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TOTAL AND REGIONAL DEPOSITION OF INHALED AEROSOLS IN HUMANS

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Abstract—Total and regional depositions of inhaled aerosols in the human respiratory tract have been calculated for a wide range of particle diameters, particle mass densities, mean flowrates and mean residence times. Good agreement is found with the recent experimental data of Heyder *et al.* (1975, 1980a) and Stahlhofen *et al.* (1980). The dependence of deposition upon particle characteristics and flow pattern is further discussed.

1. INTRODUCTION

In a given respiratory tract, the deposition of inhaled particles depends upon the particle characteristics and the pattern of breathing. Recently, Heyder *et al.* (1975, 1980a) have reported experimental data on total deposition of a spherical, uncharged aerosol of various particle diameters and mass densities under a variety of well controlled breathing conditions. They identified the physical factors responsible for deposition under this condition as being particle diameter, particle density, mean flowrate and mean residence time (Heyder *et al.*, 1980b). They also found a single deposition parameter which is a combination of all physical factors, so that deposition can be expressed as a function of this parameter alone.

In this paper, we shall compare their data with the calculated deposition results obtained from a model we have developed (Yu, 1978; Yu and Diu, 1982). A summary of this model is given in the Appendix. The purpose of comparison is two-fold. First, our deposition model was derived from a simplified respiratory tract model assuming idealized air flow profiles in the airways. Consistency with experimental data will further validate this model so that it may be used with confidence for future deposition predictions. Secondly, although regional deposition was not measured in this experiment, it can be readily determined from the model study. It is then possible to examine how regional deposition varies which each physical factor and how this variation contributes to the observed change in total deposition.

2. PHYSICAL FACTORS

For spherical, uncharged particles, the deposition of particles in the respiratory tract is due to the mechanisms of diffusion, sedimentation and impaction. It is well known that diffusion depends upon the geometrical diameter of the particle d_p, whereas sedimentation and impaction depend upon aerodynamic diameter $\sqrt{\rho} d_p$, where ρ is the mass density. It is also known that while impaction is an instantaneous process governed by the flowrate, diffusion and sedimentation, on the other hand, depend upon the residence time of the particle in the airways. Heyder *et al.* (1980a) standardized the flowrate by defining a mean flowrate at the entry of the respiratory tract to be $Q = (1/T)\int_0^T |\dot{V}|\,dt$, where $\dot{V}$ is the instantaneous volumetric flowrate and T is a single breath duration. Since particles inhaled at the beginning spend more time in the lung than those inhaled at the end of a breath, a mean residence time was also defined by Heyder *et al.* with the expression $\tau = (1/2Q)\int_0^T |V|\,dt$. Thus, deposition of particles will depend upon four physical factors d_p, ρ, Q and τ.

3. COMPARISON OF TOTAL DEPOSITION

In our deposition calculation, the breathing cycle is chosen to consist of a constant flow inspiration, a constant flow expiration of equal duration and no pause. This is consistent with the experimental condition. The lung model used in the calculation is that of Weibel, since it gives a median deposition among all existing models (Yu and Diu, 1982). Figures 1 and 2 show the comparison of the calculated total deposition and experimental data vs aerodynamic particle diameter for two different particle mass densities under two different mouth breathing conditions. The dependence of deposition on particle diameter is well established. There is a minimum deposition near 0.5 μm due to the combined effect of sedimentation and diffusion. This is shown in the figures. However, increasing particle mass density at a given particle diameter will cause an increase in deposition. For aerodynamic

