

Chapter 4

Properties of Aerosol Particles

As a counterpart of Chap. 2, this chapter covers the basic properties and dynamics of aerosol particles. An aerosol is a mixture of solid particles and/or liquid droplets suspended in a gas. The gas phase can be air or other gases. In air pollution studies, we can also call it particulate matter. In this book, particulate matter (PM) is interchangeable with *aerosol* without examining their fine differences. The particles can be either solid aerosol particles or liquid droplets with little deformation or evaporation.

This chapter starts with classic particle dynamics followed by basic terms that are widely used in air emission engineering including aerodynamic diameter, equivalent diameters, Stokes number, Stokes law, adhesion and reentrainment of particles, and diffusion of particles in the air. At the end, particle size statistics and dynamics are introduced.

4.1 Particle Motion

It is important to analyze the behavior of particles in various force fields, which guides the design and operation of many particulate air pollution control devices. In most of the cases, the particle is subject of at least two forces acting along opposite directions, one is parallel and another opposite to the direction of motion. The latter is the resistance of the surrounding gas to the particle in motion.

4.1.1 Particle Reynolds Number

In particle dynamics, the particle Reynolds number follows similar definition except that characteristic length is the particle diameter, d_p , and that the velocity in Eq. (2.69) is replaced with the magnitude of the velocity (speed) of gas with respect to that of the particle, $|u - v|$.

$$Re_p = \frac{\rho_g d_p |u - v|}{\mu} \quad (4.1)$$

In this equation, the density is the gas density and subscript g is added in order to differentiate it with the density of solid particles. With a coordinate fixed on the moving particle, $|u - v|$ should always be a positive quantity.

The particle Reynolds number can be used to estimate the flow condition around the particles. There are four regime for particle dynamics as follows.

$$\left\{ \begin{array}{l} \text{Stokes regime : } Re_p < 1 \\ \text{Transient regime : } 1 < Re_p < 5 \\ \text{Turbulent regime : } 5 < Re_p < 1000 \\ \text{Newton's regime : } Re_p > 1000 \end{array} \right.$$

For Stokes regime, the flow around the particle is laminar and the frictional force is dominant over the inertia force. In the transient regime, the flow around the particle starts to develop turbulence, both inertial and frictional forces are important. In the turbulent regime, the flow around the particle is turbulent and drag decreases with Re_p . The flow around the particle becomes highly turbulent when $Re_p > 1000$ and the drag is considered constant, and the inertial force is dominant.

4.1.2 Stokes' Law

Stokes' law is derived from the Navier-Stokes equations, which are nearly insolvable due to the nonlinear partial differential equations. Stokes solved these equations with the following assumptions:

- (1) The inertial forces are negligible compared with the viscous forces.
- (2) There are no walls or other particles nearby. Because of the small size of airborne particles, the fraction of the particles near a wall is negligible.
- (3) The particle is a rigid sphere. This means that there is a limitation of Stokes law for liquid droplets or soft particles.
- (4) The fluid is incompressible. When the fluid is a gas, say air, the assumption does not imply that air is incompressible, but that it does not compress near the surface of the particle. This is equivalent to assuming that the relative velocity between the gas and the particle is much less than the speed of sound, and it is valid for airborne particles.
- (5) There is no slipping between the fluid and particles i.e., the fluid velocity at the particle's surface is zero. When the relative velocity is not zero, a correction is needed.
- (6) The motion of the particle is constant.

With the first assumption, the drag force on the moving particle can now be described by

$$F_D = 3\pi\mu d_p |u - v| \quad (4.2)$$

where u is the velocity of air and v is that of the particle.

In Stokes regime, the resistance experienced by a moving particle in a gas is described by the above equation. In practice, this equation is not perfect. When particle $Re_p = 1.0$, the error is 12 %. The error can be reduced to 5 % at a $Re_p = 0.3$.

The same drag force can also be calculated using Eq. (4.3),

$$F_D = C_D \left(\frac{1}{2} \rho u_\infty^2 \right) A \quad (4.3)$$

which was derived from Newton's law. Substituting the cross-section area (or rigorously, the frontal area) $A = \pi d_p^2/4$ into Eq. (4.3) leads to

$$F_D = C_D \left[\frac{1}{2} \rho_g (u - v)^2 \right] \left(\frac{1}{4} \pi d_p^2 \right) \quad (4.4)$$

Comparing Eqs. (4.2) and (4.4), we can get the drag coefficient in the Stokes regime,

$$C_D = \frac{24\mu}{\rho_g d_p |u - v|} = \frac{24}{Re_p} \quad (4.5)$$

This is the equation for the dashed straight-line portion at the up-left corner of Fig. 2.4. Note that when we first introduced Fig. 2.4 and Eq. (4.3), we assumed the solid phase (the sphere) is static and only air moves around the sphere. It would be easy to understand the concepts in this section by assuming air is quiescent and only the aerosol particle is moving. Indeed $|u - v|$ represents the relative motion of particle with respect to the air.

Overall, for spherical particles, the following relationships can be used to estimate drag coefficient.

$$C_D = \begin{cases} \frac{24}{Re_p} & Re_p \leq 1 \\ \frac{Re_p}{24} \left(1 + 0.15 Re_p^{0.687} \right) & 1 < Re_p \leq 1000 \\ 0.44 & Re_p > 1000 \end{cases} \quad (4.6)$$

4.1.3 Dynamic Shape Factor

In the Stokes' analysis above, the particles were assumed rigid spheres. But in reality, most of the particles are nonspherical. Being cubic, cylindrical, crystal, or

irregular. The shape of a particle affects its aerodynamic behavior by influencing its drag resistance. Therefore, a correction factor called the dynamic shape factor is necessary to correct the Stokes' law.

The dynamic shape factor, taking symbol S_f herein, is defined as the ratio of the actual drag force of the nonspherical particle to the drag force of a sphere having the same volume and velocity as the nonspherical particle. The dynamic shape factor S_f is then given by

$$S_f = \frac{F_D}{3\pi\mu|u - v|d_e} \quad (4.7)$$

which gives the drag on a nonspherical particle in Stokes regime as

$$F_D = 3\pi\mu|u - v|d_e S_f \quad (4.8)$$

where d_e is the equivalent volume diameter. It is the diameter of a sphere having the same volume as that of the nonspherical particle. Note that the shape factor is 1 for spherical particles. Most of the dynamic shape factors are greater than 1.0.

Dynamic shape factors are usually determined experimentally by measuring the settling velocity of geometric models in liquids. For irregular particles, settling velocities were measured indirectly using the elutriation devices [11]. An elutriation device separates particles based on their size, shape and density.

