American Industrial Hygiene Association Journal

ISSN: 0002-8894 (Print) (Online) Journal homepage: https://www.tandfonline.com/loi/aiha20

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To cite this article: C.K. DIU & C.P. YU (1983) Respiratory Tract Deposition of Polydisperse Aerosols in Humans, American Industrial Hygiene Association Journal, 44:1, 62-65, DOI: 10.1080/15298668391404374

To link to this article: https://doi.org/10.1080/15298668391404374

Am. Ind. Hyg. Assoc. J. 44(1):62-65 (1983)

Respiratory Tract Deposition of Polydisperse Aerosols in Humans

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Total and regional deposition of polydisperse aerosols in the human respiratory tract are studied theoretically. The size distribution of the aerosol is assumed to be lognormal. For a given mass median particle diameter, mass deposition fraction is found to vary with the geometric standard deviation of the aerosol. The departure of the deposition pattern in various regions of the respiratory system from that of a monodisperse aerosol is interpreted in terms of the average mobility effect and deposition limitation effect of the polydisperse aerosol together with the sequential filtering effect of the respiratory tract.

Introduction

Environmental aerosols are normally composed of particles of different size, shape and composition. It has been a well established fact that particle size is the single most important characteristic affecting particle deposition in the respiratory tract. This paper deals with the deposition of polydisperse aerosols of uniform composition using a computational model. The size distribution function which characterizes a polydisperse aerosol represents the fraction of particles present in the aerosol as a function of the particle diameter. If the particle concentration is sufficiently low such that particle coagulation is negligible, the deposition of a polydisperse aerosol can be calculated by superimposing the depositions of many monodisperse aerosols, each having different diameter and concentration.

The size distribution function to be adopted for the polydisperse aerosol in this is the lognormal distribution. This is adequate for single component aerosols, although complicated distributions such as trimodal ones for some environmental aerosols have been found.(1)

The geometric standard deviation, σ_g, is defined as the ratio of the 84.13% particle diameter to that of the 50%. The count median diameter ($\bar{D}_c$) and mass median diameter ($\bar{D}_m$) are the particle diameters at 50% number and mass level, respectively. For a lognormal distribution, a simple relationship can be derived from $\bar{D}_m$, $\bar{D}_c$ and σ_g and is given by(2)

$$\ln \bar{D}_m = \ln \bar{D}_c + 3 \ln^2 \sigma_g \qquad (1)$$

It has been suggested by the Task Group on Lung Dynamics(3) that the mass median aerodynamic diameter (MMAD) is an appropriate particle size parameter to use in the lung deposition study since it represents the amount of material deposited on the airway surface. The MMAD is equal to $\bar{D}_m$ for spherical particles of unit density. In this paper, total and regional deposition are determined as functions of $\bar{D}_m$ for various values of σ_g.