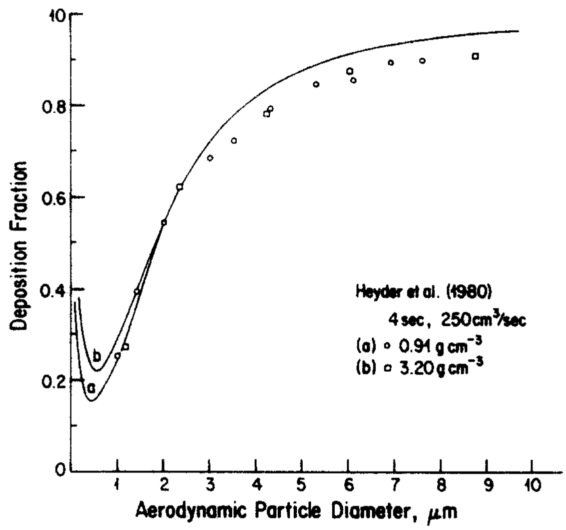

Fig. 1. Total deposition as a function of aerodynamic particle diameter at mouth breathing for $\rho = 0.91$ and $3.20\,g/cm^3$. ($Q = 250\,cm^3/sec$, $\tau = 4\,sec$.) The solid lines are the calculated values.

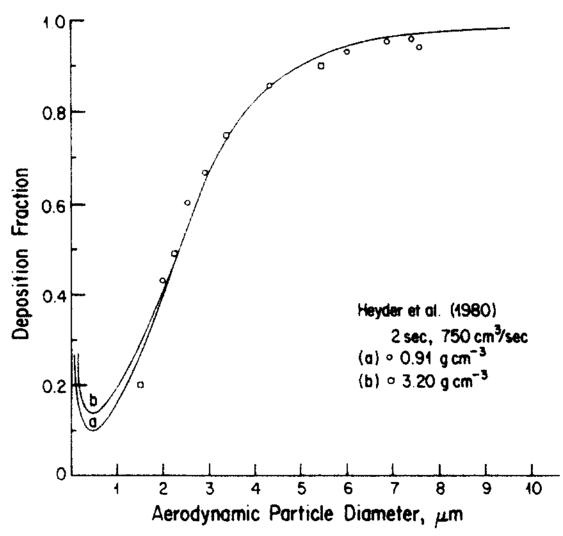

Fig. 2. Total deposition as a function of aerodynamic particle diameter at mouth breathing for $\rho = 0.91$ and $3.20\,g/cm^3$. ($Q = 750\,cm^3/sec$, $\tau = 2\,sec$.) The solid lines are the calculated values.

particle diameters larger than 2 μm, both calculation and measurement find that deposition is a function of a single aerodynamic diameter regardless of mass density. In this case, deposition is dominated by impaction and sedimentation. Below 2 μm, diffusion becomes increasingly important and deposition at a given breathing condition must be expressed as a function of both d_p and ρ.

The effect of flowrate on total deposition is illustrated in Figs. 3 and 4. In Fig. 3, the mean residence time is fixed at 1 sec so that deposition by sedimentation and diffusion is minimal. We see that total deposition increases with flowrate because of the increase of impaction deposition. The calculated results agree reasonably well with the data except for very large particles (> 6 μm), where the calculated values slightly overestimate deposition. When the mean residence time is increased to 2 sec, sedimentation and diffusion become relatively significant and Fig. 4 shows the effect of flowrate on deposition for this case. It is seen that the

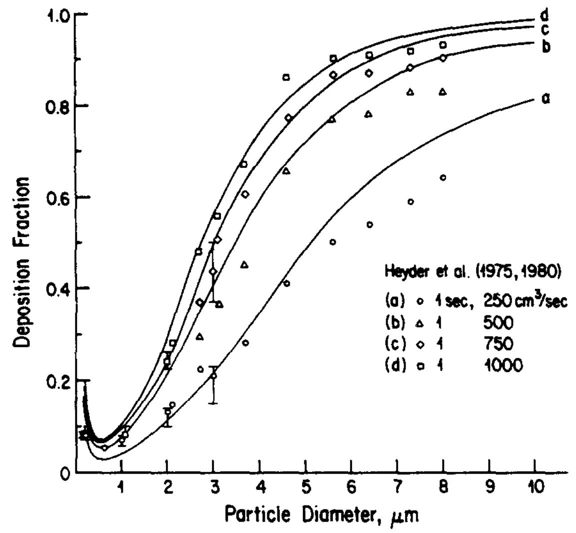

Fig. 3. Total deposition as a function of particle diameter at mouth breathing for various Q at $\tau = 1$ sec ($\rho = 0.91$ g/cm^3). The solid lines are the calculated values.

