Prediction of Particle Deposition in Human Respiratory System

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Abstract

Airborne particulate matter has caused growing public concerns with regard to their effect on human health. Knowledge of particle dosage in human bodies is of importance for risk evaluation from exposure to high concentration aerosols. The present study utilizes mathematical models to predict particle deposition in a representative human respiratory system. An anatomical model of the human respiratory system is obtained from available physiological data and morphometric measurements from the literature. The transport models employed include diffusion, gravitational settling, inertial impaction and interception. Deposition calculation has been performed for particle sizes between 0.001 and 10 μm aerodynamic diameter to study the effects of airway regions, exercise levels, functional reserve capacities and genders. The predicted deposition patterns compare satisfactorily well with those from published literature. The effect of different exercise levels, which account for different tidal volumes and breathing rates, exhibits clear differences in deposition while variation in other parameters considered has only a small effect on deposition. For a given breathing condition, submicron particles appear to deposit more and deeper into the airways than super-micron particles.

Keywords: Particle deposition, Human respiratory system, PM_{10}

1. Introduction

Particulate matter has been identified to be one of the major air pollution problems in urban environments in Thailand [1]. Numerous studies in Europe and the USA, e.g. [2, 3], have shown a strong correlation between mortality/morbidity from cardio-respiratory causes and exposure to PM_{10}, defined as particles passing through a size selective inlet with a 50% efficiency cut-off at 10 μm aerodynamic diameter. Those at great risks are infants, children, elderly people and people with chronic respiratory diseases. Thailand's recent study of the relationship between PM_{10} and daily mortality in Bangkok [4] found that a 10-μg/m^3 change in daily PM_{10} is associated with a 1-2% increase in natural death, a 1-2% increase in cardiovascular mortality, and a 3-6% increase in respiratory mortality. Airborne particles can penetrate the human respiratory system deep into the smallest respiratory tracts and parts of the lungs during inhalation and a small fraction deposits on the surface of the airways. In this way, various and potentially hazardous organic and inorganic materials can be introduced into the human body, which may damage the lung tissue and cause cancer. The hazard caused by inhaled particles depends on their chemical composition and on the site at which they deposit within the respiratory system. Information concerning particle deposition in human lungs is of special interest because it is useful for a quantitative risk evaluation from exposure to airborne particles. It is also vital to the effective administration of pharmaceutical aerosols by inhalation to targeted regions of the respiratory tracts. The deposition of particles in the lungs for given exposure conditions depends on data such as ambient concentrations, aerosol properties, and breathing parameters.

There have been many investigations on this subject experimentally and theoretically by various researchers. Some recent reviews have been carried out and reported by Hofmann et al [5], Musante and Martonen [6], and James [7]. Few comprehensive measurements of deposition efficiency in the airways are available in the literature. Existing experimental data often exhibits slight or large differences in deposition efficiency, compared to that predicted by deposition models. In the present study, an attempt has been made to theoretically predict particle deposition in the human respiratory system. The effects of particle size and breathing parameters on deposition efficiency in different regions of the human lung are investigated parametrically.

2. Mathematical Model of Human Respiratory System

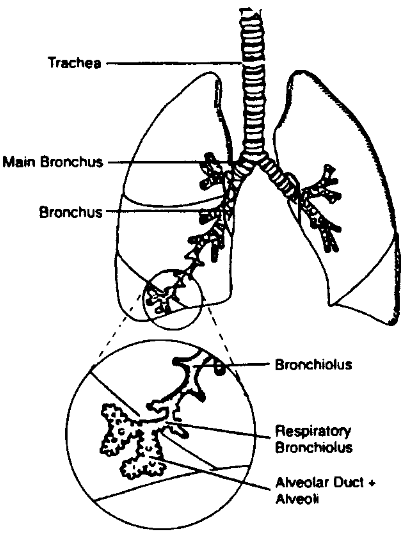

Figure 1. Regions of the respiratory system (adapted from Hinds [8])

The respiratory system can be divided into three regions (figure 1) that are different in structure, airflow patterns, function, retention time and sensitivity to deposited particles. These regions are: (i) the head airway region or the extrathoracic or nasopharyngeal region which includes the nose, mouth, pharynx, and larynx, (ii) the lung airways or tracheo-bronchial region which looks like an inverted tree, with the trachea subdividing into smaller and smaller branches and (iii) the pulmonary or alveolar region where gas exchange takes place [8]. To calculate the fraction of inhaled particles deposited within the respiratory system, it is necessary to adopt a simplified geometrical model of airway size, shape and branching.