4.1.4 The Knudsen Number and Cunningham Correction Factor

An important assumption of the Stokes' law is that there is no slipping between the gas and the aerosol particles. It is also referred to as continuum flow. However, when the particle is getting smaller and smaller, approaching the mean free path of the gas molecules, this assumption of continuum transport is no longer valid. The dimensionless parameter that defines the nature of the aerosol is the Knudsen number (Kn), which is the ratio of gas mean free path to particle radius.

$$Kn = 2\lambda/d_p \quad (4.9)$$

When $Kn \ll 1$, the particle diameter is much greater than the mean free path of the gas, and the particle is in the continuum regime. This applies to the preceding analyses. On the other hand, when $Kn \gg 1$, the particle size is much smaller than the gas mean free path, and its behavior is like a gas molecule. The particle size between these two extremes defines the transition regime.

When the system is in noncontinuum regime, *Cunningham correction factor* (C_c), is used to correct the drag force.

$$F_D = \frac{3\pi\mu d_p |u - v|}{C_c} \quad (4.10)$$

The Cunningham correction factor for aerosol particles can be determined using the following equation recommended by Allen and Raabe [2]

$$C_c = 1 + Kn \left[1.142 + 0.558 \exp\left(-\frac{0.999}{Kn}\right) \right] \quad (4.11)$$

where λ is the gas mean free path that was introduced in Sect. 2.1.7.

There are several alternative equations for the Cunningham correction factor, differing only in the numerical factors. For example, Whitby et al. [28] (cited by Otto et al. [19]) used a formula as

$$C_c = 1 + 1.392Kn^{1.0783} \quad (4.12)$$

And Flagan and Seinfeld [9] give a more complex one as follows.

$$C_c = \begin{cases} 1 + 1.257Kn \approx 1.0 & Kn < 0.001 \\ 1 + Kn \left[1.257 + 0.40 \exp\left(-\frac{1.10}{Kn}\right) \right] & 0.001 < Kn < 100 \\ 1 + 1.657Kn & Kn > 100 \end{cases} \quad (4.13)$$

Equation (4.11) is used in this book unless otherwise specified. However, readers are suggested to choose the equations in accordance to their specific applications.

Both Knudsen number and Cunningham correction factor are dimensionless parameters. Since the theoretical value of C_c is always greater than 1, the drag force experienced with slipping effect considered is always smaller than the value calculated with nonslipping assumption.

For a small particle with irregular shape, both slip factor and shape factor are supposed to be considered for particle dynamics analysis. However, the task is so complicated that it outvalues the outcome. In air emission engineering, it is well acceptable to use the approximate factor calculated for the equivalent volume sphere for most irregular particles. The slip factor for randomly oriented fibers ($L/d < 20$) is 0–12 % greater than that for the equivalent volume sphere. Drag coefficients of different particle shapes are available in the literature (e.g., [12, 15]).

4.2 Rectilinear Particle Motion

Steady rectilinear particle motion is the simplest yet important type of particle motion in particle dynamics. It is the foundation for the mechanisms of particle separation from air stream, namely particulate air pollution control.

4.2.1 Particle Acceleration

Consider a particle with constant mass m that is released in quiescent air with an initial velocity of zero. Newton's second law of motion must hold at any instant $t > 0$.

$$\sum \vec{F} = m \frac{d\vec{v}(t)}{dt} \quad (4.14)$$

where $\vec{v}(t)$ is the particle velocity in the static air at time t , and the mass of the particle is considered as a constant when there is no evaporation or growth. In this case only two forces, a constant force of gravity and a drag force, act on the falling particles. The drag force depends on the particle velocity at any instant, ignoring additional acceleration of the surrounding air.

At any instant, the drag force is given by Stokes' law. Taking the positive direction downward, the above vector equation can be described using magnitudes

$$\sum F = mg - F_D \Rightarrow mg - \frac{3\pi\mu d_p v(t)}{C_c} = m \frac{dv(t)}{dt} \quad (4.15)$$

Note that in this equation we ignored the bouyant force. This is valid for typical conditions, when the aerosol particle density is much great than that of the air.

Rearranging the above equation and integration with the initial condition of $v = 0$ at $t = 0$ leads to

$$\left(\frac{3\pi\mu d_p}{mC_c} \right) \int_0^t dt = - \int_0^{v(t)} \frac{dv(t)}{\left[v(t) - \left(\frac{mgC_c}{3\pi\mu d_p} \right) \right]} \quad (4.16)$$

Integrating both sides and replacing m with $\frac{1}{6}\pi\rho d_p^3$ leads to

$$- \frac{t}{\left(\frac{\rho_p d_p^2 C_c}{18\mu} \right)} = \ln \left(\frac{\frac{\rho_p d_p^2 g C_c}{18\mu} - v(t)}{\frac{\rho_p d_p^2 g C_c}{18\mu}} \right) \quad (4.17)$$

If we define a constant

$$\tau = \frac{\rho_p d_p^2 C_c}{18\mu} \quad (4.18)$$

then we get the settling velocity of the particle, $v(t)$, at any time, t .

$$v(t) = g\tau \left[1 - \exp\left(-\frac{t}{\tau}\right) \right] \quad (4.19)$$

This equation shows that when t approaches infinity, the settling speed of the aerosol particle approaches a constant, which is the maximum speed that the particle can reach. In aerosol dynamics, this maximum speed is called terminal settling velocity, denoted by v_{TS} .

$$v_{TS} = v(t \rightarrow \infty) = g\tau = \frac{\rho_p d_p^2 g C_c}{18\mu} \quad (4.20)$$

Then Eq. (4.19) can be simplified as

$$\frac{v(t)}{v_{TS}} = 1 - \exp\left(-\frac{t}{\tau}\right) \quad (4.21)$$

This equation gives the speed $v(t)$ of a particle at any time t after it is released in still air in a gravitational field.

Figure 4.1 is produced using Eq. (4.21) above. It shows that the particle reaches 95 % of its terminal settling speed when $t = 3\tau$. However, from a practical point of view, within ± 5 % error the particle speed reaches v_{TS} when t is 3τ and after that it remains constant.

As shown in Table 4.1, particles having aerodynamic diameters less than or equal to $10 \mu\text{m}$, reach their terminal speed in less than 1 ms. Even a $100 \mu\text{m}$ particle reaches its terminal speed in less than 0.1 s. Therefore, it is acceptable to assume that a particle reaches its terminal speed instantly with a negligible error.