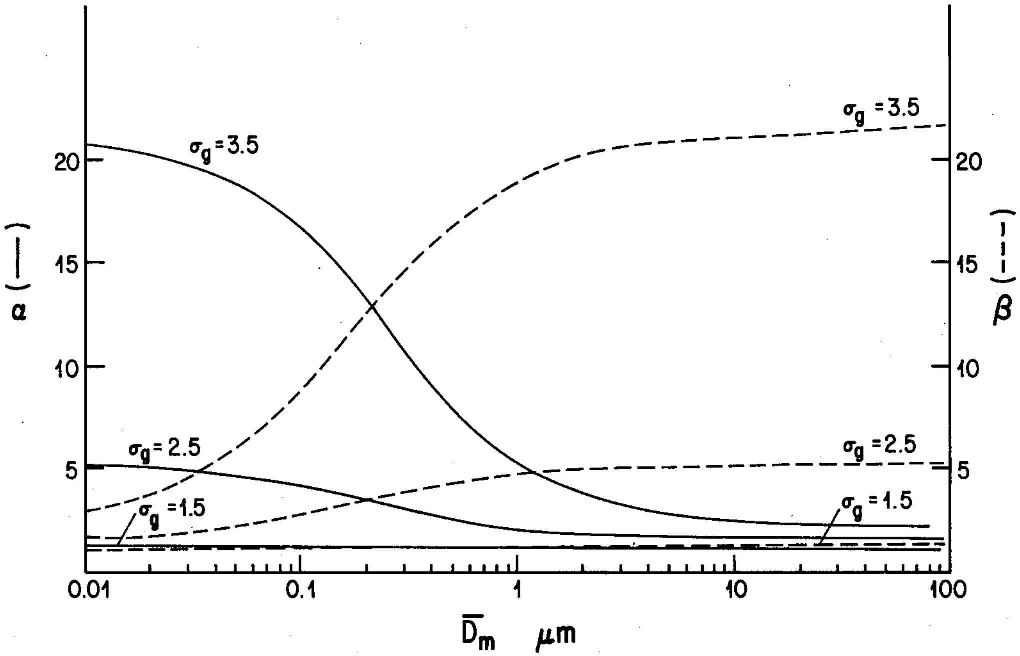

Figure 1 — Values of α (solid lines) and β (dotted lines) versus $\bar{D}_m$ for different σ_g.

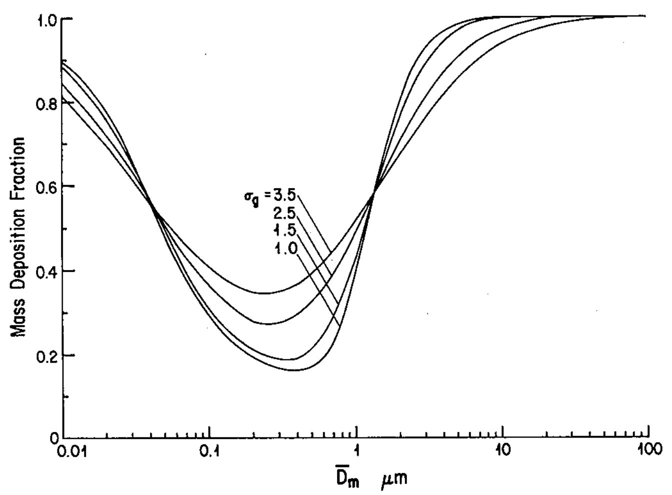

Figure 2 — Total mass deposition fraction at nose breathing calculated for a polydisperse aerosol with different values of σ_g. The breathing condition is 1000 cm^3 tidal volume and 15 resp/min. with equal period for inspiration and expiration and no pause.

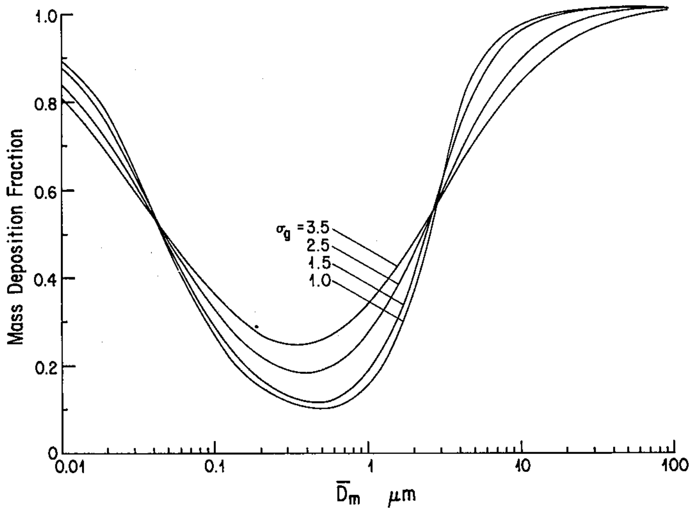

Figure 3 — Total mass deposition fraction at mouth breathing calculated for a polydisperse aerosol with different values of σ_g. The breathing condition is the same as in Fig. 2.