2.1 Airway dimensions

There are several existing morphometric models for adult lungs which are derived from morphometric measurements of a few or several individual lung casts. One of the most widely used lung models for the dimension of diameters and lengths of the airways is that provided by James [7], adopted from Wiebel [9], Yeh et al [10] and Phalen et al [11], for generation 0-15, and Haefeli-Bleuer and Weibel [12] for generation 16-23, and is shown in table 1.

Airway generations	Diameter (mm)	Length (mm)
	Trachea	
0	16.5	91.0
	Bronchi	
1	12.0	38.0
2	8.5	15.0
3	6.1	8.3
4	4.4	9.0
5	3.6	8.1
6	2.9	6.6
7	2.4	6.0
8	2.0	5.3
9	1.6	4.4
10	1.3	3.7
	Bronchioles	
11	1.1	3.2
12	0.86	2.7
13	0.71	2.2
14	0.59	1.8
15	0.50	1.6
	Bronchioles to Alveoli	
16	0.50	1.33
17	0.49	1.12
18	0.40	0.93
19	0.38	0.83
20	0.36	0.70
21	0.34	0.70
22	0.31	0.70
23	0.29	0.67

Table 1. Model of average airway dimensions

These linear dimensions are scaled to a normal functional reserve capacity (FRC) of 3300 and 2700 mL for adult male and female, respectively, using a commonly applied linear scaling procedure which is based on the assumption that all linear dimensions (diameter and length) vary with the cube root of the total lung volume or functional reserve capacity. It is also assumed that airway dimensions do not vary during inhalation and exhalation.

2.2 Number of airways

An adult's lung has a symmetrical branching airway structure similar to Weibel's model [9]. The number of airways at generation i, N_i, is;

$$N_i = 2^i \qquad \text{for} \quad 0 \leq i \leq 22$$

$$N_{23} = N_r - 2^{22} - 2^{21}$$

where N_r is the total number of airways of the last three airway generations which is about 14.7 million for a fully grown adult [13].

3. Particle Deposition Models

Deposition efficiency is defined as the ratio of the difference between inlet and outlet particle concentrations to the inlet particle concentration. Here, particles striking the airway surface are assumed to adhere (no bouncing). Deposition of particles in the human respiratory airways occurs by Brownian diffusion, gravitational settling, inertial impaction and interception. The first three physical mechanisms depend on the aerodynamic behavior of particles, whereas the last one depends on particle geometry. It is generally assumed that airflow in the small airways is fully developed laminar, disregarding modification of the primary flow profile by the complex geometry at the bifurcation zone. In the upper airways, the main mechanisms are, diffusion for small particles (diameters < 0.5 μm) and impaction for large particles. Deposition by impaction is significant at high flow rates. In the lower part of the lung, diffusion and gravitational settling become dominant for small and large particles, respectively. Deposition mechanisms have been studied by [13, 14, 15, 16] and the mathematical expressions are given below.

3.1 Diffusion

An expression for the deposition efficiency of particles by diffusion for fully developed laminar flow in a cylindrical tube is as follows:
for $\Delta > 0.0055$

$$\eta = 1 - 0.819\exp(-14.642\Delta) - 0.0975\exp(-89.25\Delta) - 0.0325\exp(-288\Delta)$$