Since we can use 95 % of the maximum settling speed to represent its terminal settling speed, the terminal settling speed equation can be simplified as

$$v_{TS} = \frac{\rho_p d_p^2 g C_c}{18\mu} \quad (4.22)$$

Note that for a particle with irregular shape the shape factor has to be taken into consideration. The analysis is identical to that for spherical particles. The terminal settling velocity becomes

Fig. 4.1 Dimensionless speed versus dimensionless time for an accelerating particle

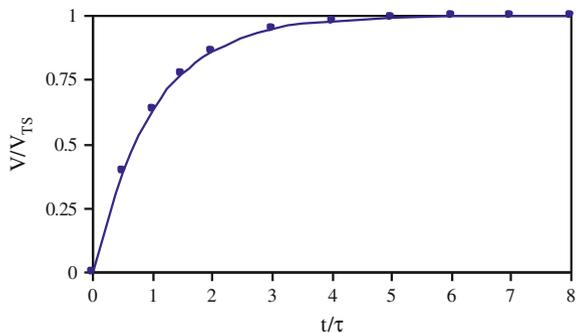


Table 4.1 Time required for particles of standard density to reach their terminal velocity at standard conditions

Particle diameter, d_p (μm)	95 % of its maximum settling speed, $0.95v_{\text{TS}}$ (m/s)	Time to reach $0.95v_{\text{TS}}$ $t = 3\tau$
0.01	0.0000001	0.0000000
0.1	0.0000008	0.0000003
1	0.0000331	0.0000107
10	0.0028980	0.0009329
100	0.2863625	0.0921817

$$v_{\text{TS}} = \frac{\rho_p d_p^2 g C_c}{18\mu\mathcal{S}_f} \quad (4.23)$$

Example 4.1: Terminal settling time

Consider a spherical glass particle with a diameter of $30\ \mu\text{m}$ and a density of $2,500\ \text{kg/m}^3$ is released from rest in still air. How long it will take to reach its terminal velocity?

Solution

From $d_p = 30\ \mu\text{m}$, $\rho_p = 2,500\ \text{kg/m}^3$, and $\mu = 1.81 \times 10^{-5}\ \text{Pa s}$, we can get

$$Kn = 2\lambda/d_p = 2 \times \frac{0.066\ \mu\text{m}}{30\ \mu\text{m}} = 0.0044$$

Since $0.001 < Kn < 100$, the Cunningham correction factor is calculated using

$$\begin{aligned} C_c &= 1 + Kn \left[1.142 + 0.558 \exp\left(-\frac{0.999}{Kn}\right) \right] \\ &= 1 + 0.0044 \left[1.142 + 0.558 \exp\left(-\frac{0.999}{Kn}\right) \right] = 1.055 \end{aligned}$$

The time it takes for the particle to reach its terminal speed is,

$$t = 3\tau = 3 \left(\frac{\rho_p d_p^2 C_c}{18\mu} \right) = 3 \left(\frac{2500 \times (30 \times 10^{-6})^2 \cdot 1.055}{18 \times 1.81 \times 10^{-5}} \right) = 0.0073\ \text{s}$$

Example 4.2: Sneezing droplet settling

Scientific research results indicated the total average size distribution of the droplets by coughing was $0.58\text{--}5.42\ \mu\text{m}$, and 82 % of droplet nuclei were centered in $0.74\text{--}2.12\ \mu\text{m}$. A spherical droplet with a diameter of $5\ \mu\text{m}$ and density of $1,000\ \text{kg/m}^3$ is discharged from the mouth horizontally in still air.

If the mouth is about 1.5 m above the floor, how long would it take for the 5- μm droplet to settle down to the floor.

Solution Given $d_p = 5 \mu\text{m}$, $\rho_p = 1,000 \text{ kg/m}^3$, and $\mu = 1.81 \times 10^{-5} \text{ Pa s}$, we can get,

$$Kn = 2\lambda/d_p = 2 \times \frac{0.066 \mu\text{m}}{5 \mu\text{m}} = 0.0264$$

$$C_c = 1 + Kn \left[1.142 + 0.558 \exp\left(-\frac{0.999}{Kn}\right) \right] = 1.033$$

$$t = 3\tau = 3 \left(\frac{\rho_p d_p^2 C_c}{18\mu} \right) = 3 \left(\frac{1000 \times (5 \times 10^{-6})^2 \times 1.0333}{18 \times 1.81 \times 10^{-5}} \right) = 0.00024 \text{ s}$$

$$v_{\text{TS}} = \frac{\rho_p d_p^2 g C_c}{18\mu} = \frac{1000 \times (5 \times 10^{-6})^2 \times 9.81 \times 1.033}{18 \times 1.81 \times 10^{-5}} = 0.000753 \text{ m/s}$$

$$\Delta t = \frac{H}{v_{\text{TS}}} = \frac{1.5 \text{ m}}{0.000753 \text{ m/s}} = 1992 \text{ s} = 33 \text{ min}$$

It could be much slower for a smaller particle.

4.2.2 Settling at High Reynolds Numbers

The particle motion is in Newton's regime for $Re > 1.0$ and the corresponding settling speed in a gravitational field can be determined by equating the drag force and the force of gravity, which gives

$$v_{\text{TS}} = \frac{4\rho_p d_p g}{3C_D \rho_g} \quad (4.24)$$

where the drag coefficient C_D was introduced before. However, it is not straightforward to find v_{TS} using this equation. Because C_D depends on the particle Reynolds number. It cannot be determined without knowing v_{TS} . One way to solve this problem is an iterative solution obtained by substituting an initial guess of v_{TS} into the above equation and by trying different values of v_{TS} until the solution converges with a desired accuracy.

4.2.3 Aerodynamic Diameter

Aerodynamic diameter (d_a) is an equivalent diameter that finds many applications in aerosol characterization and particulate emission control. It is defined as the diameter of a spherical particle with a standard density of $1,000 \text{ kg/m}^3$ that has the same settling velocity as the real particle, when both of them present in the same gravitational field.

Figure 4.2 illustrates the aerodynamic diameter of an irregular particle. Imagine two particles, one is spherical with a standard density (ρ_0) and a diameter (d_a) and another is nonspherical, are released in the same calm air. They have the same aerodynamic diameter if they fall with the same settling velocity. In another word, the aerodynamic diameter of the nonspherical particle is d_a .

For the same gravitational settling velocity, it can be written in terms of aerodynamic diameter and equivalent geometric diameter as

$$v_{\text{TS}} = \frac{\rho_p d_e^2 g C_c}{18\mu S_f} = \frac{\rho_0 d_a^2 g C_c}{18\mu} \quad (4.25)$$

where ρ_0 is the standard particle density, $1,000 \text{ kg/m}^3$, which is the same as water at normal condition.

The aerodynamic diameter of a particle is the key particle property for evaluating or comparing the performances of different types of particulate air cleaners, as to be introduced later in this book. Many particulate matter emission control devices, such as cyclones and filters, separate particles from the gas/air stream aerodynamically.