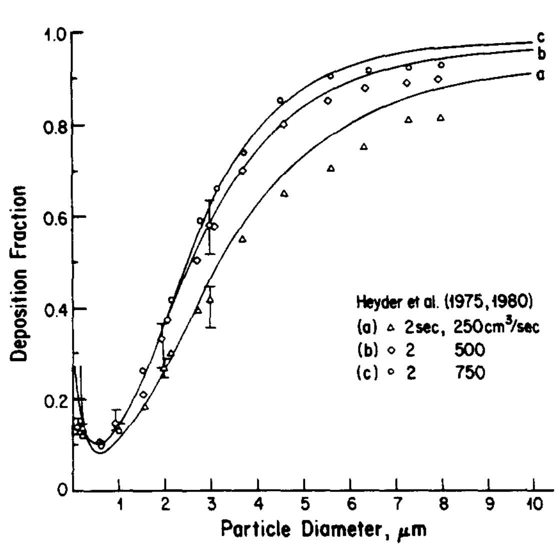

Fig. 4. Total deposition as a function of particle diameter at mouth breathing for various Q at $\tau = 2$ sec ($\rho = 0.91$ g/cm^3). The solid lines are the calculated values.

comparison of calculation and data is improved and the flowrate has a smaller effect on deposition than that shown in Fig. 3.

To gain a further understanding of the flowrate effect, Fig. 5 depicts the calculated deposition for various flowrates at $\tau = 1$ sec. It shows that for $Q > 500\,cm^3/sec$ the increase in total deposition is due to the increase in impaction deposition in the head and tracheobronchial regions. Alveolar deposition in this case remains nearly unchanged since

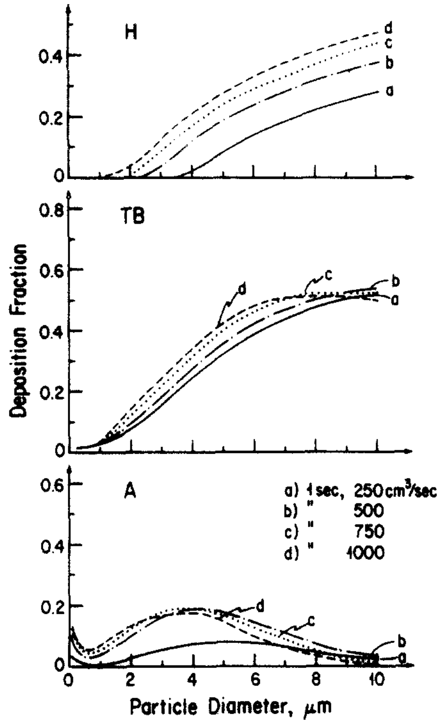

Fig. 5. Calculated regional deposition as a function of particle diameter at mouth breathing for various Q at $\tau = 1$ sec ($\rho = 0.91\ g/cm^3$).

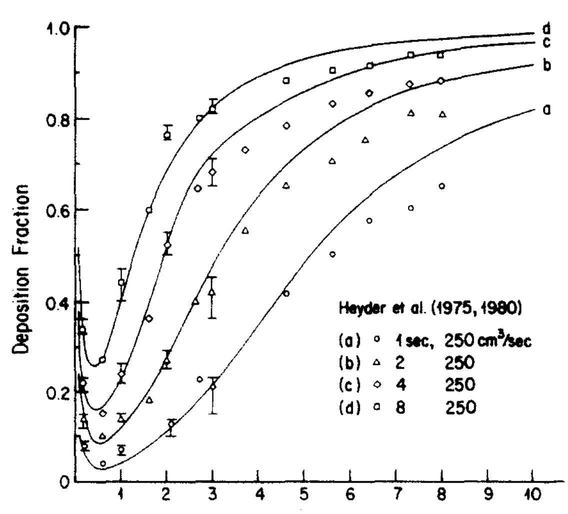

Fig. 6. Total deposition as a function of particle diameter at mouth breathing for various τ at $Q = 250\,cm^3/sec$ ($\rho = 0.91\ g/cm^3$). The solid lines are the calculated values.

deposition in this region is governed by sedimentation and it increases only with the residence time. However, there is a dramatic increase in alveolar deposition when Q increases from 250 to 500 cm^3/sec. This is the tidal volume effect, due to a rapid increase of aerosol entering the alveolar region.