for $\Delta < 0.0055$

$$\eta = 6.461\Delta^{2/3} - 4.80\Delta$$

where
$\Delta = LD_f/(D^2u)$ in which L and D are the airway length and diameter, respectively, u is the air velocity in the airway and $D_f = CkT/(3\pi\mu d)$ is the diffusion coefficient with k being the Boltzmann constant, T the absolute temperature, μ the air viscosity, Cunningham correction factor, $C = 1 + Kn[1.257 + 0.40\, e^{(-1.10/Kn)}]$ in which Knudsen number, $Kn = 2\lambda/d$, λ is the gas mean free path and d is the particle diameter. The above expression is applicable for both inspiration and expiration. During pause, or breath holding, the expression for diffusion efficiency is

$$\eta = 1 - \sum_{i=1}^{3} \frac{4}{k_i^2}\exp(-k_i^2\tau_d) - (1 - \sum_{i=1}^{3}\frac{4}{k_i^2})\exp\left[\frac{-4\tau_d^{1/2}}{\pi^{1/2}}(1 - \sum_{i=1}^{3}\frac{4}{k_i^2})\right]$$

where
$\tau_d = 4D_f\tau/(D^2)$ in which τ is the breath holding time, and k_1, k_2 and k_3 are the first three roots of the Bessel function of the zeroth order,

$$J_0(k) = 0$$

3.2 Gravitational settling

For a system with laminar flow in a cylindrical tube, the gravitational deposition efficiency is

$$\eta = \frac{2}{\pi}\left(2\varepsilon\sqrt{1-\varepsilon^{2/3}} - \varepsilon^{1/3}\sqrt{1-\varepsilon^{2/3}} + \sin^{-1}\varepsilon^{1/3}\right)$$

where
$\varepsilon = 3\pi u_s L/(16uD)$ and $u_s = gC\rho d^2/(18\mu)$ is the particle settling velocity, ρ is the particle density. The above expression is applicable for

both inspiration and expiration whereas the following is applicable during pause:
for $0 < \tau_s < 1$

$$\eta = 1.1094\tau_s - 0.2604\tau_s^2$$

for $\tau_s > 1$

$$\eta = 1 - 0.0069\tau_s^{-1} - 0.0859\tau_s^{-2} - 0.0582\tau_s^{-3}$$

where $\tau_s = u_s\tau/D$

3.3 Inertial impaction

Inertial impaction of particles occurs primarily near the bifurcations.

$$\eta = 0.768(St)\ \ \theta$$

where
$St = C\rho d^2 u/(9\mu D)$ is the particle Stokes number, and $\theta = L/(4D)$ is the bend angle. This is for inspiration only since there is no impaction during expiration and pause.

3.4 Interception

In a laminar flow, the deposition efficiency by direct interception at an airway bifurcation during inspiration for a spherical particle is

$$\eta = \frac{8}{3\pi}\left(\frac{d}{D} - \frac{d^3}{8D^3}\right)$$

with no interception during expiration and pause.

4. Calculation of Deposition Efficiency

4.1 Breathing conditions

Deposition calculations have been performed for a variety of monodispersed particles, ranging from 0.001 to 10 μm for adults at three levels of exercise: sitting, light exercise, and heavy exercise. Breathing parameters used in the calculations are given in table 2, similar to that in Hinds [8]. The respiratory cycle adopted in this work is an idealistic one. It is assumed to consist of a constant flow of inhalation, pause or breath holding, and a constant flow of exhalation with corresponding period fractions equal to 43.5, 5.0 and 51.5 % respectively. For a similar lung structure, parametric studies of different functional reserve capacity and gender on tracheo-bronchial deposition are carried out. The baseline deposition case is designated to be that of an adult male at rest or sitting. The air temperature as well as properties such as viscosity, and density are taken at standard conditions. Density of particles is assumed to be 1000 kg/m^3 for a unit density sphere. The particle characteristics are representative of typical ambient particulate matter. In this study, inhalability or efficiency of entry of particles into the nose or mouth is also taken into account. Further details can be found in Hinds [8].