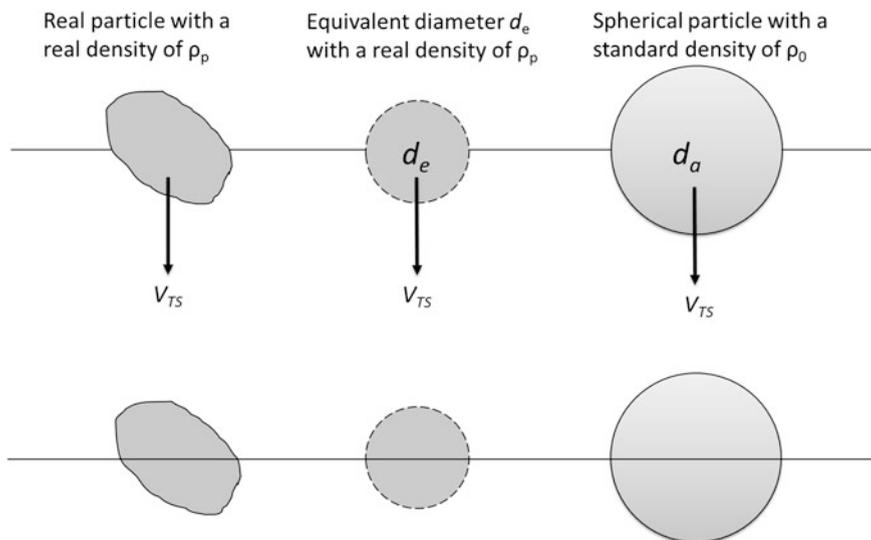


Fig. 4.2 An irregular particle and its equivalent volume diameter and aerodynamic diameter

Consequently, it is not necessary to know the physical size, shape or density of a particle if its aerodynamic diameter is determined.

From the above equation, one can get the formula for aerodynamic diameter,

$$d_a = d_e \left(\frac{\rho_p}{\rho_0 S_f} \right)^{1/2} \quad (4.26)$$

Example 4.3: Aerodynamic diameter

Estimate the aerodynamic diameter of a spherical steel particle with a geometric equivalent diameter $d_e = 10 \mu\text{m}$ and $\rho_p = 8,000 \text{ kg/m}^3$.

Solution

Since the particle is spherical, its shape factor, $S_f = 1$

$$d_a = d_e \left(\frac{\rho_p}{\rho_0 S_f} \right)^{1/2} = 10 \times 10^{-6} \left(\frac{8000}{1000 \times 1} \right)^{1/2} = 2.83 \times 10^{-5} \text{ m} = 28.3 \mu\text{m}$$

For a particle with this great density, its aerodynamic particle diameter is much greater than its geometric equivalent diameter.

4.2.4 Curvilinear Motion of Aerosol Particles

Curvilinear motion is a motion when a particle follows a curved path. A classic example of curvilinear motion is the projectile of a particle with a horizontal initial velocity in the still air. It is more complicated for a particle-air mixture that flows around an obstacle. Very small particles with negligible inertia tend to follow the gas while large and heavy particles tend to continue in a straight line due to the great inertia.

The inertia of a particle in curvilinear motion is characterized by the Stokes number (Stk), like the Reynolds number in fluid mechanics for the characterization of a fluid flow. The Stokes number is defined as the ratio of the stopping distance of a particle to a characteristic dimension of the obstacle.

$$Stk = \frac{\tau u_0}{d_c} = \frac{\rho_p d_p^2 C_c u_0}{18 \mu d_c} \quad (4.27)$$

where the characteristic dimension d_c in the above equation can be defined differently according to applications. And the definition of Stokes number may be application specific. u_0 is the undisturbed air speed. In standard air, a particle with $Stk \gg 1.0$ will continue in a straight line as the fluid turns around the obstacle. But for a particle with $Stk \ll 1$, it will follow the fluid streamlines closely.

Example 4.4: Stokes number

Estimate the Stokes number of a 1 μm spherical particle with a density of 8,000 kg/m^3 in an air flowing at 1 m/s normal to a cylinder of diameter 10 cm , assuming standard conditions.

Solution

Given $d_e = 1 \mu\text{m}$, $u_o = 1 \text{ m/s}$, $d_c = 10 \text{ cm}$, $\rho_p = 8000 \text{ kg/m}^3$, we get

$$Kn = 2\lambda/d_p = 2\lambda/d_e = 2 \times 0.066/1 = 0.132$$

$$C_c = 1 + Kn \left[1.142 + 0.558 \exp\left(-\frac{0.999}{Kn}\right) \right] = 1.166$$

$$Stk = \frac{\rho_p d_p^2 C_c u_o}{18\mu d_c} = \frac{8000 \times (1 \times 10^{-6})^2 \times 1.166 \times 1}{18 \times 1.81 \times 10^{-5} \times 0.1} = 2.86 \times 10^{-4}$$

Note that the geometric diameter is used in calculating the Knudsen number because Kn is a geometric ratio rather than an aerodynamic property.

The small Stokes number indicates that this particle follows the air under standard conditions and it is difficult to separate the particle from the air simply by inertia. However, it is feasible under other conditions, when the particle viscosity is reduced and the particle Cunningham correction factor is enhanced by great air mean free path. In-depth analysis will be introduced in Chap. 13.

4.2.5 Diffusion of Aerosol Particles

Diffusion of gas borne particles takes place when there is a gradient of particle concentration in the space. It results in a net transport of particles from a region of higher concentration to that of lower concentration. The transport flux of the gas borne particles is defined by Fick's first law of diffusion. In the absence of external forces, Fick's law is the same as that for gases,

$$J = -D_p \frac{dn}{dx} \quad (4.28)$$

where J = flux of particles, expressed in terms of the number of particles per unit area per unit time ($\#/s \cdot \text{m}^2$), D_p = diffusivity of the particles in the gas (m^2/s), and dn/dx = gradient in number concentration of particles ($1/\text{m}$).

The diffusion coefficient for an aerosol particle is given by the Stokes-Einstein equation [12].

$$D_p = \frac{kTC_c}{3\pi\mu d_p} \quad (4.29)$$

The particle diffusion coefficient has a unit of m^2/s . For large particles when $C_c = 1$, the particle diffusion coefficient is inversely proportional to the particle size. For smaller particles when the slip effect becomes significant, D_p approaches a value that is inversely proportional to d_p^2 , which is very similar to the diffusion coefficient for gas molecules. This is because the behavior of finer particles approaches that of gas molecules.

Example 4.5: Particle diffusion coefficients

Calculate the diffusion coefficients for 100 nm and 10 μm particles at standard conditions.

Solution

We know that $k = 1.3806 \times 10^{-23} \text{kg} \cdot \text{m}^2/(\text{s}^2 \text{K})$, $T = 288 \text{K}$; $\lambda = 66 \text{nm}$.