Analysis

A deposition model of monodisperse aerosols was developed by Yu[(4)] and modified by Yu and Diu.[(5)] This model has proved capable of providing accurate prediction of total and regional deposition of inhaled monodisperse aerosols under various breathing conditions. In this study, we generalize the model to polydisperse aerosols.

Assuming a polydisperse aerosol with a lognormal distribution in particle diameter D in the form

$$f(D) = \frac{1}{\sqrt{2\pi}\; n\sigma_g D} \exp\left[-(\ell nD - \ell n\bar{D}_c)^2 / 2(\ell n\sigma_g)^2\right] \qquad (2)$$

Let F(D) be the deposition fraction in the respiratory tract for a monodisperse aerosol with particle diameter D, then the mass deposition fraction for a polydisperse aerosol with size distribution given by (2) can be written as

$$\bar{F}(\bar{D}_c,\sigma_g) = \frac{\int_0^\infty F(D)\, f(D)\, D^3 dD}{\int_0^\infty f(D)\, D^3 dD}$$

$$= \frac{1}{\sqrt{2\pi}\; n\sigma_g} \int_{-\infty}^{\infty} F(e^y) \exp\{-[y - (\ell n\bar{D}_c + 3\ell n^2\sigma_g)]^2 / (2\ell n^2\sigma_g)\} dy \qquad (3)$$

where y = nD.

We may also express $\bar{F}$ as a function of $\bar{D}_m$ and σ_g with the use of (1). Thus, for a polydisperse aerosol, deposition fraction in various regions of the respiratory tract can be computed from (3) at given $\bar{D}_m$ and σ_g once F(D) is known.

In order to gain a better understanding on the deposition result of a polydisperse aerosol, it will be useful to define a mass median particle deposition property in the following manner. Let P(D) be the deposition property of a particle with diameter D. The mass median particle deposition property of a polydisperse aerosol is defined as

$$\bar{P}(\bar{D}_m,\sigma_g) = \frac{\int_0^\infty P(D)\, f(D)\, D^3 dD}{\int_0^\infty f(D)\, D^3 dD} \qquad (4)$$

Thus, $\bar{P}$ has the meaning of average particle deposition property with respect to the particle mass distribution. A large value of $\bar{P}$ will result in a higher mass deposition if no other effects are present.

It has also been established that the deposition of aerosol particles in the respiratory tract is due to three major mechanisms. These are impaction, gravitational settling and Brownian diffusion. The particle deposition properties P(D) associated with these mechanisms are, respectively, particle inertia, settling velocity and diffusion coefficient. The first two quantities are proportional to $D^2C(D)$ while the diffusion coefficient is proportional to C(D)/D in which C(D) is the slip correction factor and is given by the expression

$$C(D) = 1 + 2\frac{\lambda}{D}\left[1.257 + 0.4\exp\left(-\frac{0.55D}{\lambda}\right)\right] \qquad (5)$$

where λ is the mean free path of gas molecules. Using the above relation, we may obtain a ratio for the particle deposi-

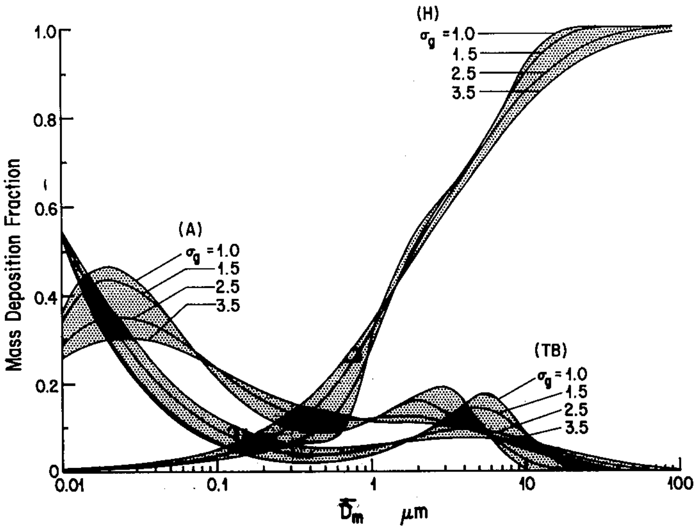

Figure 4 — Regional mass deposition fraction for nose breathing. H is for head deposition, TB for tracheobronchial and A for alveolar.

