For spheres, once you know the diameter, then you can determine others such as volume

$\left(\frac{\pi d_p^3}{6}\right)$ **, surface are** (πd_p^2) **. For non-spheres, particle volume and surface area are independent.**

First, let us consider spherical particles. $\Rightarrow$ **n(d_p)**
Often we need to tell about "Some representative particles" instead of detailed distributions.

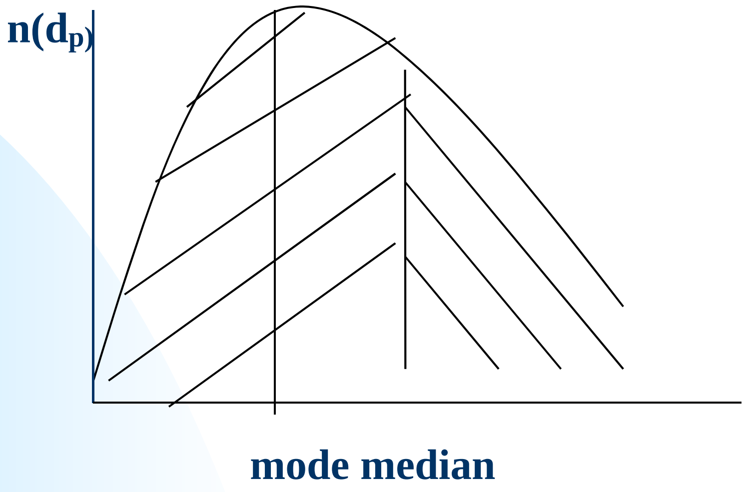
- Mean diameters

① mean (arithmetic average)

$$\overline{d}_p = \frac{\sum d_i}{N} = \frac{\sum n_i d_i}{\sum n_i} = \int_0^\infty \frac{n(d_p) d_p dd_p}{N}$$

② median: diameter for which one half the total number of particles are smaller and one half are larger

- or the diameter to cut half the area under the size distribution function curve



- or the diameter at which the cumulative distribution function is equal to 0.5

$$F(d_p) = \int_0^{d_p} f(d_p)\, dd_p$$

$$f(d_p) = \frac{dF}{dd_p}$$

③ **mode: most frequent size: the diameter that have the highest number**

$$\frac{dn(d_p)}{dd_p} = 0$$

If particle size distribution function is symmetric (like normal distribution), mean= median = mode.

However, we usually have asymmetric distribution with the tail at larger sizes.
mode < median < mean

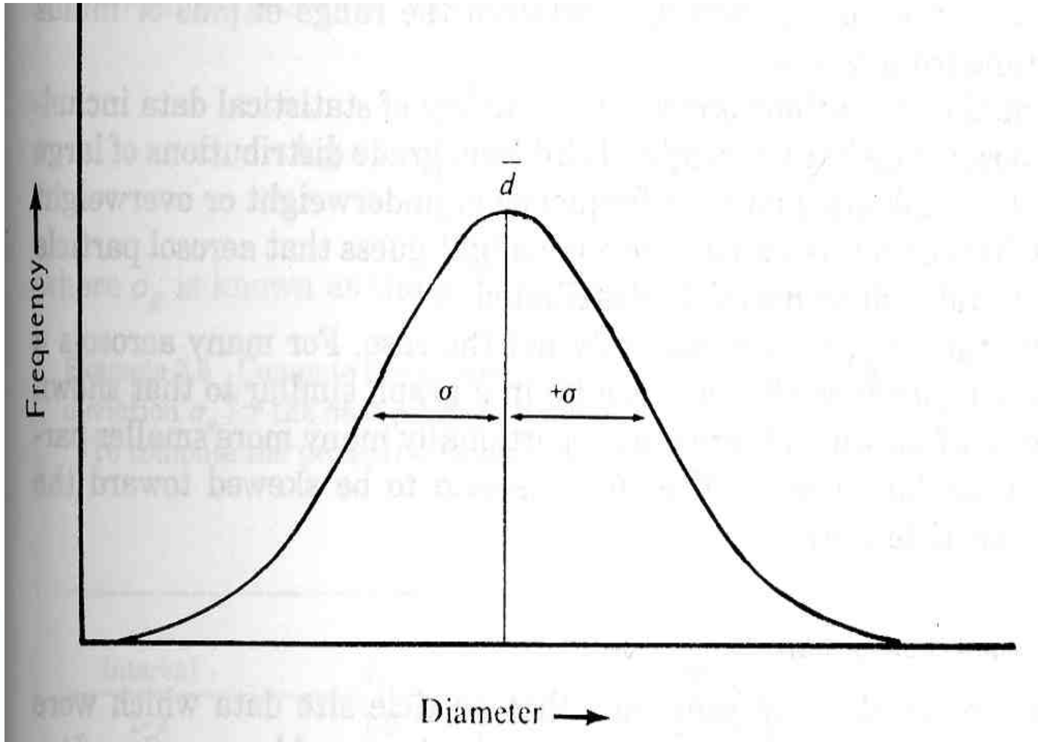


Figure 2.4a The normal distribution.

In real case most aerosols do not have symmetric distribution

: skewed distribution (if particle formation ends)