Case I For particles with $d_p = 100 \text{nm}$

$$Kn = 2\lambda/d_p = 2\lambda/d_e = 2 \times 66/100 = 1.32$$

$$C_c = 1 + Kn \left[1.257 + 0.40 \exp\left(-\frac{1.10}{Kn}\right) \right] \quad 0.001 < Kn < 100$$

$$C_c = 1 + 1.32 \left[1.257 + 0.40 \exp\left(-\frac{1.10}{1.32}\right) \right] \approx 2.66$$

$$\begin{aligned} \text{The particle diffusion coefficient } D_p &= \frac{kTC_c}{3\pi\mu d_p} \\ &= \frac{1.3806 \times 10^{-23} \times 288 \times 2.66}{3\pi \times 1.81 \times 10^{-5} \times 100 \times 10^{-9}} \\ &= 6.21 \times 10^{-10} \text{m}^2/\text{s} \end{aligned}$$

Case II For particles with $d_p = 10 \mu\text{m}$, repeat the calculation and we get

$$C_c = 1.0166$$

$$D_p = \frac{kTC_c}{3\pi\mu d_p} = \frac{1.3806 \times 10^{-23} \times 288 \times 1.0166}{3\pi \times 1.81 \times 10^{-5} \times 10 \times 10^{-6}} = 2.33 \times 10^{-17} \text{m}^2/\text{s}$$

4.2.6 Particle Deposition on Surface by Diffusion

As introduced above, most of the fine particles adhere when they impact on a surface. In this case, the particle concentration in the space where the surface is can be assumed to be zero and there is a concentration gradient established in the region near the surface. This results in a continuous diffusion of particles to the surface and a gradual decrease in particle concentration in the gas.

Consider a plane vertical surface that is immersed in a large space filled with gas and particles. It can be assumed that the gas velocity near the surface is zero. Then the rate at which particles are removed from the space, by deposition onto the surface can be determined following the analysis below. Let x be the horizontal distance from the surface. Then the particle concentration, $n(x, t)$, in the space at x at any time t , must satisfy Fick's second law of diffusion.

$$\frac{dn}{dt} = -D_p \frac{d^2n}{dx^2} \quad \left\{ \begin{array}{l} n(x, 0) = n_0 \quad \text{for } x > 0 \\ n(0, t) = 0 \quad \text{for } t > 0 \end{array} \right\} \quad (4.30)$$

It is assumed that the initial particle concentration in the entire space is n_0 . The boundary condition of $n(0, t) = 0$ is based on the assumption that all particles will adhere on the surface once they come into contact. The general solution of this equation is

$$n(x, t) = \frac{n_0}{\sqrt{\pi D_p t}} \int_0^x \exp\left(-\frac{z^2}{4D_p t}\right) dz \quad (4.31)$$

where z is the dummy variable for integration.

Then the concentration gradient at the surface, dn/dx at $x = 0$, is

$$\left. \frac{dn}{dx} \right|_{x=0} = \frac{d}{dx} \left[\frac{n_0}{\sqrt{\pi D_p t}} \int_0^x \exp\left(-\frac{z^2}{4D_p t}\right) dz \right] \Bigg|_{x=0} = \frac{n_0}{\sqrt{\pi D_p t}} \quad (4.32)$$

The rate of deposition of particles onto a unit area of surface at any time, t , is then described as

$$J = -D_p \left. \frac{dn}{dx} \right|_{x=0} = -n_0 \sqrt{\frac{D_p}{\pi t}} \quad (4.33)$$

Integrating over time in this equation from 0 to t , the cumulative number of particles, $N(t)$, deposited per unit area of surface is

$$N(t) = \int_0^t n_0 \sqrt{\frac{D_p}{\pi z}} dz = 2n_0 \sqrt{\frac{D_p t}{\pi}} \quad (4.34)$$

where $N(t)$ has a unit of ($\#/m^2$).

Again, z is the dummy variable for integration. In engineering practice, there is always limited space for containers, and therefore, this equation can only be used to set the upper limit of losses to the walls of the container.

The preceding analyses were based on the properties of a single particle without considering the particle size distribution. The same principles may be applied to a group of particles with a uniform size well dispersed in air, which is referred to as monodisperse aerosol.

4.3 Particle-Surface Interaction

The particle is subjected to adhesion force between the particle and the solid surface and pull-off force. When the adhesion force is greater than or equal to the pull-off force, the particle adhere to the surface, otherwise, the particle leaves the surface. The former is called attachment and the latter reentrainment. The adhesion force is primarily the van der Waals force between two rigid spheres [3] and the pull-off force can be quite different including, but are not limited to, drag, shear, and impaction from other aerosol particles.

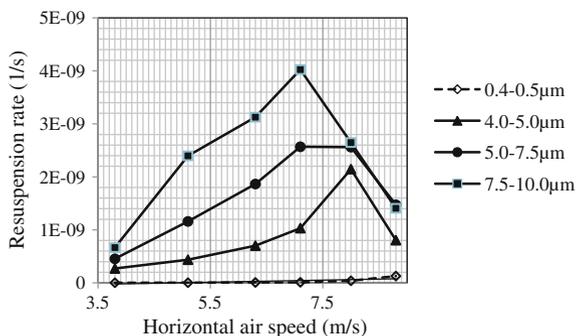
Unlike a gas molecule, most aerosol particles, especially the submicron sized ones, attach firmly to a surface they come in contact. When the particle comes in contact with another particle, both particles adhere to each other, and the process is referred to as coagulation. Various particle separation devices such as fiber filters are designed to separate particles from the gas stream by taking advantage of the adhesion. It is especially important for submicron particles because the adhesive forces on submicron particles exceed other common forces by orders of magnitude.

Closely related to adhesion of particles are the processes of resuspension and reentrainment. They are important for the buildup and removal of particles on surfaces. For example, for fugitive dust emissions caused by vehicles on paved and unpaved roads.

Wang et al. [27] investigated the resuspension of micron sized particles (0.4–10 μm) from a flat surface simulating a ventilation duct. The results in Fig. 4.3 show that the resuspension rate depends on the time, air speed, and the particle size. In-depth analyses suggest that more particles slide and roll off rather than being lifted into the air flow.

Not all airborne particles adhere to the surfaces in contact. It depends on the properties of both the particle and the surface, and the nature of the impact between the particle and the surface. A large solid particle impacting a hard surface at high

Fig. 4.3 Particle reentrainment versus bulk air velocity



velocity can rebound from the surface. When the speed of the particles is great enough, part of its kinetic energy is dissipated in the deformation process during the particle-surface impact, and part is converted elastically to kinetic energy of rebound. If the rebound energy exceeds the energy required to overcome the adhesive forces, the particle will bounce away from the surface rather than adhering to it.

Particle bounce has been studied for solid particle from impactor and fibrous filters. Overall, the bounce is likely to take place for the large particles of hard materials traveling at a great speed. In addition, the roughness of the surface plays an important role. Bouncing does not occur for droplets of liquid or easily deformed materials. The coating of surfaces with oil improves particle adhesion but reduces the bounce. On the other hand, when particles are small enough, they also may rebound because of the high thermal speed. This is called thermal rebound (see Chap. 14).