The effect of mean residence time on deposition is caused by the mechanisms of sedimentation and diffusion. Figures 6–8 show the change in deposition with mean residence time at two different flowrates. There is a good agreement between the calculated deposition and data in this case, and the result shows that deposition increases with mean residence time for all flowrates. The calculated regional deposition shown in Fig. 9 illustrates that this increase occurs in the alveolar region, and is due to longer residence time and deeper aerosol penetration.

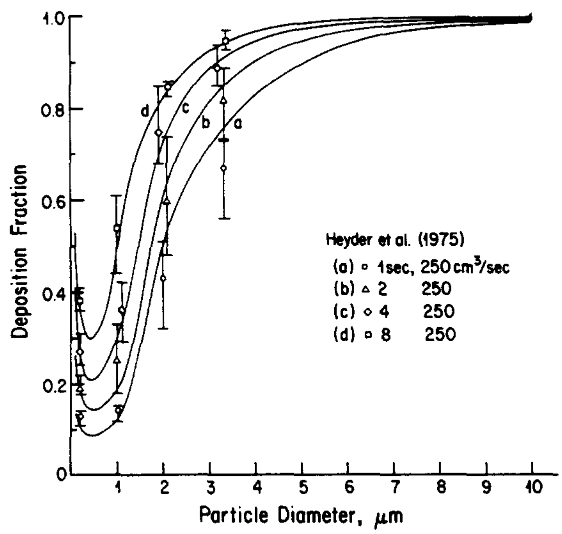

Fig. 7. Total deposition as a function of particle diameter at nose breathing for various τ at $Q = 250 cm^3/sec$ ($\rho = 0.91 g/cm^3$). The solid lines are the calculated values.

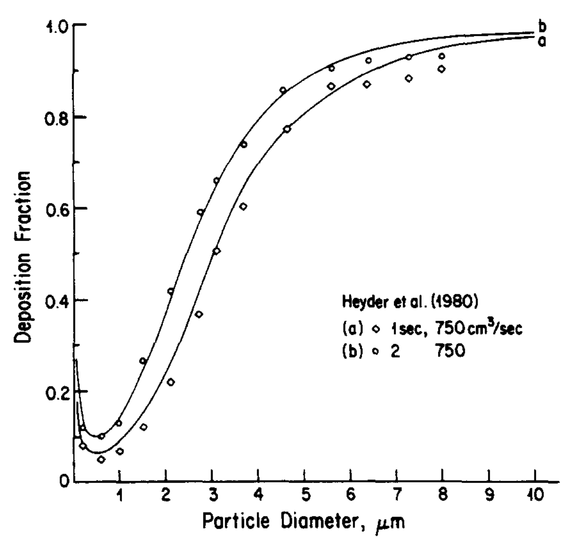

Fig. 8. Total deposition as a function of particle diameter at mouth breathing for various τ at $Q = 750 cm^3/sec$ ($\rho = 0.91 g/cm^3$). The solid lines are the calculated values.

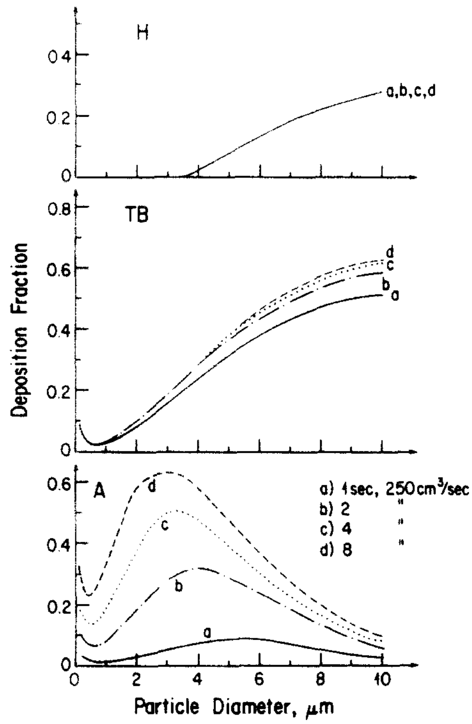

Fig. 9. Calculated regional deposition as a function of particle diameter at mouth breathing for various τ at $Q = 250\,cm^3/sec$ ($\rho = 0.91\ g/cm^3$). The solid lines are the calculated values.