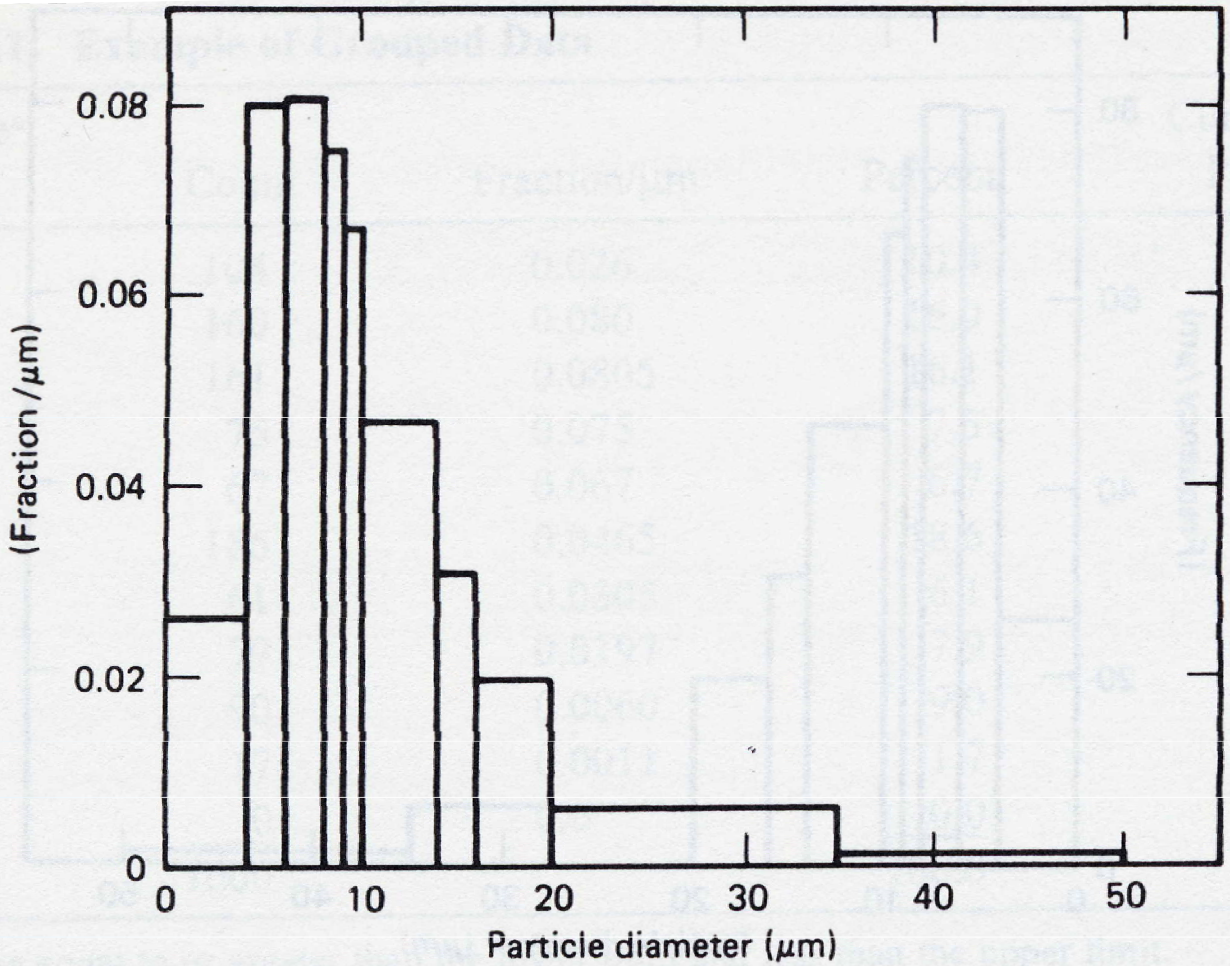


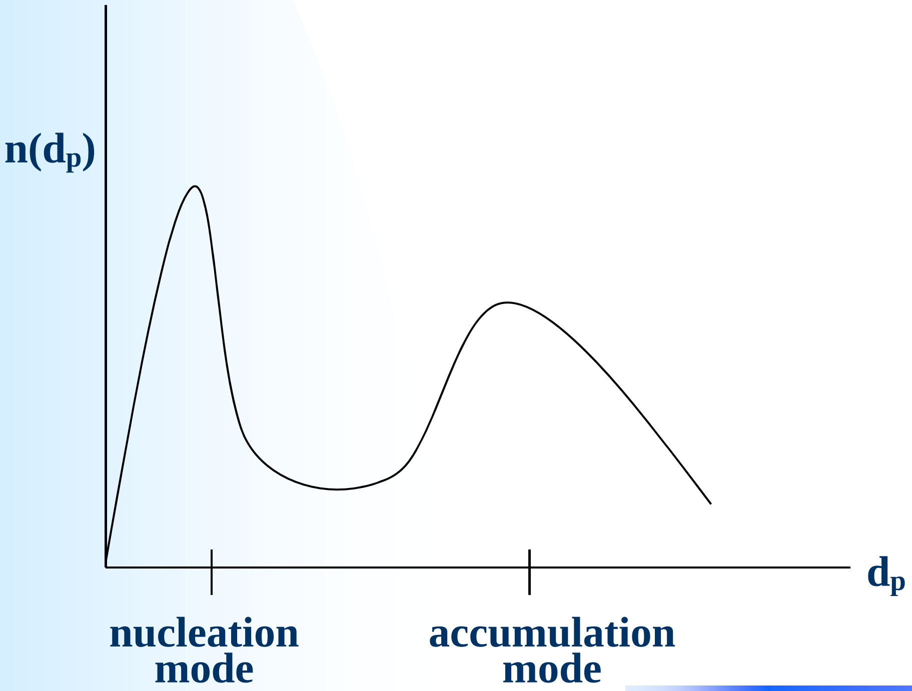
FIGURE 4.3 Fraction/μm versus particle size, count distribution.

1. If particle size distribution has one mode,

uni-modal distribution

2. Well grown single component aerosol two-modes

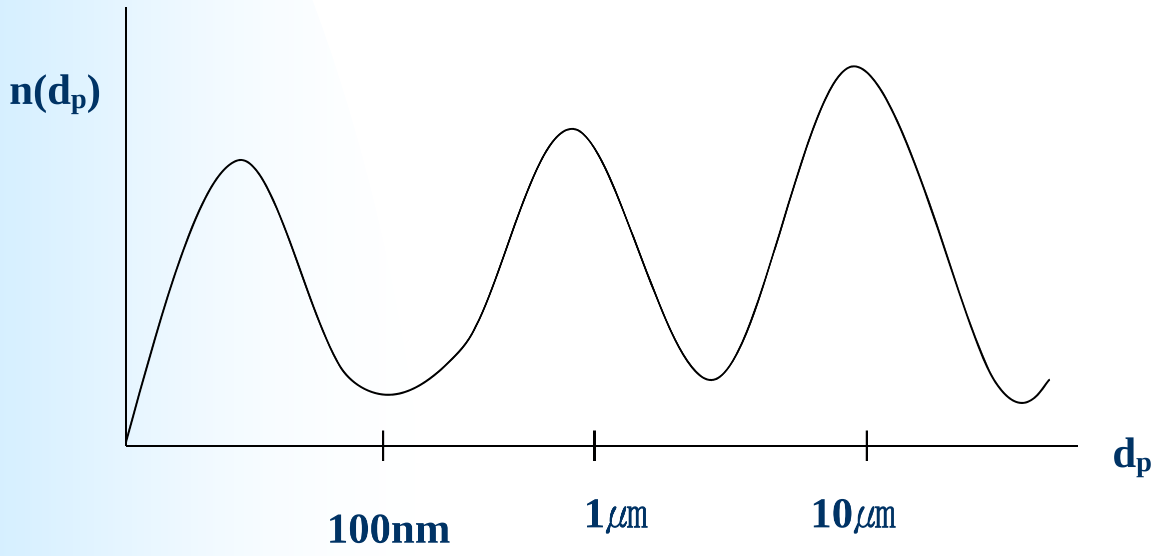
: bi-modal: formation + growth



$n(d_p)$
d_p
nucleation mode
accumulation mode

3. three-modes: tri-modal: atmospheric aerosols generated by different mechanisms

① formation ② growth ③ generation by mechanical means



Multi-modal nature of atmospheric aerosols

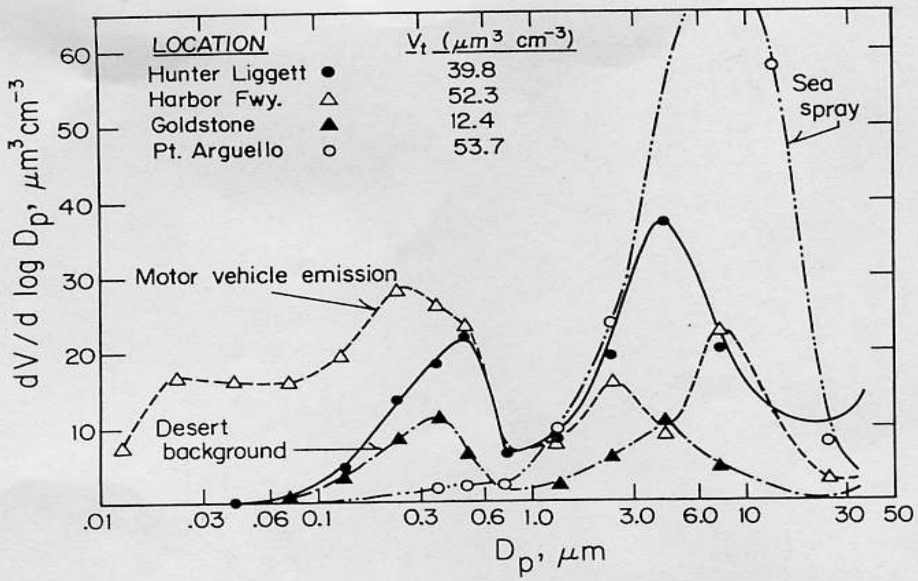


Figure 7.4. Comparison of aerosol volume distributions at four locations in the Southern California area: (1) Hunter Liggett—a non-urban background site; (2) Harbor Freeway—motor vehicle source enriched site; (3) Goldstone—a remote desert site; (4) Pt. Arguello—a site dominated by marine aerosol. V_t is the total volume concentration of aerosol (μm^3 cm^{-3}) as estimated from the particle measurements. (Hidy, 1975). Reprinted with permission from Journal of the Air Pollution Control Association.

④ geometric mean

$$d_g = (d_1 d_2 \ldots)^{1/N}$$

$$= (d_1^{n_1} d_2^{n_2} \ldots)^{1/N}$$

$$\ln d_g = \frac{\sum n_i \ln d_i}{N}$$

*** Log-normal distribution**

- normal distribution

$$n(d_p) = \frac{N}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(d_p - \overline{d_p})^2}{2\sigma^2} \right]$$

σ **: standard deviation** $= \left[\frac{\sum n_i (d_i - d_p)^2}{N-1} \right]^{1/2}$