4.4 Particle Coagulation

Particle size distribution in the air is constantly changing over time, primarily because of coagulation. When particles collide on each other by certain mechanisms, they may attach to each other by the van de Waals force and form larger ones. This phenomenon is referred to as particle coagulation or agglomeration or coalescence. The mechanisms for particle coagulation may include, but are not limited to, Brownian motion, collision, electrostatics, gravity, and gas phase turbulence.

Many models have been developed for aerosol particle coagulation and they are available in the literature. Most of them are based on the classic Smoluchowski [23] equation (Cited by Geng et al. [10]), by ignoring evaporation and condensation.

$$\frac{\partial}{\partial t} f(v, t) = \frac{1}{2} \int_0^v K(u, v-u) f(u, t) f(v-u, t) du - f(v, t) \int_0^\infty K(u, v) f(u, t) du \quad (4.35)$$

where $K(u, v)$ specifies the collision rate between particles of volume u and v . f is the size distribution density function.

It is assumed in conventional aerosol analysis that particles attach to each other upon collision, therefore, the collision rate can also be considered as the coagulation rate.

Because of the dynamic change of the size distribution, the Smoluchowski [23] equation can only be solved numerically. However, analytical solutions can be obtained for simple cases with assumptions.

4.4.1 Monodisperse Aerosol Coagulation

The analysis is simplified if we only consider monodisperse coagulation, where the particle diameters are within a narrow range. Smoluchowski [23] developed a model for Brownian coagulation of monodisperse particles in the continuum regime. It is applicable to particles with sizes in a narrow range, say $1 < d_{pA}/d_{pB} < 1.25$. The corresponding Brownian monodisperse coagulation efficient for the continuum regime ($Kn \ll 1$) and free molecule regime ($Kn \gg 1$) are simplified as

$$K = \begin{cases} 8kT3\mu & \text{continuum regime, } Kn \ll 1 \\ 9.8\sqrt{kT\rho_p d_p} & \text{free molecule regime, } Kn \gg 1 \end{cases} \quad (4.36)$$

where k is Boltzmann's constant and μ is the dynamic viscosity of the carrier gas. Otto et al. [19] introduced an analytical model for the regime in between, but its form is complicated.

Integration of Smoluchowski equation using the initial condition of $N(t=0) = N_0$ leads to the solution for the total particle concentration as a function of time and the coagulation coefficient above.

$$N(t) = \frac{2N_0}{2 + KN_0 t} \quad (4.37)$$

where N_0 is the initial particle concentration ($\#/m^3$).

By defining the characteristic dimensionless time

$$\tau = \frac{2}{KN_0} \quad (4.38)$$

Equation (4.37) becomes,

$$N(t) = \frac{N_0}{1 + t/\tau} \quad (4.39)$$

Since $N = N_0/2$ when $t = \tau$, τ is also referred to as the half-value time, which is the time it takes for the particle number concentration to drop to half of its initial value.

Example 4.6: Half value time of monodisperse aerosol

Calculate the half-value time of spherical monodisperse aerosol with an initial concentration of 10^3 particles/cm³ and an initial particle diameter of $d_p = 1$ nm. Assume standard condition and only Brownian coagulation is considered.

Solution

The Knudsen number of 1 nm particle is

$$Kn(1\text{nm}) = 2 \times 0.066/0.001 = 132 > 100$$

It is within the free molecule region. Therefore,

$$K = 9.8 \sqrt{\frac{kT}{\rho_p d_p}} = 9.8 \sqrt{\frac{(1.38 \times 10^{-23}) \times 298}{1,000 \times (1 \times 10^{-9})}} = 6.28 \times 10^{-7}$$

Then the half-value time is

$$\tau = \frac{2}{KN_0} = \frac{2}{6.28 \times 10^{-7} \times 10^3 \left(\frac{1}{\text{cm}^3}\right) \times 10^6 \left(\frac{\text{cm}^3}{\text{m}^3}\right)} = 0.003 \text{ s}$$

As seen from the result, particles at 1 nm do not have a great life time. While this is practically inaccurate, it does qualitatively show that aerosol particle diameter is a dynamic parameter.

4.4.2 Polydisperse Coagulation

Coagulation coefficients for different mechanisms have been summarized by Geng et al. [10]. Brownian motion is the dominating mechanisms for the coagulation of very fine particle under normal atmospheric condition; for this reason, our analysis is focused on Brownian coagulation.

One of the widely used Brownian coagulation coefficients is the Fuchs (1964) equation for binary collision.

$$K(a, b) = \frac{4\pi(a+b)(D_A + D_B)}{\frac{a+b}{a+b+\delta_{AB}} + \frac{4(D_A+D_B)}{(a+b)\bar{c}_{AB}}} \quad (4.40)$$

where a and b are the radii of the particles of concerns, \bar{c}_{AB} is the average particle thermal velocity, δ_{AB} is the jump distance, and D_i is the diffusivity of the particle of size i ($=A$ or B). If we use particle diameters, d_{pA} and d_{pB} , instead of the radii, Eq. (4.40) becomes

$$K(d_{pA}, d_{pB}) = \frac{2\pi(d_{pA} + d_{pB})(D_A + D_B)}{\frac{d_{pA}+d_{pB}}{d_{pA}+d_{pB}+2\delta_{AB}} + \frac{8(D_A+D_B)}{(d_{pA}+d_{pB})\bar{c}_{AB}}} \quad (4.41)$$

The particle diffusion coefficient is calculated using

$$D_i = \frac{kTC_c}{3\pi\mu d_{pi}} \quad (4.42)$$

and the mean thermal velocity are calculated using

$$\bar{c}_{AB} = (\bar{c}_A^2 + \bar{c}_B^2)^{1/2} \quad (4.43)$$

where the mean thermal velocity of the particle can be calculated using the equation for gas molecules (Eq. 2.7) by replacing the mass of a molecule with the mass of the particle.

$$\bar{c}_i = \sqrt{\frac{8kT}{\pi m_i}} \quad (4.44)$$

Similar to Eq. (4.43), the jump distance, δ_{AB} , is determined as

$$\delta_{AB} = (\delta_A^2 + \delta_B^2)^{1/2} \quad (4.45)$$

where the individual jump distance is calculated with

$$\delta_i = \frac{(d_{pi} + l_i)^3 - (d_{pi}^2 + l_i^2)^{1.5}}{3d_{pi}l_i} - d_{pi} \quad (4.46)$$

$$l_i = \frac{8D_i}{\pi\bar{c}_i} \quad (4.47)$$

It is obviously a very tedious work to accurately predict the particle size change by polydisperse coagulation. Readers are referred to the literature for more complicated models for polydisperse coagulation.

4.5 Aerosol Particle Size Distribution

Although monodisperse particles are used in describing particles with a narrow size distribution in nanoparticle manufacturing, threat agents and bioaerosols, most engineers deal with polydisperse aerosol. Polydisperse aerosol is a group of particles with different sizes suspended in the air. In typical urban atmosphere, particle concentration can reach as high as 10^7 – $10^8/\text{cm}^3$; their diameters can range from a few nanometers to around $100\ \mu\text{m}$ [22].