Another way of examining the effects of Q and τ is to vary each of their values but keeping $Q\tau$ = constant. This corresponds to a fixed tidal volume for which the effect of aerosol penetration on deposition is no longer a factor. Figures 10 and 11 are the calculated deposition and experimental data for this case at mouth and nose breathing respectively. As pointed out by Heyder *et al.* (1980a), for particle diameter larger than 1 μm, sedimentation and impaction are the two major deposition mechanisms competing with each other. For example, deposition for 1 μm particles is governed by sedimentation which depends upon τ. A

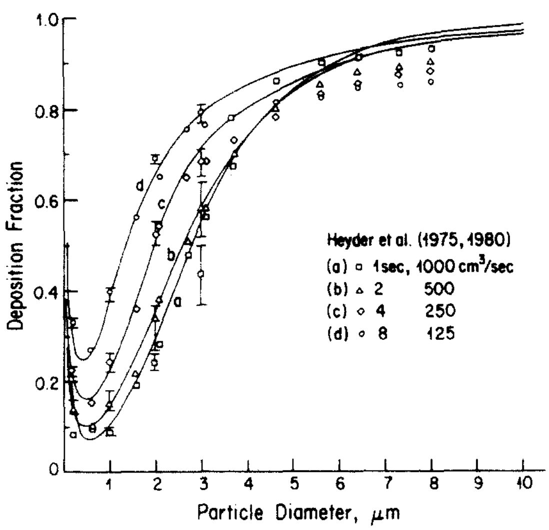

Fig. 10. Total deposition as a function of particle diameter at mouth breathing for $Q\tau = 1000\,cm^3$ ($\rho = 0.91\ g/cm^3$). The solid lines are the calculated values.

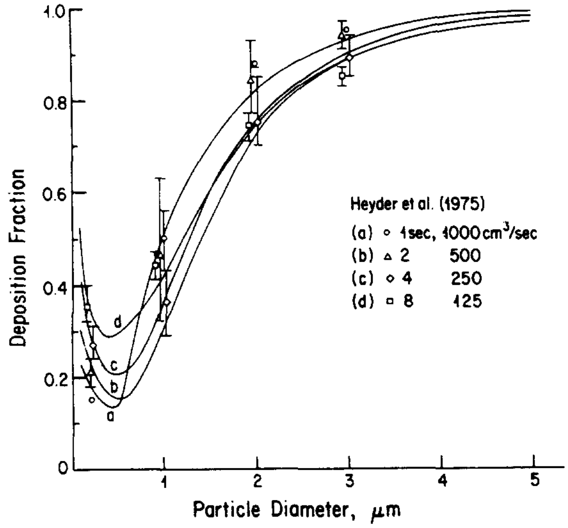

Fig. 11. Total deposition as a function of particle diameter at nose breathing for $Q\tau = 1000\,\mathrm{cm}^3$ ($\rho = 0.91\ \mathrm{g/cm}^3$). The solid lines are the calculated values.

larger value of τ will lead to a higher deposition regardless of flowrate. However, for 8 μm particles for which impaction deposition dominates, a larger Q will leave a larger deposition for all values of τ. There exists a transition particle diameter at which deposition shifts from a sedimentation dominated regime to an impaction dominated one. For mouth breathing, this was found to be about 4 μm by Heyder *et al.* while our calculation shows a value of 6 μm. For nose breathing, impaction is more important and the transition particle diameter decreases to a value of 1 μm as found by both calculation and experiment in Fig. 11. Regional deposition for constant $Q\tau$ product at mouth breathing is also calculated and presented in Fig. 12. It