$\overline{d}$ **: mean diameter** $= \frac{\sum n_i d_i}{N}$

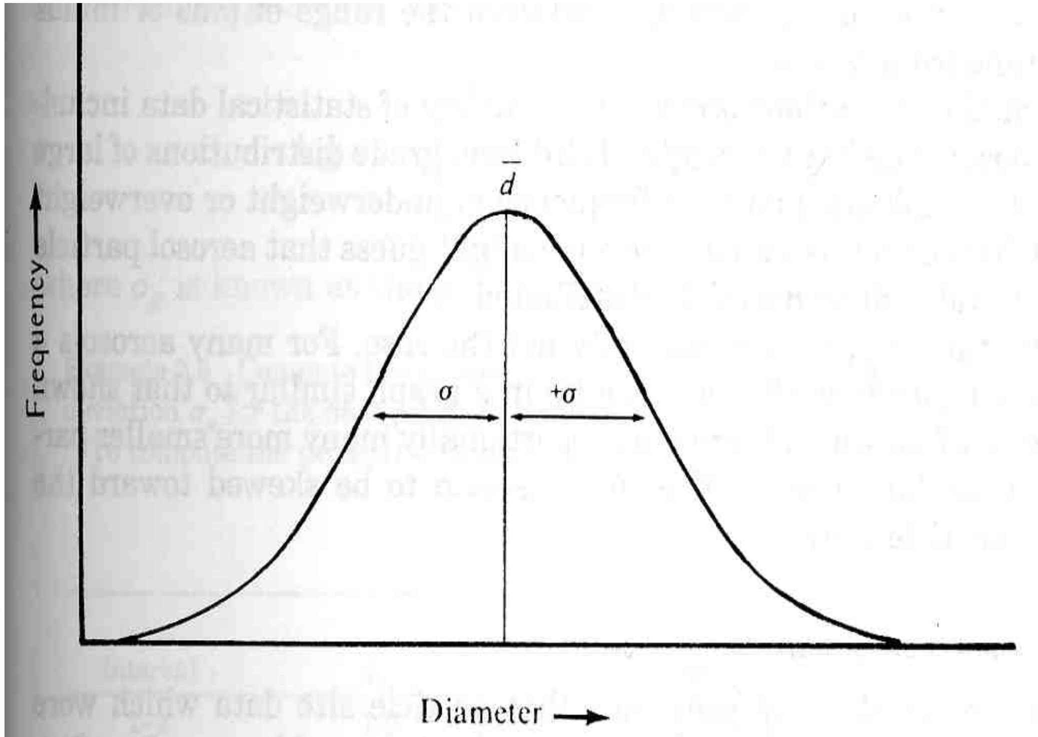


Figure 2.4a The normal distribution.

However, in real case most aerosols do not have symmetric distribution

: skewed distribution (if particle formation ends)

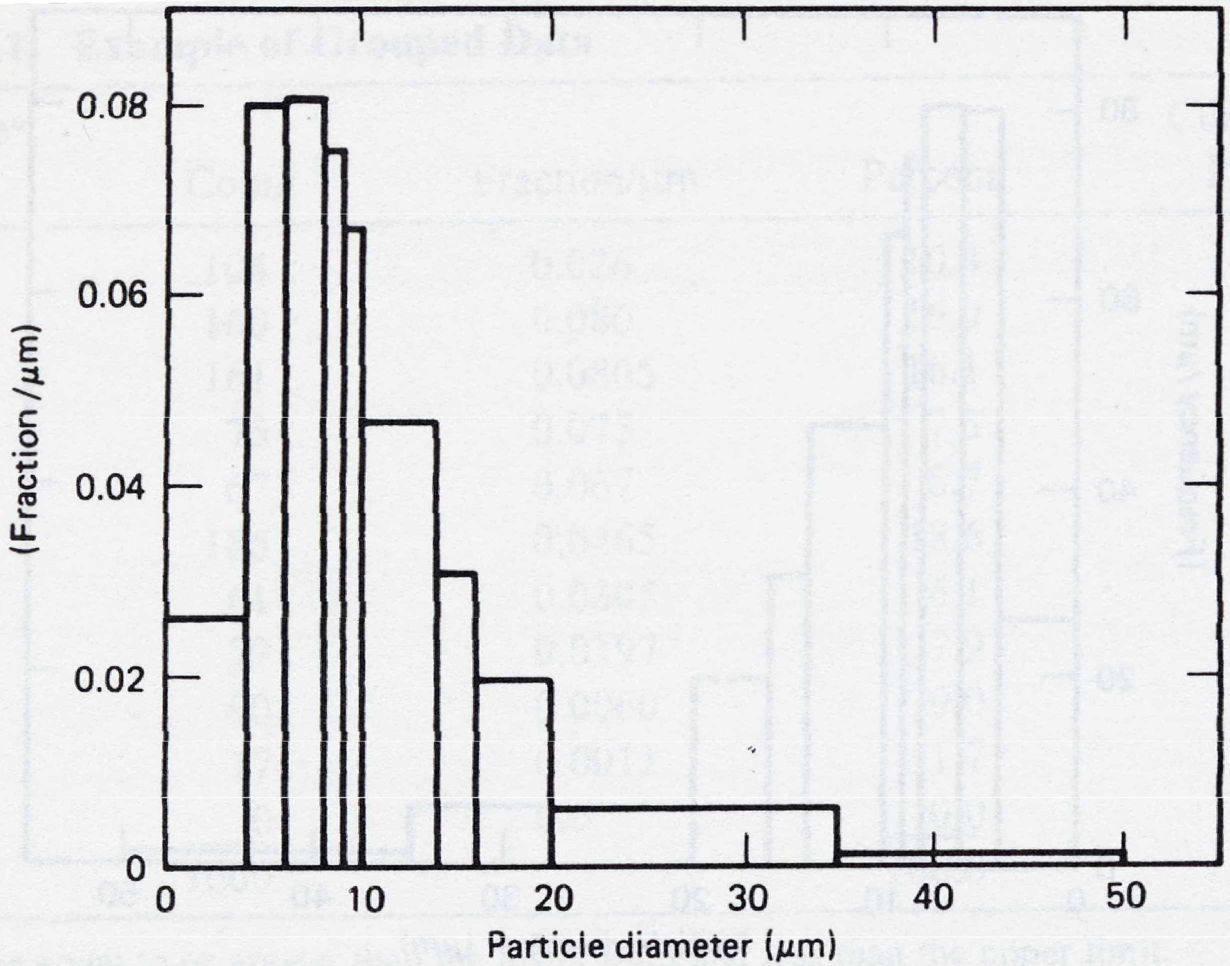


FIGURE 4.3 Fraction/μm versus particle size, count distribution.

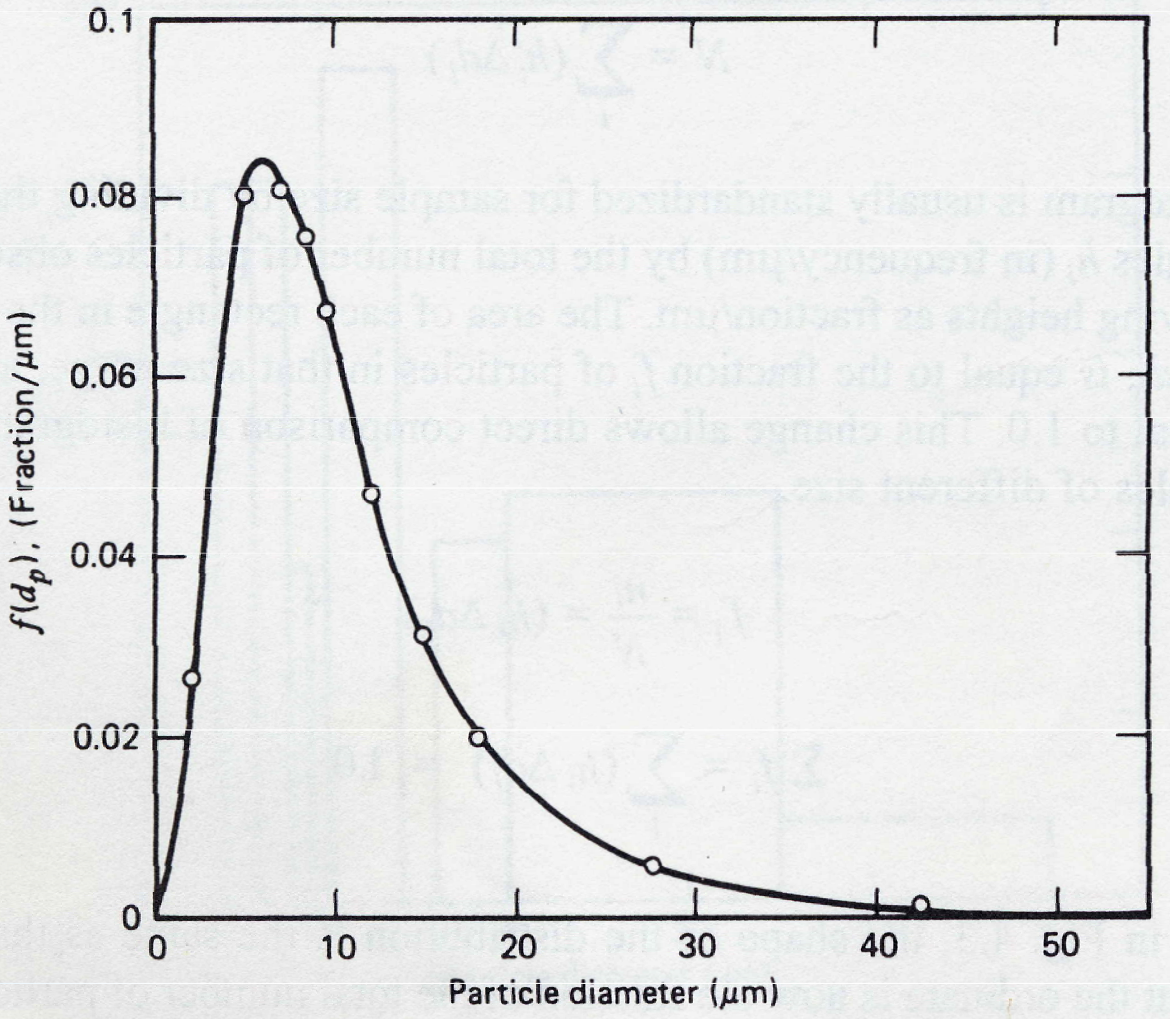


FIGURE 4.4 Frequency distribution curve.