In this study, particle penetration or the fraction of particle penetrating through each airway has been calculated as the product of the fractions penetrating the particular airway due to each individual mechanism. Deposition has been calculated by subtraction of particle penetration from unity (η = 1 – penetration). Total and regional depositions are estimated by taking into account particle deposition in all corresponding airway generations. It should be noted that calculation is carried out from generation 0 (trachea) to generation 23, hence, neglecting the effect due to headway or nasopharyngeal region. Deposition is normalized to the number of particles entering the trachea.

	Functional reserve capacity (mL)	Breathing frequency (min^{-1})	Tidal volume (mL)
Female			
sitting	2700	14	460
light exercise	2700	21	990
heavy exercise	2700	33	1360
Male			
sitting	3300	12	750
light exercise	3300	20	1250
heavy exercise	3300	26	1920

Table 2. Human respiratory parameters

4.2 Results and discussion

Effect of airway region and particle size

Figure 2 shows deposition efficiency of monodispersed particles, if they are available, in each region of the airways, starting from trachea

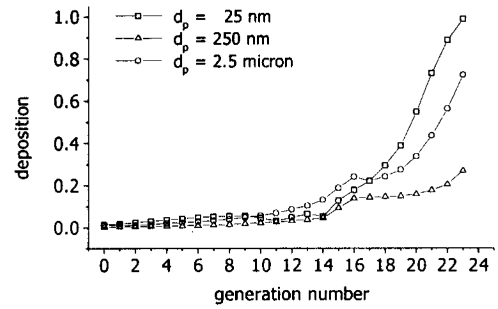

Figure 2. Variation of particle deposition patterns in different airway generations of representative adult male lung under resting conditions for three particle sizes.

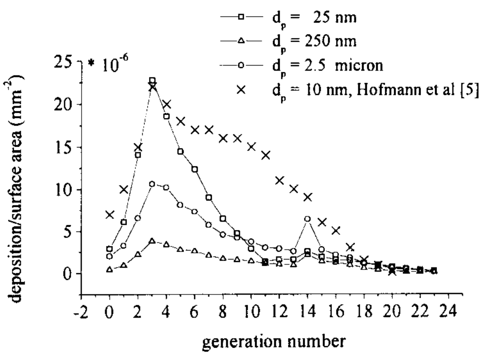

Figure 3. Variation of deposition per unit surface area with the airway generation number in representative adult male lung under resting conditions for four particle sizes

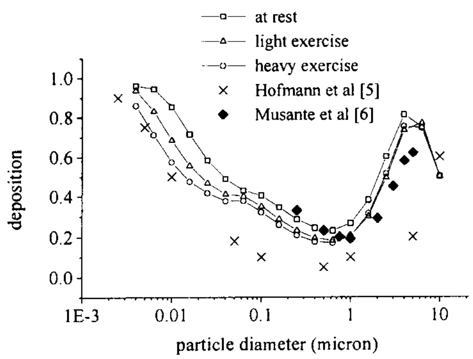

Figure 4. Tracheo-bronchial deposition under resting conditions as a function of particle diameter for three different exercise levels

(generation 0) to transitional bronchioles-alveolar ducts (generation 23) for three different particle aerodynamic diameters for an adult male at rest (750 mL tidal volume, 12 breaths per minute).

It was found that, if particles of these sizes (25 nm, 250 nm and 2.5 μm) are available in the inspiratory flow and reach every airway generation considered, the large fraction is expected to deposit in pulmonary regions. This is because deeper into the lung, airway size decreases. Airways are divided and branched, and so is the inspiratory flow. This results in an extremely slow flow, hence, high residence time and tendency for particles to deposit within bronchial and pulmonary regions. Nonetheless, when deposition rate per available surface area in each airways region, which may be more appropriate in terms of risk assessment (shown in figure 3) is considered instead, it can be seen that deposition in tracheo-bronchial region becomes more significant than that in the pulmonary region. Also plotted in figure 3 are results from Hofmann et al [5] for a 10 nm particle. A similar trend to the calculated results can be clearly observed. Data is mixed 10nm>25nm>2500nm.250nm from fig.3

