dahneke (1973) and Raabe (1976):

$$F(v) = -3\pi\eta\, d_{ve}\kappa_0 v / C(\psi d), \tag{A1}$$

where η is the viscosity of the air.

The drag force acting on the volume equivalent sphere of a doublet, moving with the same velocity as the slip equivalent sphere through the fluid, is given by

$$F_{ve} = -3\pi\eta\, d_{ve} v / C(d_{ve}). \tag{A2}$$

With the definition of the dynamic shape factor, equation (1), this yields

$$\kappa = \frac{F(v)}{F_{ve}(v)} = \kappa_0 \frac{C(d_{ve})}{C(\psi d)} \tag{A3}$$

Since the diameter of the volume equivalent sphere of a doublet is given by

$$d_{ve} = d2^{1/3}, \tag{A4}$$

and the slip correction factor by

$$C(d) = 1 + Kn(d) \times \left[f_A + f_Q \exp\left(-f_b\, Kn(d)^{-1}\right)\right], \tag{A5}$$

where $Kn(d)$ is the Knudsen number, the dynamic shape factor of the doublets is given by

$$\kappa = \kappa_0 \frac{1 + \frac{Kn(d)}{\sqrt[3]{2}}\left[f_A + f_Q \exp\left(-f_b \frac{\sqrt[3]{2}}{Kn(d)}\right)\right]}{1 + \frac{Kn(d)}{\psi}\left[f_A + f_Q \exp\left(-f_b \frac{\psi}{Kn(d)}\right)\right]} \tag{A6}$$

with the constants $f_A = 1.142$, $f_Q = 0.558$, and $f_b = 0.999$ given by Allen and Raabe (1985).

NOMENCLATURE

c	Particle number concentration
c_0	Initial particle number concentration
$C(d)$	Slip correction factor of a sphere with diameter d
d	Diameter of a sphere
d_s	Diameter of the slip equivalent sphere of a nonspherical particle
d_{ve}	Diameter of the volume equivalent sphere of a nonspherical particle
D	Diffusion coefficient of a nonspherical particle
D_{ve}	Diffusion coefficient of the volume equivalent sphere of a nonspherical particle
DE	Deposition of aerosol particles $= 1 - c/c_0$
f	Constant in the equation of the dynamic shape factor
f_A, f_b, f_Q	Constants in the equation of the slip correction factor
$F(v)$	Drag force acting on the nonspherical particle moving with velocity v through a viscous fluid
$F_{ve}(v)$	Drag force acting on the volume equivalent sphere of a nonspherical particle moving with velocity v through a viscous fluid
Kn	Knudsen number $= 2\lambda/d$
R	Radius of a cylindrical tube
t	Time
v	Velocity of an aerosol particle
β_ν	νth zero of the Bessel function of zero order
μ	Diffusion parameter $= Dt/R^2$
η	Viscosity of air
λ	Mean free path of air molecules
κ	Dynamic shape factor of a nonspherical particle
κ_0	Dynamic shape factor of a large nonspherical particle with vanishing Knudsen number
ψ	Adjusted sphere factor of a nonspherical particle

REFERENCES

Allen, M. D., and Raabe, O. G. (1985). *Aerosol Sci. Technol.* 4:269–286.

Buchwald, E. (1921). *Ann. Phys.* 66:1–24.

Cheng, Y. S., Allen, M. D., Gallegos, D. P. (1985). *Annual Report of Inhalation Toxicology Research Institut.* LMF 114, UC 48, pp. 12–16.

Cheng, Y. S., Allen, M. D., Gallegos, D. P., Yeh, H.-C., and Peterson, K. (1987). *Aerosol Sci. Technol.* (in press).

Dahneke, B. (1973). *J. Aerosol Sci.* 4:163–170.

Davies, C. N. (1946). *Proc. R. Soc. B.* 133:282–299.

Davies, C. N. (1973). *J. Aerosol Sci.* 4:317–328.

Fuchs, N. A. (1964). *The Mechanics of Aerosols.* Pergamon Press, London.

Gebhart, J., Heyder, J., Roth, C., Stahlhofen, W. (1980). *Staub-Reinhal. Luft.* 40:1–8.

Gormley, P. G., and Kennedy, M. (1949). *Proc. R. Ir. Acad. A.* 52:163–169.

Heyder, J., Roth, C., Stahlhofen,W. (1972). *J. Aerosol Sci.* 2:341–352.

Heyder, J., and Scheuch, G. (1985). *Aerosol Sci. Technol.* 2:41–44.

Hochrainer, D., and Hänel, G. (1975). *J. Aerosol Sci.* 6:97–103.

Horvath, H. (1974). *Staub-Reinhal. Luft.* 34:251–286.

Horvath, H. (1979). *J. Aerosol Sci.* 10:309–315.

Ingham, D. B. (1975). *J. Aerosol Sci.* 6:125–132.

Kasper, G. (1982). *Aerosol Sci. Technol.* 1:187–199.

Kasper, G., Niida, T., and Yang, M. (1985). *J. Aerosol Sci.* 16:535–556.

Maltoni, G. G., Melandri, C., Prodi, V., Tarroni, G., De Zaiacomo, A., Bompane, G. F., and Formignani, M. (1973). *J. Aerosol Sci.* 4:447–455.

Megaw, W. J., and Wells, A. C. (1971). *J. Aerosol Sci.* 2:161–164.

Raabe, O. G. (1976). *J. Air Pollut. Contr. Assoc.* 26:856–860.

Soderholm, S. C. (1979). *J. Aerosol Sci.* 10:163–175.

Tan, C. W., and Hsu, C.-J. (1971). *J. Aerosol Sci.* 2:117–124.

Thomas, J. W. (1967). *Assessment of Airborne Radioactivity.* International Atomic Energy Agency, Wien, pp. 701–712.

van de Vate, J. F., van Leeuwen, W. F., Plomp, A., and Smit, H. C. D. (1980). *J. Aerosol Sci.* 11:67–75.

Zeller, W. (1985). *Aerosol Sci. Technol.* 4:45–63.

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