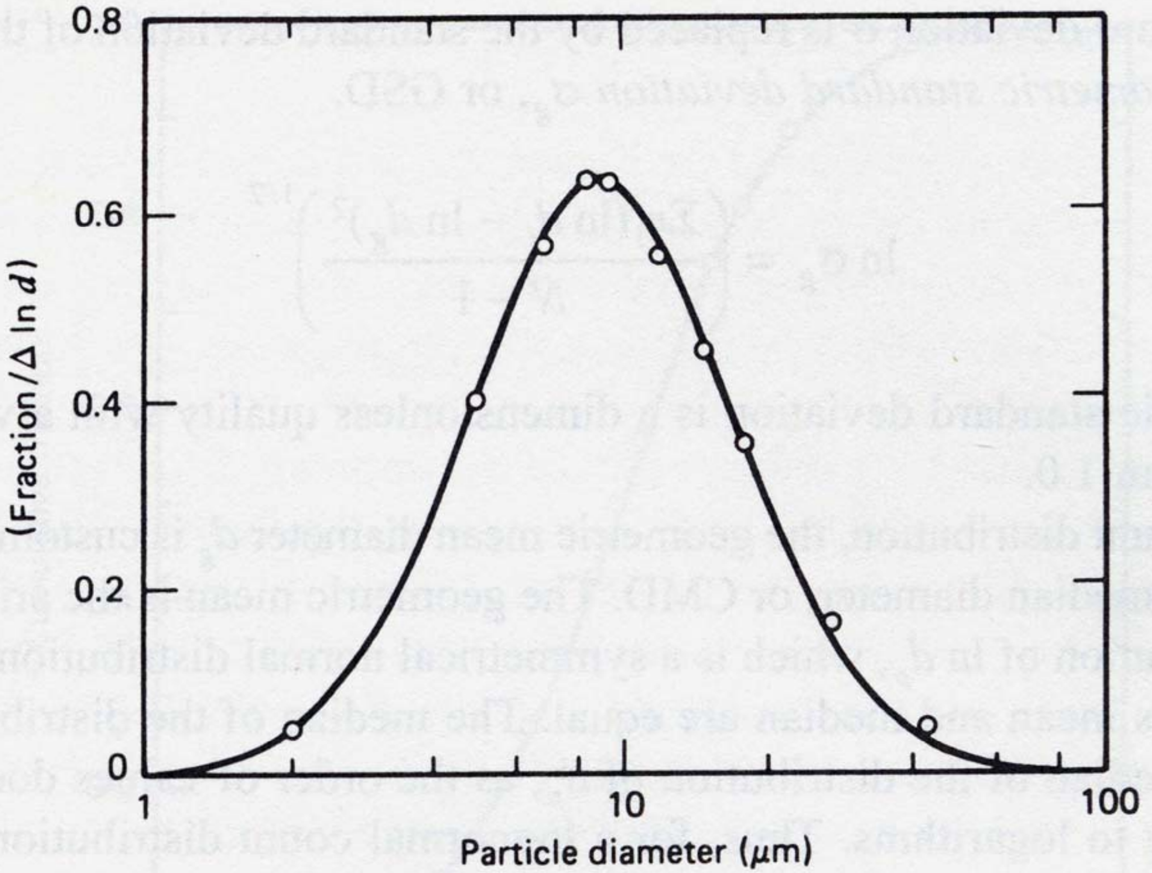
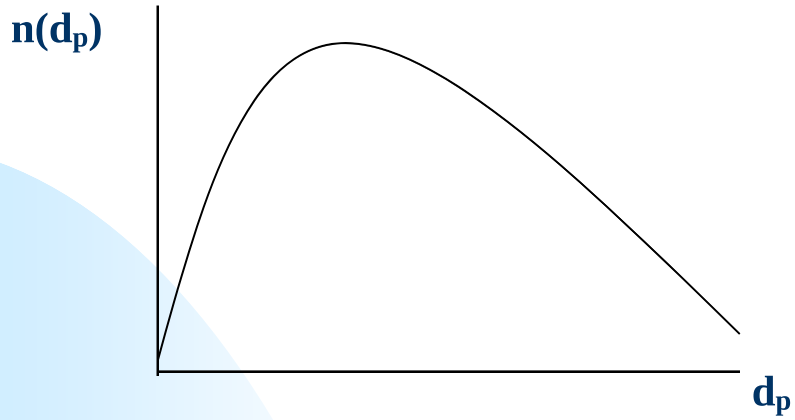


FIGURE 4.8 Frequency distribution curve (logarithmic size scale).



Log-norml distribution

$$n(\ln d_p) = \frac{N}{\sqrt{2\pi}\ln\sigma_g}\exp\left[-\frac{(\ln d_p - \ln d_g)^2}{2\ln^2\sigma_g}\right]$$

$$\ln d_g = \frac{\sum n_i \ln d_i}{N}$$

$$\ln \sigma_g = \left[\frac{\sum n_i (\ln d_i - \ln d_g)^2}{N-1}\right]^{1/2}$$

d_g **: geometric mean diameter**

σ_g **: geometric standard deviation**

Monodisperse aerosols should have $\sigma = 0$ **or** $\sigma_g = 1$

Particle numbers between $\ln d_p$ **and** $\ln d_p + d\ln d_p = dN_i = n(\ln d_p)d\ln d_p$

$$= n(\ln d_p)\frac{1}{d_p}dd_p = n(d_p)dd_p$$

$$\therefore n(d_p) = \frac{1}{d_p}n(\ln d_p)$$

For log-normal distributions

$$d_g = d_{median}$$

To completely define the log-normal distributions, you should know N, d_g , σ_g

(only three parameters), then you know the complete distributions

*** Log-probability graph**

$F(d_p)$ **: cumulative distribution function**

$$F(\ln d_p) = \int_{-\infty}^{\ln(d_p)} \frac{n(\ln d_p)}{N} d\ln d_p$$

$$= \frac{1}{2} + \frac{1}{2} erf\left(\frac{\ln(d_p / d_g)}{\sqrt{2}\ln\sigma_g} \right)$$ if log-normal

$$erf^{-1}\left\{ (F - \frac{1}{2})2 \right\} = \frac{1}{\sqrt{2}\ln\sigma_g}\ln d_p - \frac{1}{\sqrt{2}\ln\sigma_g}\ln d_g$$

*Revised

*Revised

$$erf^{-1}\left\{(F-\frac{1}{2})2\right\}=\frac{1}{\sqrt{2}\ln\sigma_g}\ln d_p-\frac{1}{\sqrt{2}\ln\sigma_g}\ln d_g$$

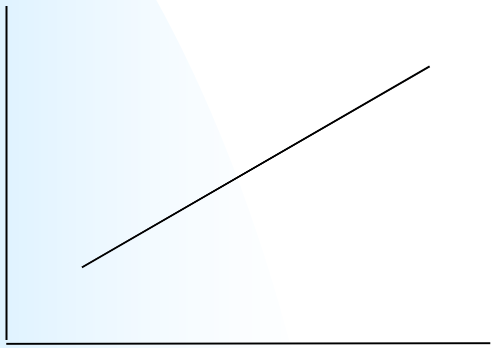
If $\ln(d_p/\ d_g)=\ln\sigma_g$

$$F=\frac{1}{2}+\frac{1}{2}erf\,(\frac{1}{\sqrt{2}})=0.841$$

$$\ln \sigma_g = \ln d_p - \ln d_g = \ln d_{84\%} - \ln d_{50\%}$$

$$\sigma_g = \frac{d_{84\%}}{d_{50\%}}$$

$\ln d_p$



$$erf^{-1}\left\{(F - \frac{1}{2})^2\right\}$$

CMD(Count median diameter) or Dg (geometric mean diameter can be determined from this log-probability graph by reading the diameter corresponding to 50% cumulative farction. GSD(geometric standard deviation) can be also determined directly from this graph by finding the diameter corresponding to 84% cumulative fraction.