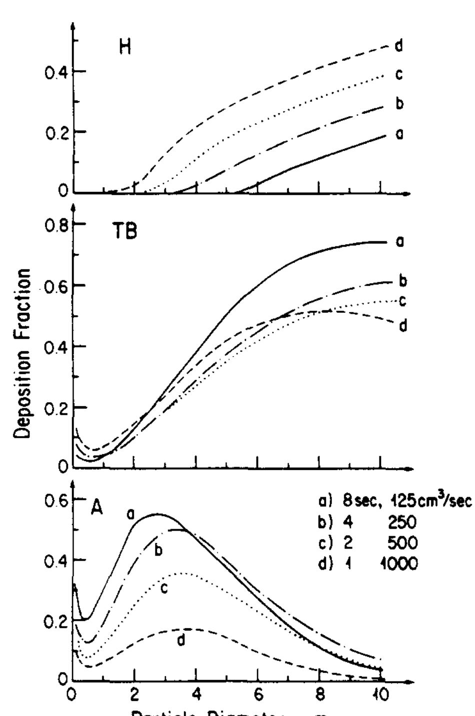

Fig. 12. Calculated regional deposition as a function of particle diameter at mouth breathing for $Q\tau = 1000\,\mathrm{cm}^3$ ($\rho = 0.91\ \mathrm{g/cm}^3$). The solid lines are the calculated values.

shows that high head deposition is always associated with high flowrate, and alveolar deposition increases normally with the mean residence time.

4. COMPARISON OF REGIONAL DEPOSITION

There are not enough data on regional deposition for a well controlled experiment under various conditions of particle mass density, mean flowrate and mean residence time. Recent measurements by Stahlhofen *et al.* (1980) using iron oxide particles tagged with ^{198}Au covered a wide range of particle sizes. Their data are used for comparison with our calculated deposition. The alveolar deposition in this experiment was obtained by back extrapolation in time of particle retention curves, a definition somewhat different from that introduced by Lippmann and Albert (1969) based upon 24 hr activity measurement after inhalation.

The data of Stahlhofen *et al.* show that at mouth breathing, the head and tracheobronchial depositions are insignificant if aerodynamic particle diameter is below 2 μm. Figures 13 and 14 present these data together with the calculated deposition for three subjects at two different breathing conditions. The calculation was based upon a different lung model (Yeh and Schum, 1980), which has the same structure as Weibel's model but with larger tracheobronchial airway dimensions (Yu and Diu, 1982). The agreement between calculation and experiment appears very good although a small tracheobronchial deposition was found from calculation for aerodynamic particle diameter below 2 μm. If Weibel's model is used in the calculation, the tracheobronchial deposition would be even higher. In fact, other deposition data recently obtained by Chan and Lippmann (1980) consistently show a significant tracheobronchial deposition for small particles. Thus, the question of whether or not any deposition occurs in the head and tracheobronchial regions when the aerodynamic particle diameter is below 2 μm remains unanswered at this time.

5. CONCLUDING REMARKS

It has been shown that deposition calculated from our model gives a reasonably accurate estimate of total and regional depositions in the respiratory tract for a wide range of particle diameters, mass densities and breathing conditions. Within the error of intersubject

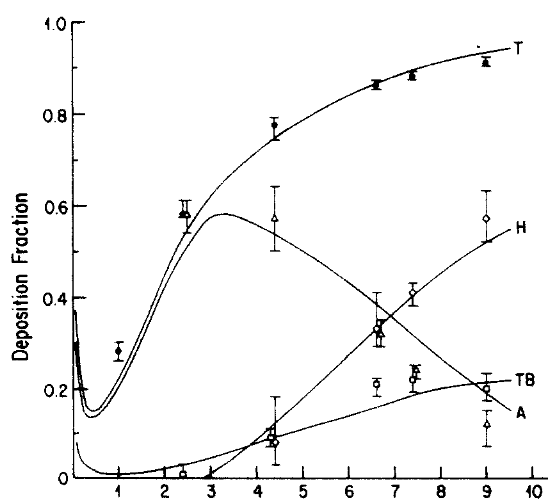

Fig. 13. Regional deposition as a function of aerodynamic particle diameter at mouth breathing for $Q = 250\,cm^3/sec$ and $\tau = 4$ sec. The solid lines are the calculated values for head (H), tracheobronchial (TB), alveolar (A) and total (T) deposition.