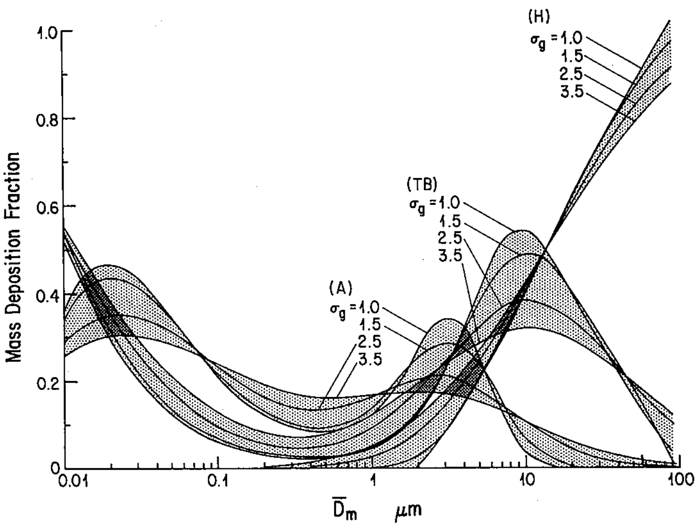

Figure 5 — Regional mass deposition fraction for mouth breathing.

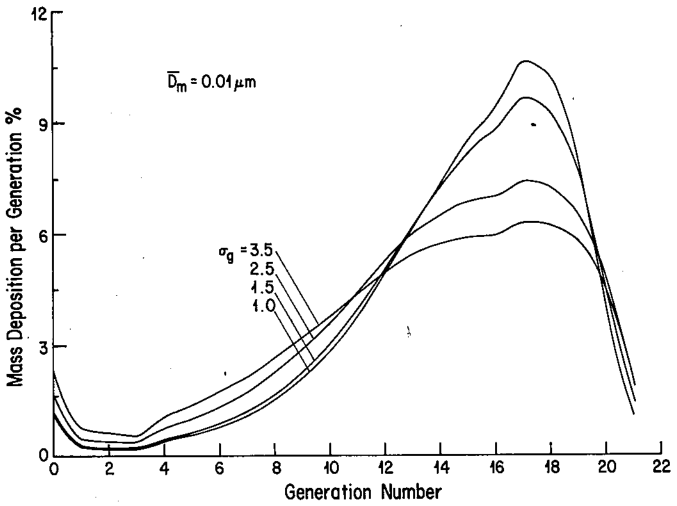

Figure 6 — Mass deposition profile at mouth breathing along airway generation for $\bar{D}_m$ = 0.01 μm and different values of σ_g.

tion property of a polydisperse to a monodisperse aerosol as follows:

$$\alpha = \frac{\bar{P}(\bar{D}_m,\sigma_g)}{\bar{P}(\bar{D}_m,\sigma_g = 1)} = \frac{\int_0^\infty C(D)\, f(D)\, D^5 dD}{C(\bar{D}_m)\bar{D}_m{}^2 \int_0^\infty f(D)\, D^3 dD} \tag{6}$$

for impaction and settling, and

$$\beta = \frac{\bar{D}_m \int_0^\infty C(D)\, f(D)\, D^2 dD}{C(\bar{D}_m) \int_0^\infty f(D)\, D^3 dD} \tag{7}$$

for diffusion.

Figure 1 displays the values of α and β versus $\bar{D}_m$ for various values of σ_g. It shows that α and β are always greater than unity and they increase as σ_g increases. Thus, a higher mass deposition fraction is expected for polydisperse aerosols from this effect, which we shall call the "average mobility effect".