The cumulative fraction scale (or percent) is converted to a probability scale. This probability scale compresses the percent scale near the median (50%) and expands the scale near the ends such that a cumulative plot of a log-normal distribution will yield a straight line. When the particle diameter scale is logarithmic, the graph is called a log-probability plot. When the size scale is linear, the graph will yield a straight line for a normal distribution and is called a probability graph.

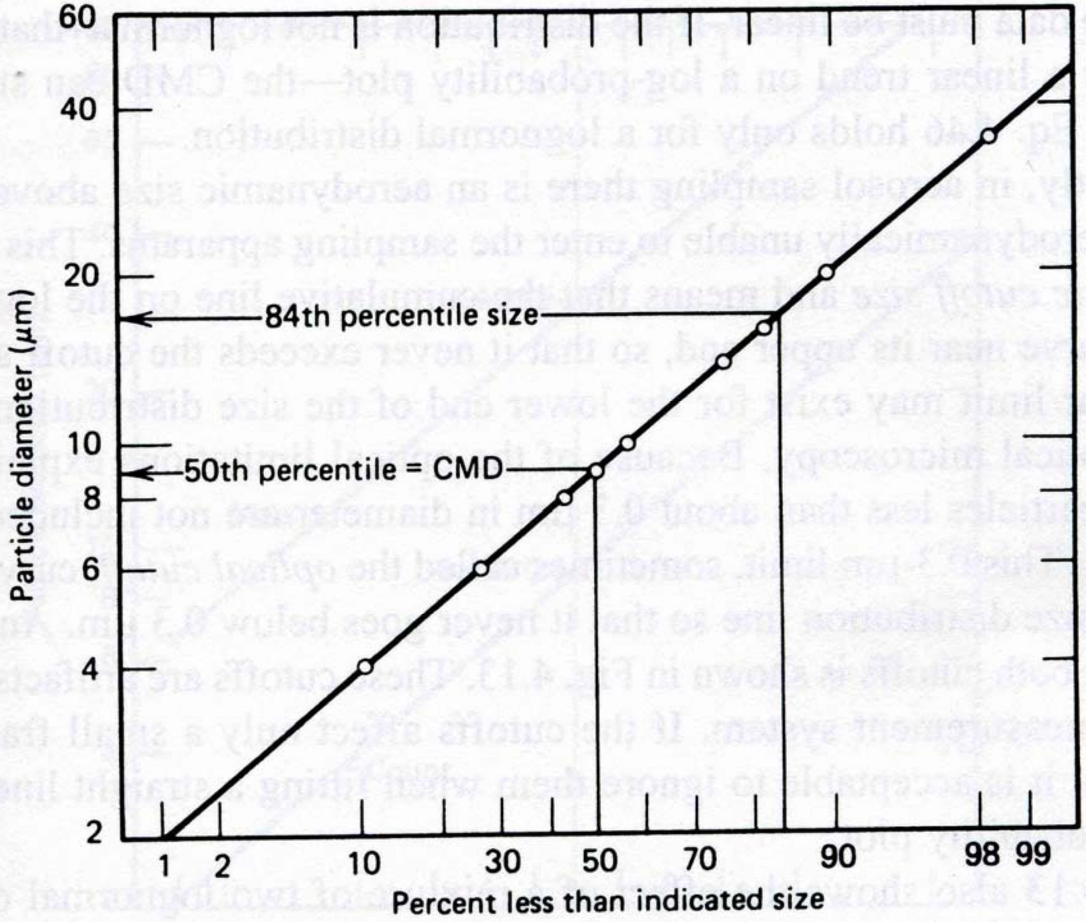


FIGURE 4.12 Log-probability graph.

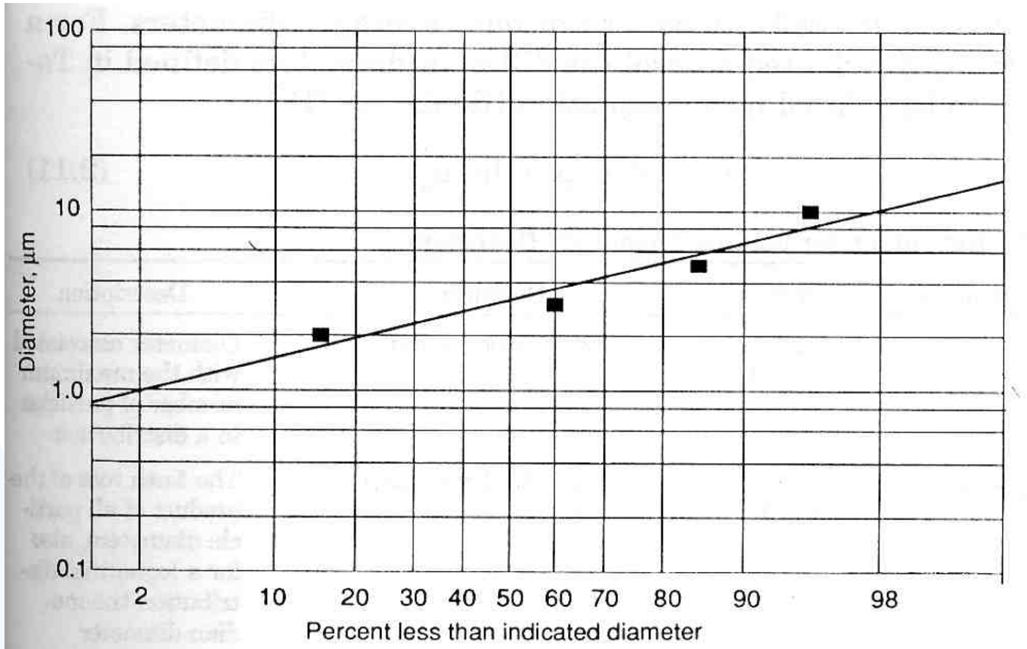


Figure 2.5 Log probability plot using the data from Example 2.1.

Steepness of the curve on log-probability curve indicates "broadness of the log-normal size distribution". Less steep curve represents ⇒ narrower distribution (with small σ_g)

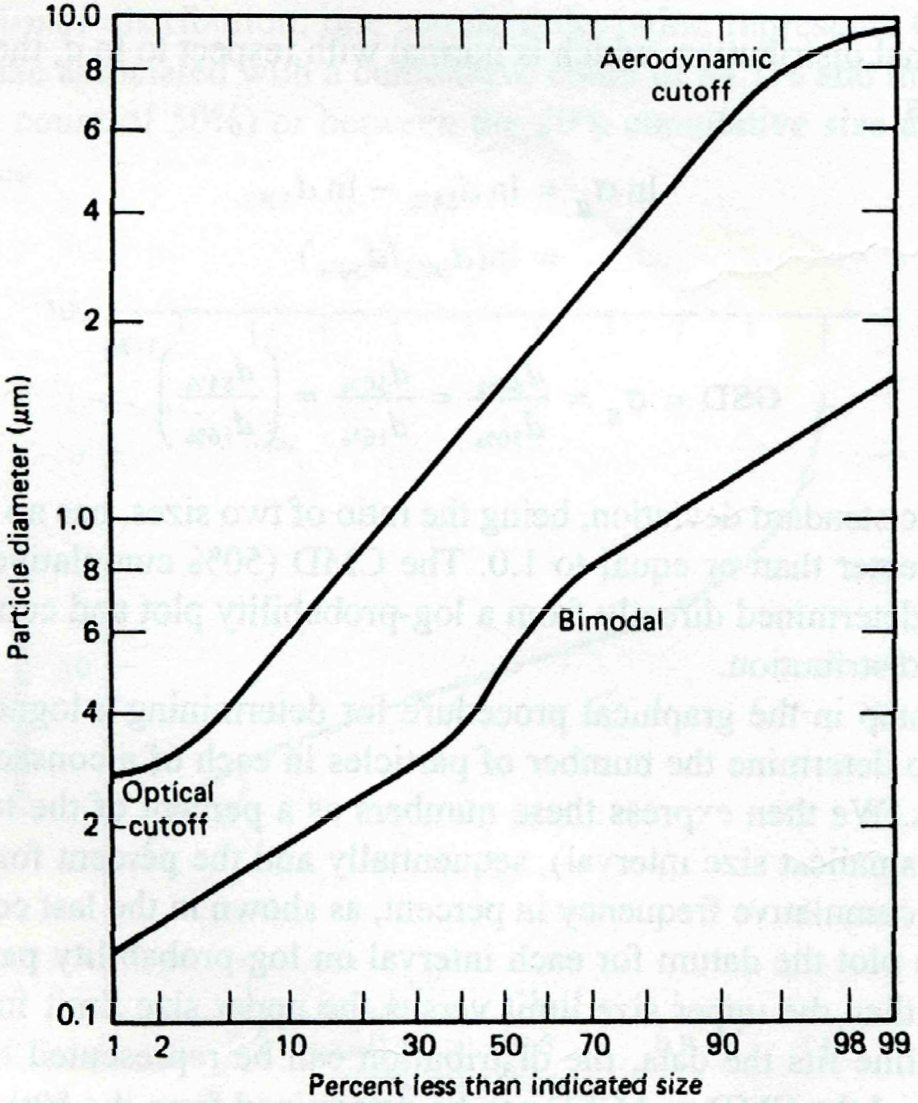


FIGURE 4.13 Nonlinear log-probability graphs.