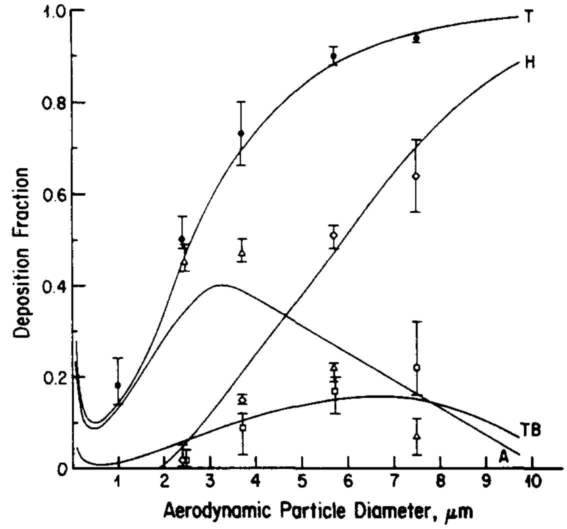

Fig. 14. Regional deposition as a function of aerodynamic particle diameter at mouth breathing for $Q = 750\,\text{cm}^3/\text{sec}$ and $\tau = 2$ sec. The solid lines are the calculated values of head (H), tracheobronchial (TB), alveolar (A) and total (T) deposition.

variability, this model can be used with confidence in predicting particle deposition for the assessment of health hazard.

A more interesting approach in studying particle deposition in the respiratory tract is dimensional analysis. Rather than considering the physical factors discussed earlier, it would be meaningful to consider four independent, dimensionless parameters for the problem as follows:

$$X_1 = \frac{\text{tidal volume}}{\text{FRC}} = C_1 Q\tau, \tag{1}$$

$$X_2 = \frac{\text{stop distance}}{\text{airway size}} = C_2 \rho d_p^2 Q, \tag{2}$$

$$X_3 = \frac{\text{residence time}}{\text{sedimentation time}} = C_3 \rho d_p^2 \tau, \tag{3}$$

$$X_4 = \frac{\text{residence time}}{\text{diffusion time}} = C_4 \frac{\tau}{d_p^2}, \tag{4}$$

where C_1 to C_4 are constants depending upon the airway geometry and the physical properties of the air. The parameter X_1 given by equation (1) is a measure of aerosol penetration in the lung. X_2, X_3 and X_4 are respectively parameters for impaction, sedimentation and diffusion. It can be shown that increasing X_1 to X_4 individually will lead to an increase of deposition, and the experimental results of Heyder *et al.* discussed above can be explained more easily with the use of these parameters.

In principle, it should also be possible to find total and regional depositions as functions of X_1 to X_4. Heyder *et al.* have successfully found a deposition parameter x_M which is a function of d_p, ρ, Q and τ such that total deposition depends only upon x_M. Their approach was based upon data deduction and it can be shown that x_M obtained in this manner does not serve as a useful parameter for regional deposition. The finding of a single deposition parameter for each region remains a challenge for future deposition studies.

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APPENDIX

Yu (1978) proposed a continuous deposition model for inhaled particles in which he derived a partial differential equation for particle concentration C as a function of the airway generation number z and time t. This equation was solved using the method of characteristics. For a respiratory cycle consisting of inspiration and expiration with constant flowrate and equal duration, the solution for C may be cast into the following form.