A great amount of literature shows that the size distribution of most polydisperse aerosol particles is lognormal. To understand lognormal distribution, it is necessary to revisit what we learned about normal distribution. Normal distribution is also called Gaussian distribution. For a variate x with a mean of \bar{x} and standard deviation of σ , the normal probability fractional distribution function in the domain $-\infty < x < \infty$ is described as

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\left(\frac{x - \bar{x}}{\sigma\sqrt{2}}\right)^2\right] \quad (4.48)$$

where $f(x) \leq 1$. The corresponding cumulative distribution, which describes the probability of the variable below certain value, is

$$\Phi(u) = f(x < u) = \frac{1}{2} \left[1 + \operatorname{erf}\left(\frac{u - \bar{u}}{\sigma_u\sqrt{2}}\right) \right] \quad (4.49)$$

where the error function is used to characterize the measurement errors. It is described as

$$\operatorname{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y \exp(-z^2) dz \quad (4.50)$$

An error function $\operatorname{erf}(y)$ is symmetric about its origin. For a quantity that is log-normally distributed, its logarithm is governed by normal distribution by replacing x with $\log x$, \bar{x} with $\log \bar{x}$ and σ with $\log \sigma$.

$$f(\log x) = \frac{1}{\log \sigma \sqrt{2\pi}} \exp\left[-\left(\frac{\log x - \log \bar{x}}{\sqrt{2} \log \sigma}\right)^2\right] \quad (4.51)$$

For its specific applications to aerosol particles, the probability of the particle number fraction can be described as

$$f(\log d_p) = \frac{1}{\log \sigma \sqrt{2\pi}} \exp\left[-\left(\frac{\log d_p - \log \bar{d}_{pg}}{\sqrt{2} \log \sigma}\right)^2\right] \quad (4.52)$$

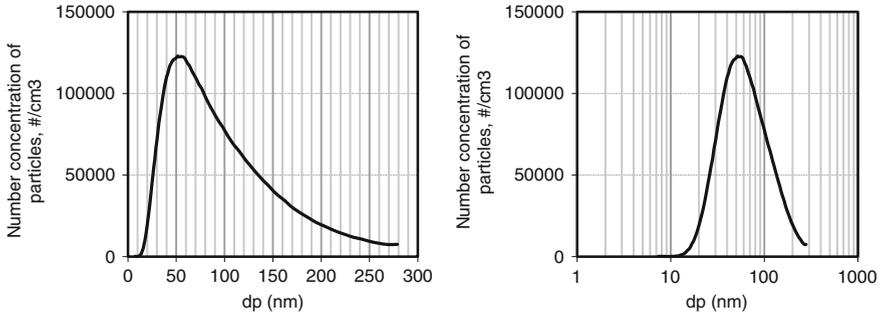


Fig. 4.4 Aerosol size distribution (*left* linear scale x-axis, *right* logarithm x-axis)

Since $f(\log d_p) = d_p \times f(d_p)$ [9], the equation can be transformed into

$$f(d_p) = \frac{1}{\sqrt{2\pi}d_p \log \sigma} \exp \left[- \left(\frac{\log d_p - \log \bar{d}_{pg}}{\sqrt{2} \log \sigma} \right)^2 \right] \quad (4.53)$$

Figure 4.4 shows how the curves look like when the particle number concentrations are presented in linear scale x-axis and logarithm scale x-axis.

The corresponding cumulative distribution is then similar to Eq. (4.49)

$$\emptyset(d_p) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\log d_p - \log \bar{d}_{pg}}{\sqrt{2} \log \sigma} \right) \right] \quad (4.54)$$

This equation can be used to explain the physical meanings of \bar{d}_{pg} and σ . When $d_p = \bar{d}_{pg}$, $\emptyset(d_p) = 0.5$ and it indicates that 50 % of the particles are less than \bar{d}_{pg} . Therefore, \bar{d}_{pg} is the *median* diameter of the particles. The role of σ can be better understood letting $d_p = \sigma \bar{d}_{pg}$, which gives $\emptyset(d_p) = 0.84$. This means that 84 % of the particles are smaller than $(\sigma \bar{d}_{pg})$. So σ is the geometric standard deviation. Similarly, we can get that 95 % of the particles are smaller than $(2\sigma \bar{d}_{pg})$ and 99.5 % are smaller than $(3\sigma \bar{d}_{pg})$.

In aerosol technology, we usually are also interested in the absolute number of particles besides the probability function in Eq. (4.54). Multiplying both sides of Eq. (4.54) with the total number of the particles gives us a practical equation as

$$F(d_p) = N\emptyset(d_p) = N \left[1 + \operatorname{erf} \left(\frac{\log d_p - \log \bar{d}_{pg}}{\sqrt{2} \log \sigma} \right) \right] \quad (4.55)$$

It describes the total number below particles of size d_p in a population. Equation (4.55) can also be extended to describing the surface and volume distributions, by replacing $n(d_p)$ with $\pi d_p^2 \cdot n(d_p)$ and $(\pi d_p^3 / 6) \cdot n(d_p)$ for surface and

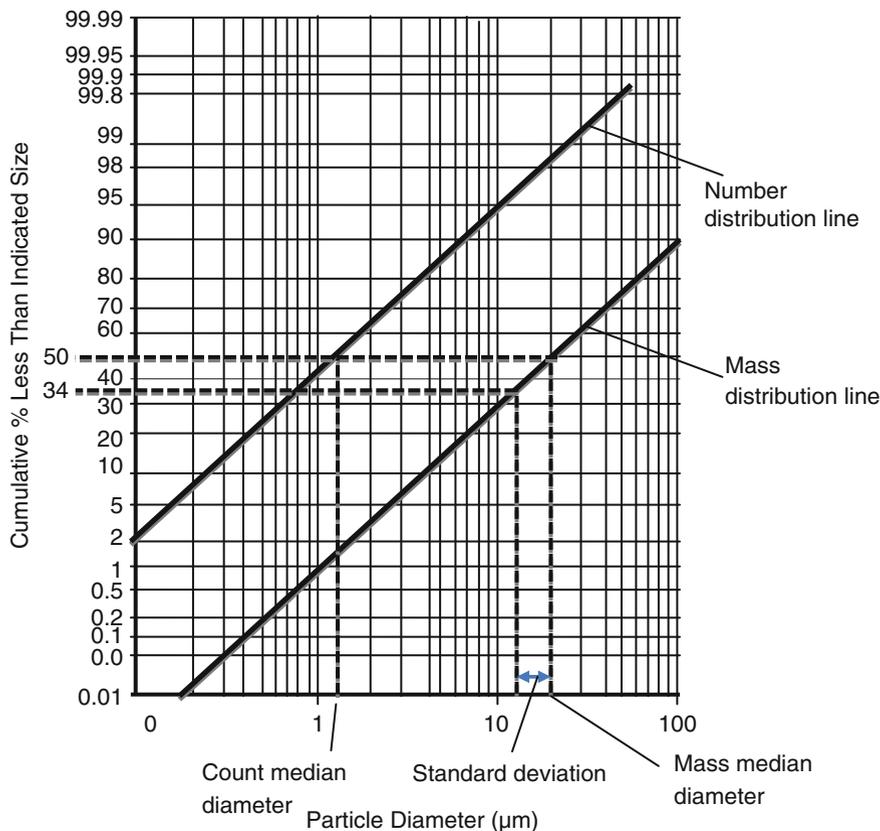


Fig. 4.5 Cumulative lognormal distributions for the same aerosol sample

volume, respectively. We can see that both surface and volume also follow log-normal distributions with the same standard deviation but with different median diameters. They are related to the number geometric mean diameter as follows.