Up to this point, we have dealt with number distribution as a function of particle size. Sometimes, we may need to define mass distribution, surface area distribution as a function of particle size. For example, catalytic application of particles, surface area is an important factor, and the surface area distribution is needed to be known.

$$n_s(d_p) = \pi d_p^2 n(d_p)$$ ㎛²/ cm² ·㎛

$$S = \int_0^\infty n_s(d_p)dd_p$$ ⇒ total surface area concentration

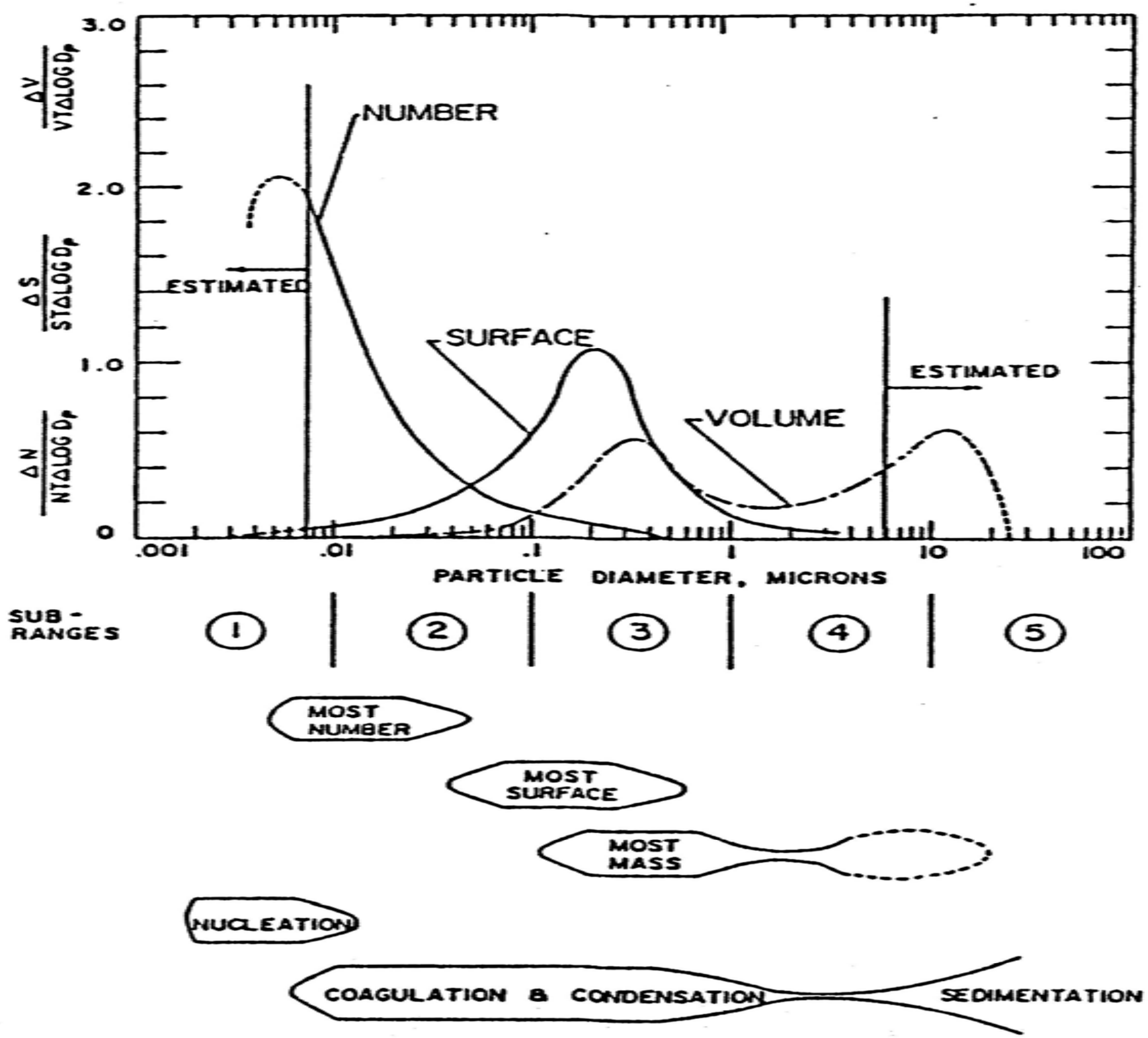
$$n_v(d_p) = \frac{\pi}{6} d_p^3 n(d_p)$$ ㎛³/ cm³ ·㎛

$$V = \int_0^\infty n_v(d_p)dd_p$$ **: total volume concentration**

⇒ Weighted Distributions

$$n_q(d_p) = a_q d_p^q n(d_p)$$

Since particle diameters vary over several orders, horizontal axis is generally using log-scale: log d_p


3.0
2.0
1.0
0
ΔV / VTΔLOG Dp
ΔS / STΔLOG Dp
ΔN / NTΔLOG Dp
NUMBER
ESTIMATED
SURFACE
VOLUME
ESTIMATED
.001
.01
.1
1
10
100
PARTICLE DIAMETER, MICRONS
SUB-RANGES
1
2
3
4
5
MOST NUMBER
MOST SURFACE
MOST MASS
NUCLEATION
COAGULATION & CONDENSATION
SEDIMENTATION

trol

$$\therefore\ n_q(\log d_p)\, d\log d_p = n_q(d_p)\, dd_p$$

$$n_q(\log d_p) = n_q(d_p)\frac{dd_p}{d\log d_p} = 2.303 d_p n_q(d_p)$$

For example) if you know $n_m(m),$ **can you find** $n_m(\log d_p)?$

$$n_m(m)\, dm = n_m(\log d_p)\, d\log d_p$$

$$m = \frac{\pi}{6}\rho_p d_p^3 \longrightarrow dm = \frac{\pi}{6}\rho_p 3 d_p^2\, dd_p$$

$$d\log d_p = \frac{dd_p}{2.303 d_p}$$

$$\therefore n_m(\log d_p) = 6.9\, m n_m(m)$$

If you know n(m) instead of $n_m(m)$ **, then**

*Revised

$$n_m(m) = mn(m)$$

$$\therefore n_m(\log d_p) = 6.9m^2 n(m)$$

- Moment average

Definition of moments of distribution function

$$M_v = \int_0^\infty n(d_p) d_p^v dd_p$$

Zeroth moment $M_0 = \int_0^\infty n(d_p) dd_p = N$

First moment $M_1 = \int_0^\infty n(d_p) d_p dd_p : \overline{d_p} = M_1 / M_0$

: mean diameter

The need to use the moment average for particle statistics arises because aerosol size is frequently measured indirectly. For example, if you have a basket of apples of different sizes, you could determine the average size by measuring each apple with calipers, summing the results and dividing by the total numbers of apples. This is the direct measurement. If, however, each apple were weighted on a balance and the weights summed and divided by their number, the average mass would be first obtained. Then assuming the apple as spheres, you can indirectly calculate the average diameter of apple corresponding to the average mass.

2nd moment

$$M_2 = \int_0^\infty n(d_p) d_p^2 \, dd_p$$

$$\pi M_2 = S$$

$$\pi d_{\bar{s}}^2 = \frac{\sum \pi d_i^2}{N} = \frac{\pi}{N} \int_0^\infty n(d_p) d_p^2 \, dd_p$$

$d_{\bar{s}}^2 = M_2 / M_0$ **: 2nd moment average**

$d_{\bar{s}}$ **: diameter of average surface area**

3rd moment

$$M_3 = \int_0^\infty n(d_p) d_p^3 \, dd_p$$

$$\frac{\pi}{6} \rho_p d_{\bar{m}}^3 = \frac{\frac{\pi}{6} \rho_p M_3}{N}$$

$d_{\bar{m}}^3 = M_3 / M_0$ **: 3rd moment average**

$$d_{\bar{p}} = \left(\frac{\sum n_i d_i^{\,p}}{N} \right)^{1/P}$$

*** Weighted mean diameters - arithmetic mean (count mean)**

$$\overline{d_p} = \sum \frac{d_i n_i}{N} = \frac{M_1}{M_0}$$

- surface area mean diameter

$$d_{sm} = \frac{\pi \sum n_i d_i^{\,2} d_i}{\pi \sum n_i d_i^{\,2}} = \frac{M_3}{M_2}$$

or

$$= \frac{d_{\bar{m}}^{\,3}}{d_{\bar{s}}^{\,2}}$$

d_{sm} **: sauter diameter (mean volume-surface diameter)**

- **mass mean diameter**

$$d_{mm} = \frac{\frac{\pi}{6} d_p \sum n_i d_i^3 d_i}{\frac{\pi}{6} \rho_p \sum n_i d_i^3} = \frac{M_4}{M_3}$$

$$d_{sm} = \left(\frac{6}{\rho_p}\right) \frac{M}{S}$$

S/M: specific surface area can be measured by nitrogen gas adsorption, so called, BET method then you can measure d_{sm}.