At inspiration

$$C(z,t) = C_0 \exp\left(-\sum_{j=0}^{J} \eta_j\right) \quad \text{for } z \leqslant z' \tag{A-1}$$

$$C(z,t) = 0 \quad \text{for } z \geqslant z', \tag{A-2}$$

where C_0 is the particle concentration entering the trachea, z' denotes the position of the aerosol front, given by

$$\frac{V_{z'}}{V_l} = \frac{t}{t+\tau} \tag{A-3}$$

and at expiration

$$C(z,t) = C(\xi,\tau) \exp\left(-\sum_{j=z}^{\xi} \eta_j\right) \quad \text{for } z < z' \tag{A-4}$$

$$C(z,t) = 0 \quad \text{for } z > z', \tag{A-5}$$

where ξ is related to z' and t by the expression

$$\frac{V_l - V_{z'}}{V_l - V_\xi} = \frac{\tau}{2\tau - t}. \tag{A-6}$$

In equations (A-3) and (A-6), V_l is the total lung volume at rest, $V_{z'}$ and V_ξ are respectively the accumulated lung volume for the first z' and ξ generations. Also, in equations (A-1) and (A-4), η_j is the combined particle collection efficiency at the jth generation airways, given by

$$\eta_j = \eta_{Ij} + \eta_{Sj} + \eta_{Dj}, \tag{A-7}$$

where η_{Ij}, η_{Sj} and η_{Dj} are respectively contributions from the mechanisms of impaction, sedimentation and diffusion. It has been derived that

$$\eta_{Ij} = 0.768(St_j)\theta_j, \tag{A-8}$$

$$\eta_{Sj} = \frac{2}{\Pi}\left[2\varepsilon_j\sqrt{1-\varepsilon_j^{2/3}} - \varepsilon_j^{1/3}\sqrt{1-\varepsilon_j^{2/3}} + \sin^{-1}\varepsilon_j^{1/3}\right], \tag{A-9}$$

$$\begin{aligned}\eta_{Dj} = 1 &- 0.819\exp(-14.63\Delta_j) - 0.0976\exp(-89.22\Delta_j) \\ &- 0.0325\exp(-228\Delta_j) - 0.0509\exp(-125\Delta_j^{2/3}),\end{aligned} \tag{A-10}$$

for both inspiration and expiration except that $\eta_{Ij} = 0$ at expiration. Here

$St_j = \rho d_p^2 u_j/(9\mu d_j)$,
$\theta_j = l_j/(4d_j)$,
$\varepsilon_j = 3\pi u_g l_j/(16 u d_j)$,
$\Delta_j = D l_j/(d_j^2 u_j)$,

in which

ρ = particle mass density,
d_p = particle diameter,
u_j = air velocity at the jth airway generation,
μ = air viscosity,
u_g = particle settling velocity,
D = particle diffusion coefficient,
l_j = length of the jth generation of airways,
d_j = diameter of the jth generation of airways.

For Weibel's lung model, the fraction of particle deposition in the tracheobronchial region TB and that in the alveolar region A over a respiratory cycle were calculated using the formulas

$$\mathrm{TB} = \frac{1}{Q_0 C_0 \tau} \int_0^{2\tau} \left(\sum_{j=0}^{16} C_j A_j u_j \eta_j \right) \mathrm{d}t \tag{A-11}$$

and

$$\mathrm{A} = \frac{1}{Q_0 C_0 \tau} \int_0^{2\tau} \left(\sum_{j=17}^{23} C_j A_j u_j \eta_j \right) \mathrm{d}t \tag{A-12}$$

in which A_j and C_j are, respectively, the summed cross-sectional area of the airways and particle concentration at the jth generation. It should be pointed out that equations (A-9) and (A-10) were derived for laminar flow and for an average airway inclination angle of $\sin^{-1} \pi/4$. The inclusion of turbulent particle diffusion in equation (A-10) and the use of measured values of inclination angle in equation (A-9) did not lead to any significant change in deposition results.

Particle deposition in the head via mouth breathing was calculated using the empirical formulas derived by Yu *et al.* (1981). These are

$$H = -1.117 + 0.324 \log \frac{\rho d_p^2 Q}{(\mathrm{g}\,\mu\mathrm{m}^2\,\mathrm{sec}^{-1})} \qquad \text{for } \rho d_p^2 Q > 3000\,\mathrm{g}\,\mu\mathrm{m}^2\,\mathrm{sec}^{-1} \tag{A-13}$$

$$H = 0 \qquad \text{for } \rho d_p^2 Q < 3000\,\mathrm{g}\,\mu\mathrm{m}^2\,\mathrm{sec}^{-1} \tag{A-14}$$

and no deposition occurs at expiration.