$$\log \bar{d}_{pgA} = \log \bar{d}_{pg} + 2(\log \sigma)^2 \tag{4.56}$$

$$\log \bar{d}_{pgV} = \log \bar{d}_{pg} + 3(\log \sigma)^2 \tag{4.57}$$

where \bar{d}_{pgA} and \bar{d}_{pgV} are the geometric surface and volume median diameters. Respectively.

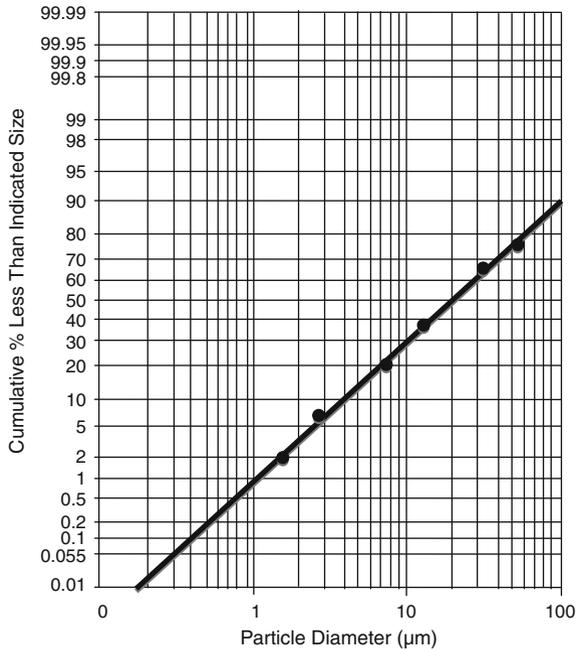
A log-probability paper based on Eq. (4.55) has been widely used to aerosol particle size distribution analysis. If we plot the number, surface, and volume cumulative distributions in the same log probability paper, they are parallel straight lines, as seen in Fig. 4.5. We can determine the median size of particles (based on number or mass) and the geometric standard deviation using a chart like this.

In an engineering practice, log probability paper is often used in engineering practice to determine the aerosol particle size distribution. One kind of log probability paper is given in Fig. A.1 as an example. Note that the x-axis is for the probability and the y-axis is for the particle diameter.

4.6 Practice Problems

1. Calculate the aerodynamic diameter for an iron oxide spherical particle with geometric equivalent diameter, $d_p = 0.21 \mu\text{m}$ and density, $\rho_p = 5,200 \text{ kg/m}^3$.
2. Calculate the aerodynamic diameter for a sand particle with geometric equivalent diameter, $d_p = 0.3 \mu\text{m}$ and density, $\rho_p = 3,500 \text{ kg/m}^3$.
3. A spherical grain of concrete dust is falling down to the floor through standard calm air. The particle geometric diameter is $2 \mu\text{m}$ and the particle density is $2,500 \text{ kg/m}^3$. Determine
 - (a) the aerodynamic particle diameter of the particle
 - (b) how long it will take for the particle to reach its terminal velocity
 - (c) terminal settling velocity of the particle
 - (d) flow condition around this particle, laminar or turbulent
 - (e) how long it will take this particle will take to fall down a distance of 1 m?
 Given: standard room air density = 1.21 kg/m^3 , viscosity = $1.81 \times 10^{-5} \text{ Pa s}$. Air mean free path = $0.066 \mu\text{m}$.
4. A spherical particle with a diameter of $2 \mu\text{m}$ and a density of $5,200 \text{ kg/m}^3$ is released from rest in still air. How long it will take to reach its terminal velocity?
5. A dust grain with a diameter of $5 \mu\text{m}$ and a density of $5,000 \text{ kg/m}^3$ is released from rest in still air. Calculate the terminal settling velocity and drag force exerted on this particle.
6. A particle with a diameter of $0.08 \mu\text{m}$ and a density of $2,000 \text{ kg/m}^3$ is released from rest in still air. What is the terminal velocity and drag force if particle is released from rest in still air?
7. Calculate the diffusion coefficient of a $2\text{-}\mu\text{m}$ particle in air at $25 \text{ }^\circ\text{C}$ and 1 atm.
8. Calculate the diffusion coefficient of a smoke particle having $0.05 \mu\text{m}$ diameter in air at $45 \text{ }^\circ\text{C}$ and 1 atm.
9. Calculate the Cunningham correction factor for the following particles at 373 K and 1 atm. (a) $0.055 \mu\text{m}$, (b) $0.55 \mu\text{m}$, and (c) $5.5 \mu\text{m}$.
10. A dust particle having $0.75 \mu\text{m}$ diameter escapes through a filter of vacuum cleaner at a height 1 m above the floor. Assume that the particle is spherical and its density is $1,200 \text{ kg/m}^3$. How long it will take to settle on the floor?
11. Two particles having diameters 1 and $10 \mu\text{m}$, respectively, are released from a height of 25 m above the ground. Assume that the particles are spherical with $1,200 \text{ kg/m}^3$ of density and ambient air is still. How long will they take to settle on the ground?

12. Starting from Eq. (4.55) derive the fractional distribution equation the surface and volume distributions to show that both surface and volume also follow lognormal distributions with the same standard deviation but with different median diameters.
13. A 1- μm cubic particle discharged from a 20-m tall stack travels with a horizontal wind at a constant speed of 10 m/s. Assuming its density is 1,500 kg/m^3 , estimate
- its volume *equivalent* diameter,
 - its aerodynamic diameter, and
 - the horizontal distance it travels before it falls to the ground.
14. Calculate the half-value time of spherical monodisperse aerosol with initial concentration of 10^6 particles/ cm^3 and initial particle diameter of $dp = 100 \mu\text{m}$. Assume standard condition and only Brownian coagulation is considered.
15. The figure below shows the cumulative mass distribution of a sample taken from coal fly ash. Assume the particles are lognormally distributed. Find the geometric standard deviation, and mass median diameter using the figure below.



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