- If you have log-normal distribution or you force or approximate the distribution as log-normal, then you can easily obtain other mean values from one mean value.

Weighted Distributions

If number distribution is log-normal, which distributions do weighted distributions have ?

$$n_s(d_p) = \pi d_p^{\,2} n(d_p) \qquad n_\upsilon(d_p) = \frac{\pi}{6} d_p^{\,3} n(d_p)$$

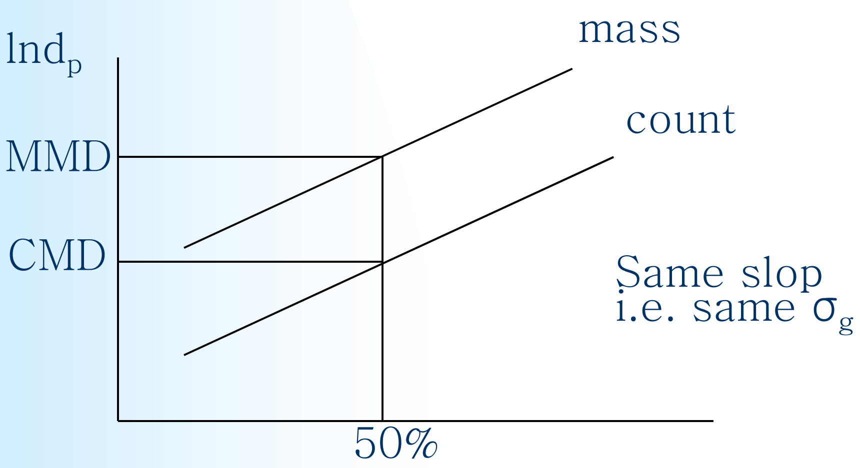
$$n_q(d_p) = a_q d_p^{\,q} n(d_p)$$

$$\therefore n_q(d_p) = \frac{a_q N d_p^{\,q}}{\sqrt{2\pi} d_p \ln\sigma_g} \exp\left[-\frac{(\ln d_p - \ln d_g)^2}{2\ln^2\sigma_g}\right]$$

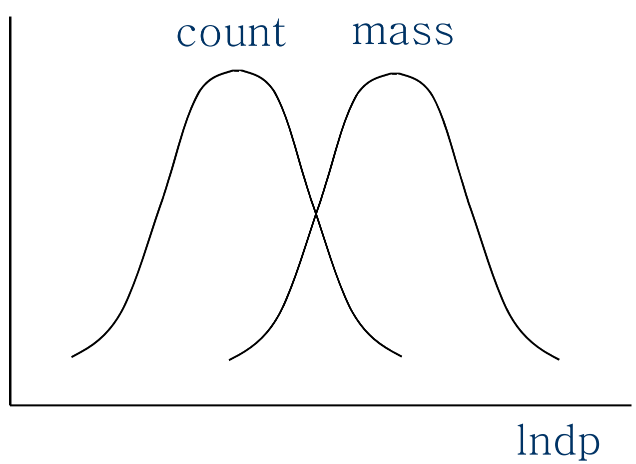
since $d_p^{\,q} = \exp(q \ln d_p)$

$$n_q(d_p) = \frac{a_q N}{\sqrt{2\pi} d_p \ln\sigma_g} \exp\left(q \ln d_g + \frac{q^2}{2}\ln^2\sigma_g\right) \exp\left[-\frac{\{\ln d_p - (\ln d_g + q\ln^2\sigma_g)\}^2}{2\ln^2\sigma_g}\right]$$

$\therefore n_q(dp)$ **is also log-normal with geometric standard deviation,** σ_g **and median diameter,** $\ln d_{g\,median} = \ln d_g + q \ln^2 \sigma_g$



Log-probability graph



① $\frac{qMD}{CMD} = \exp(q \ln^2 \sigma_g)$ **: median diameter of q weighted distribution**

e.g. mass median diameter: q=3

② **d_{qm} : mean diameter of qth moment distribution**

e.g. surface area mean: q=2

mass mean: q=3

$$d_{qm} = \frac{M_{q+1}}{M_q}$$

$$\frac{d_{qm}}{CMD} = \exp\left[\left(q + \frac{1}{2}\right)\ln^2 \sigma_g\right]$$

③ $$d_{\bar{p}} = \left(\overline{d_p}\right)^{1/p} = CMD \exp\left(\frac{p}{2}\ln^2 \sigma_q\right)$$

e.g. diameter of average volume

p=3

$$d_{\bar{p}} = CMD \exp\left(\frac{3}{2}\ln^2 \sigma_g\right)$$

mode $$\hat{d} = CMD \exp\left(-\ln^2 \sigma_g\right)$$

4.10 APPENDIX 3: DERIVATION OF THE HATCH–CHOATE EQUATIONS

The diameter of average d^p, where $p = 2$ for surface area and 3 for mass, is given by Eq. 4.22 as

$$d_{\bar{p}} = (\overline{d^p})^{1/p} = \left(\int_0^\infty d^p f(d) dd\right)^{1/p} \tag{4.65}$$

To evaluate $d_{\bar{p}}$ for a lognormal distribution, we must first express the quantity $d^p f(d)$ in terms of the CMD, σ_g, and p. Expressing $f(d)$ in terms of Eq. 4.42 and making the substitution $d^p = \exp(p \ln d)$ gives

$$d^p f(d) = \frac{e^{p \ln d}}{\sqrt{2\pi}\, d \ln \sigma_g} \exp\left(\frac{-(\ln d - \ln \text{CMD})^2}{2 \ln^2 \sigma_g}\right) \tag{4.66}$$

Combining and expanding the exponent yields

$$d^p f(d) = \frac{1}{\sqrt{2\pi}\, d \ln \sigma_g} \times \exp\left(\frac{+2(\ln^2\sigma_g)p \ln d - \ln^2 d + 2(\ln d) \ln \mathrm{CMD} - \ln^2 \mathrm{CMD}}{2 \ln^2 \sigma_g}\right) \quad (4.67)$$

We can complete the square in the exponential term of Eq. 4.67 by multiplying the entire equation by

$$1 = \left[\exp\left(p \ln \mathrm{CMD} + \frac{p^2}{2} \ln^2 \sigma_g\right)\right]\left[\exp\left(-p \ln \mathrm{CMD} - \frac{p^2}{2} \ln^2 \sigma_g\right)\right] \quad (4.68)$$

The second factor of Eq. 4.68 is combined with the exponential term in Eq. 4.67 to give a new exponential term,

$$\frac{-1}{2\ln^2\sigma_g}[\ln^2 d - 2(\ln d)(\ln \mathrm{CMD} + p\ln^2\sigma_g)$$

$$+ \ln^2\mathrm{CMD} + 2p(\ln \mathrm{CMD})\ln^2\sigma_g + (p\ln^2\sigma_g)^2] \quad (4.69)$$

which is equal to

$$\frac{-[\ln d - (\ln \mathrm{CMD} + p\ln^2\sigma_g)]^2}{2\ln^2\sigma_g} \quad (4.70)$$

Thus,

$$d^p f(d) = \exp\left(p \ln \text{CMD} + \frac{p^2}{2} \ln^2 \sigma_g\right)$$

$$\times \left[\frac{1}{\sqrt{2\pi}\, d \ln \sigma_g} \exp\left(-\frac{[\ln x - (\ln \text{CMD} + p \ln^2 \sigma_g)]^2}{2 \ln^2 \sigma_g}\right)\right] \quad (4.71)$$

We can now substitute Eq. 4.71 into Eq. 4.65 and integrate the resulting expression. The first exponential in Eq. 4.71 is a constant term. The bracketed term is identical in form to the frequency function of a lognormal distribution. Equation 4.65 becomes

$$d_{\bar{p}} = \left(\overline{d^p}\right)^{1/p} = \exp\left[p \ln \text{CMD} + \frac{p^2}{2} \ln^2 \sigma_g\right]^{1/p} \quad (4.72)$$

$$\ln d_{\bar{p}} = \frac{1}{p} \ln \overline{d^p} = \frac{1}{p}\left[p \ln \mathrm{CMD} + \frac{p^2}{2} \ln^2 \sigma_g \right] \tag{4.73}$$

$$\ln d_{\bar{p}} = \ln \mathrm{CMD} + \left(\frac{p}{2}\right) \ln^2 \sigma_g \tag{4.74}$$

and $d_{\bar{p}}$, the diameter of average d^p, is

$$d_{\bar{p}} = \mathrm{CMD} \exp\left[\frac{p}{2} \ln^2 \sigma_g \right] \tag{4.75}$$

which is identical to Eq. 4.52.