Effect of breathing behavior

Figure 4 shows variation of deposition with particle diameter for three different typical exercise levels as observed in daily life. The tidal volume is varied over a range from 750 mL to about 2000 mL and the breathing frequency varies over a range from 12 to 20 per minute. The curves show the proportion of deposition calculated to occur in the tracheo-bronchial region. It was found that almost all ultrafine particles (< 0.05 μm diameter) are deposited in the bronchi, as a result of diffusion and a large fraction of supermicron particles are deposited due to the effect of gravitational settling. The curves also show a minimum at particle size around 0.5 μm. It was also found that fractional deposition under resting conditions is higher than that under heavy exercise conditions up to about 20% for each breathing cycle. This may be due to the fact that residence time of particles spent in the respiratory tracts during resting conditions is slightly longer than that during heavy exercise conditions. Also shown in figure 4 is the comparison between the results with those from Hofmann et al [5] and Musante and

Martonen [6] for similar conditions. The calculated results are found to be in qualitative hot with Musante agreement with data from the published literature.

Effect of lung functional residual capacity

The fractions of particles deposited are shown as a function of particle diameter for different values of FRC in figure 5. It was found that there is no significant shift in deposition when the FRC increases from 2300 mL to 4300 mL, contrary to Yu's results [15] which exhibit a decrease in fractional deposition as the FRC increases. The indifference in deposition may be due to identical values of tidal volume and breathing frequency in each FRC used. Changes in airway dimensions as a result of scaling procedure for each FRC appear not to have a significant effect on deposition.

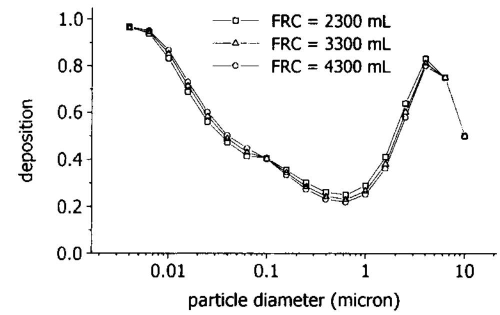

Figure 5. Tracheo-bronchial deposition under resting condition as a function of particle diameter for three different functional reserve capacities (FRC)

Effect of gender

The influence of gender or sex has also been studied. Lung airway dimensions for male and female adults differ. They also have different breathing characteristics for similar levels of exercise. Deposition of particles in representative male and female respiratory systems under resting conditions is illustrated in figure 6. The proportion of particle deposition for both genders under the same breathing conditions is similar, contrary to expectations.

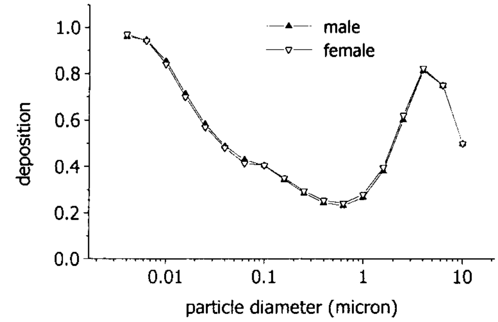

Figure 6. Tracheo-bronchial deposition under resting conditions as a function of particle diameter for male and female respiratory tracts

5. Concluding Remarks

The models described in this work are examples of the application of the currently available knowledge on particle deposition to a practical engineering problem. Calculation of particle deposition in the human respiratory system has been performed in this study. A lung model and expressions for particle transport from the literature have been used. For different airway generations, particle aerodynamic sizes, exercise levels, lung volumes and human genders, deposition efficiencies have been evaluated. The comparison with the deposition data from the literature by Hofmann et al [5] and Musante and Martonen [6] shows reasonably agreement. Slight discrepancies observed may be due to the use of different lung models and different mathematical expressions and assumptions.

Also, in this study, a particle clearance mechanism has not been taken into account. However, they show applicability of the models at a level sufficient for practical purposes. It should be noted that realistic airway geometry and breathing patterns are normally complex and irregular. The analysis presented here is relatively simple and is intended to demonstrate that reasonable predictions of particle deposition in human lungs can be obtained. It can, therefore, be a useful tool for the estimation of particle deposition rates.

6. Acknowledgement

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