Discussion of Deposition Results

Total mass deposition fraction via nose and mouth breathing has been calculated using (3) for a breathing condition of 1000 cm^3 tidal volume with 15 respirations per minute. The breathing cycle consists of equal duration of inspiration and expiration without pause. Weibel's lung model with initial lung volume of 3000 cm^3 has been used in the calculation. Figures 2 and 3 present the total deposition results of a polydisperse aerosol with unit mass density. For 0.04 μm < $\bar{D}_m$ < 2 μm, it is seen that a higher size dispersion will result in a larger deposition due to the average mobility effect that we noted above. However, as $\bar{D}_m$ becomes larger than 2 μm or smaller than 0.04 μm, Fig. 2 shows that the effect of σ_g on deposition is reversed. This reversal is caused by the fact that total deposition in the respiratory system approaches 100% for a monodisperse aerosol when particle diameter is greater than 10 μm or smaller than 0.005 μm. As the mass median diameter of a polydisperse aerosol is close to these values, deposition is expected to be lower than that of the monodisperse aerosol because there are particles in the polydisperse aerosol which have much lower deposition efficiencies. This

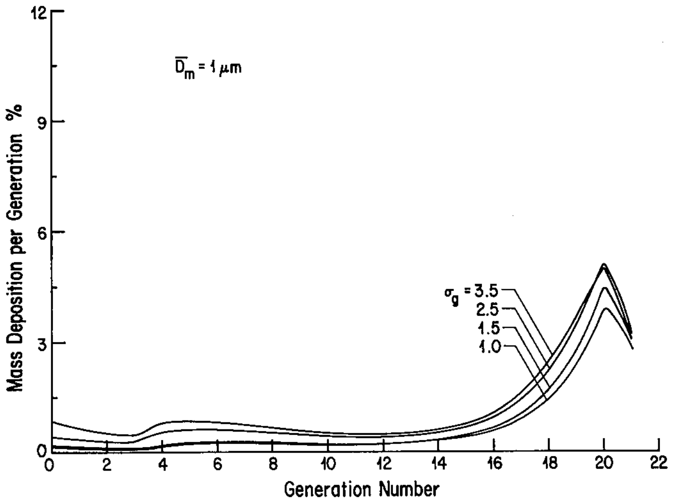

Figure 7 — Mass deposition profile at mouth breathing along airway generation for $\bar{D}_m$ = 1.0 μm and different values of σ_g.

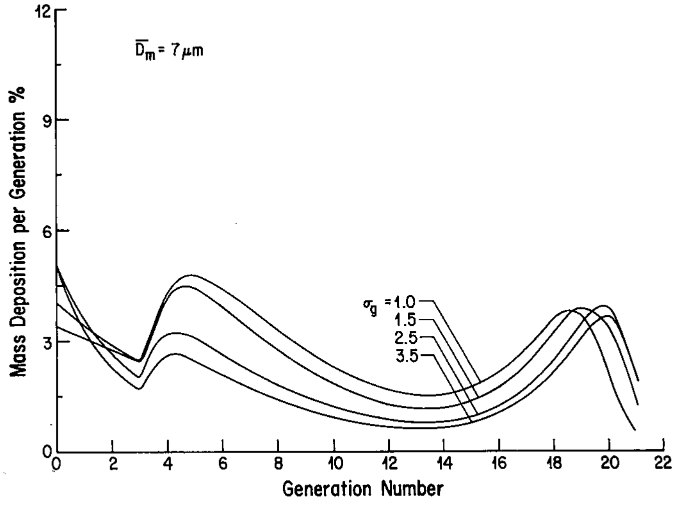

Figure 8 — Mass deposition profile at mouth breathing along airway generation for $\bar{D}_m$ = 7.0 μm and different values of σ_g.

effect, which occurs only when deposition fraction is high will be called the "deposition limitation effect".