To obtain the conversion equation for the median (qMD) of the qth moment distribution, we start with the distribution function, Eq. 4.35. Substituting Eq. 4.71, with p replaced by q, for the numerator and using the procedure just outlined in Eqs. 4.66–4.72 to evaluate the integral of Eq. 4.71 for the denominator, we get

$$df_q = \frac{1}{\sqrt{2\pi}\ d \ln \sigma_g} \exp\left(-\frac{[\ln d - (\ln \text{CMD} + q \ln^2 \sigma_g)]^2}{2 \ln^2 \sigma_g} \right) \tag{4.76}$$

This equation has the form of a lognormal distribution, Eq. 4.42, with a median diameter given by

$$\begin{aligned} \ln q\text{MD} &= \ln \text{CMD} + q \ln^2 \sigma_g \\ q\text{MD} &= \text{CMD} \exp(q \ln^2 \sigma_g) \end{aligned} \tag{4.77}$$

which is identical to Eq. 4.48.

We can use Eq. 4.71 to get d_{qm}, the mean of the qth moment distribution. This mean is the ratio of two moments of diameter and has the general form

$$d_{qm} = \frac{\int_0^\infty x^{q+1} f(x)\, dx}{\int_0^\infty x^q f(x)\, dx} \tag{4.78}$$

Both the numerator and denominator of Eq. 4.78 are equivalent to the integrals of Eq. 4.71. Evaluating Eq. 4.78 using the procedure followed in Eqs. 4.66–4.72 gives

$$d_{qm} = \frac{\exp\left[(q+1)\ln \mathrm{CMD} + \dfrac{(q+1)^2}{2}\ln^2\sigma_g\right]}{\exp\left[q \ln \mathrm{CMD} + \dfrac{q^2}{2}\ln^2\sigma_g\right]} \tag{4.79}$$

$$\ln d_{qm} = \ln \mathrm{CMD} + \frac{[(q+1)^2 - q^2]\ln^2\sigma_g}{2} \tag{4.80}$$

$$d_{qm} = \mathrm{CMD}\exp[(q + ½)\ln^2\sigma_g] \tag{4.81}$$

which is identical to Eq. 4.50.

Log-normal distribution : different representative diameters

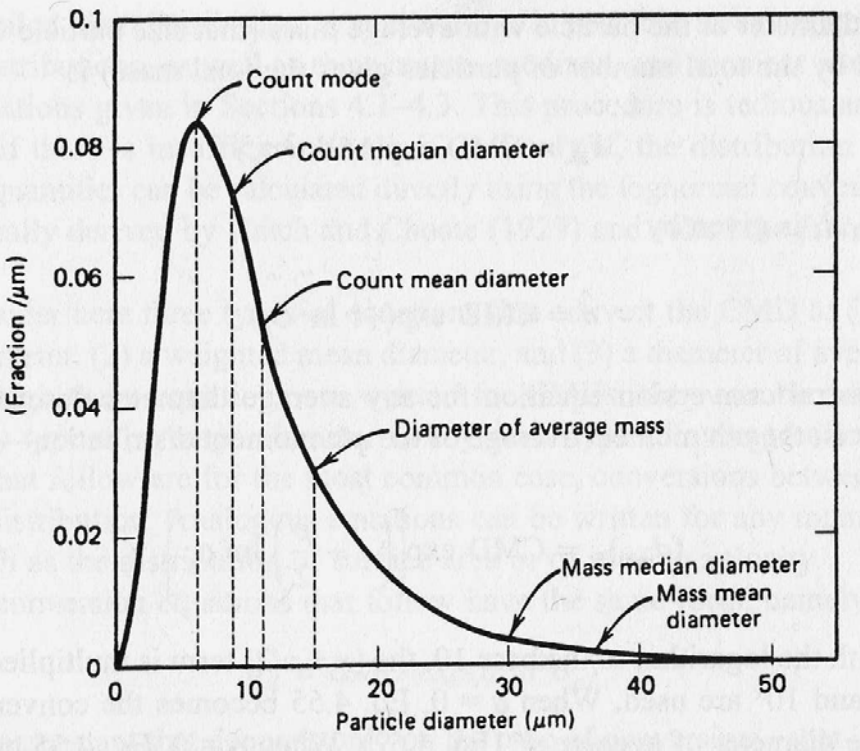


FIGURE 4.15 Arithmetic plot of the size data from Table 4.1 (count distribution with CMD = 9.0 μm and GSD = 1.89), showing the locations of various average diameters.

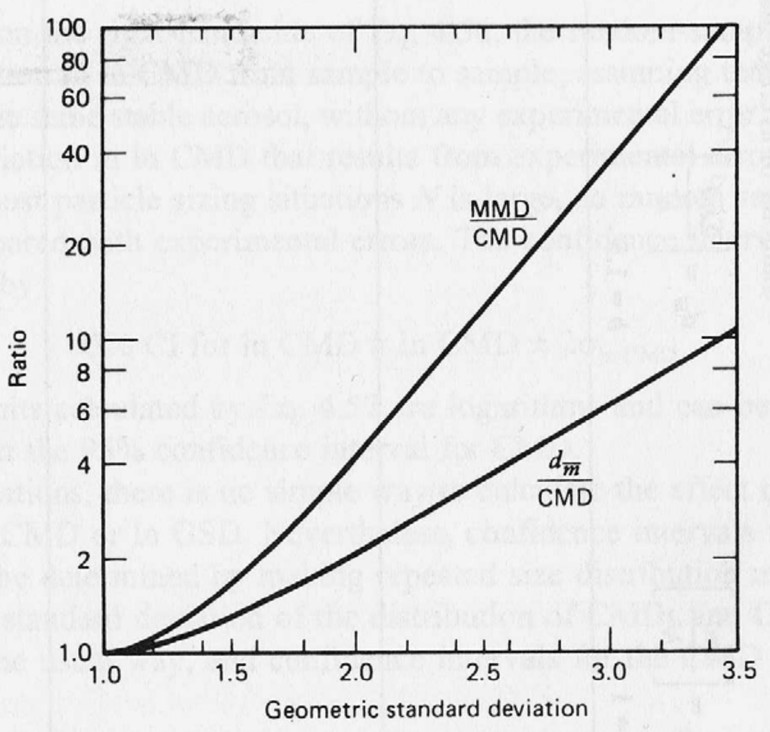


FIGURE 4.16 Ratios of mass median diameter and diameter of average mass to count median diameter versus geometric standard deviation.

Different weighted distributions of atmospheric aerosols

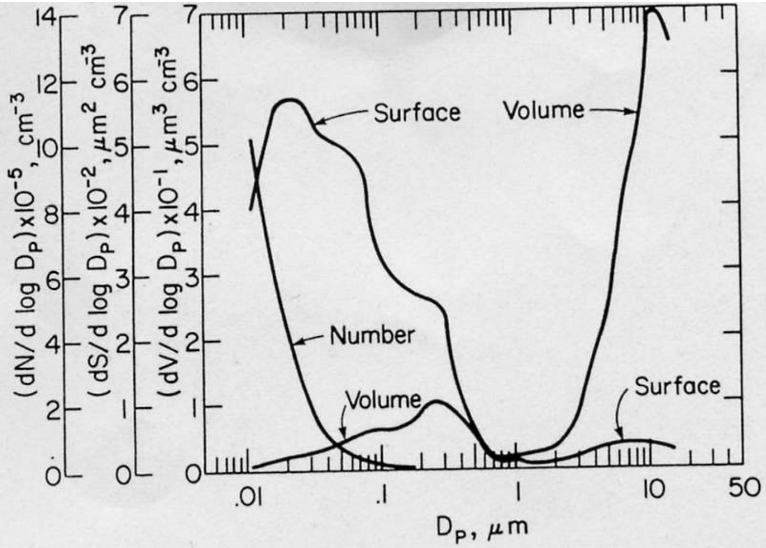


Figure 7.3. Normalized aerosol number, surface area, and volume distributions for the grand average October 1971 measurements at Denver's City Maintenance Yard. (Willeke and Whitby, 1975). Reprinted with permission from Journal of the Air Pollution Control Association.