For the regional deposition of aerosols, the effect of particle size dispersion is further complicated by the sequential filtering effect of the various compartments in the respiratory system. Figures 4 and 5 show mass deposition in the head, tracheobronchial and alveolar region for nose and mouth breathing respectively. It is seen in Fig. 4 that for $0.01\ \mu m < \bar{D}_m < 0.07\ \mu m$, higher values of σ_g lead to larger tracheobronchial deposition and smaller alveolar deposition. Although the larger tracheobronchial deposition is caused by the average mobility effect, the lower alveolar deposition is due to the deposition limitation effect and the sequential filtering effect because of less aerosol entering the pulmonary region. For $0.07\ \mu m < \bar{D}_m < 1\ \mu m$, all regions exhibit higher deposition with increasing σ_g because the average mobility effect predominates. Between 1 μm and 6 μm, the effect of σ_g on deposition is reversed in all regions as the deposition limitation effect takes over. Beyond 6 μm, the effect on the alveolar deposition again reverses, caused by the sequential filtering effect. The regional deposition of polydisperse aerosols via mouth-breathing follows a similar pattern except the effect of σ_g on the tracheobronchial and alveolar deposition is considerably larger. This is due to lower deposition obtained in the head for mouth-breathing.

The various effects on regional deposition can be further illustrated from Figs. 6 to 8 where deposition profiles along the airway generation are plotted for three characteristic particle diameters. For $\bar{D}_m = 0.01\ \mu m$ which is the diffusion dominated case, a higher σ_g leads to a larger mass deposition in the first 13 airway generations because of the average mobility effect. Beyond the 13th generation, both the sequential filtering and deposition limitation effect predominate and deposition decreases as σ_g increases. At a particle size $\bar{D}_m = 1.0\ \mu m$ for which sedimentation deposition is most important, consistently higher depositions are found in all generations due to the increase of σ_g, as illustrated in Fig. 7. Also, for an impactional particle with $\bar{D}_m = 7\ \mu m$, Fig. 8 shows that the effect of σ_g on deposition is governed by the deposition limitation effect.everywhere except in the first and last two to three generations. Figure 8 also shows that aerosols with larger size dispersion but with same mass median diameter will penetrate deeper into the pulmonary region.

Conclusion

The effect of particle size dispersion of deposition in the respiratory system has been investigated. Predicted total and regional deposition results of a polydisperse aerosol show that they are considerably different from that of a monodisperse counterpart. These differences are explained in terms of average mobility effect, deposition limitation effect, and sequential filtering effect. It has recently been found by Morrow$^{(6)}$ that for $\sigma_g < 2.0$ the mass deposition of a polydisperse aerosol does not deviate profoundly from the value of a monodisperse aerosol. The present results appear to support this conclusion. However, even for small σ_g, the difference in deposition depends upon the mass median diameter of the aerosol and the deposition site, as illustrated in Figures 6 to 8.

Another complication in dealing with the deposition of polydisperse aerosols is that the mobility of large particles ($D > 0.5\ \mu m$) is governed by their aerodynamic diameter while geometric diameter is responsible for diffusion. Thus, for aerosols with different particle mass densities, deposition calculated from (3) will have different results when even $\bar{D}_m$ and σ_g are the same. Nevertheless, because large particles contribute to most of the mass in a polydisperse aerosol, it is reasonable to use aerodynamic diameter to account for this particle mass density effect. Deposition results presented above are therefore valid for aerosols with any particle mass density provided that aerodynamic diameter is used for D.

Experimental determination of particle deposition in the respiratory tract has mostly been conducted for monodisperse aerosols,$^{(7)}$ the present results need to be validated by future experimental studies using polydisperse aerosols.

Acknowledgements

This work was supported by Grant No. ES-02565 from the National Institute of Environmental Health Sciences and from Grant No. OH-00923 from the National Institute for Occupational Safety and Health. We appreciate a discussion with Dr. T.T. Soong.

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25 January, 1982; Revised 8 July, 1982