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COMPARISON OF COMPUTED LUNG DEPOSITION DATA WITH EXPERIMENTAL RESULTS

VERGLEICH VON BERECHNETEN LUNGENDEPOSITIONSDATEN MIT EXPERIMENTELLEN ERGEBNISSEN

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Abstract

Deposition fractions of inhaled particles predicted by different computational models vary with respect to physical and biological factors and mathematical modeling techniques. These models must be validated by comparison with published experimental data. Experimental data supplied by different deposition studies with surrogate airway models or lung casts have been employed in this study to validate the stochastic deposition model IDEAL at the airway generation level. Furthermore, different analytical equations derived for the three major deposition mechanisms, namely diffusion, impaction and sedimentation have been applied to different cast or airway models to investigate their effect on calculated particle deposition fractions. From this comparative study it can be concluded that structural differences of lung morphologies among different individuals seem to be responsible for the apparent variability in particle deposition in each generation. The use of different deposition equations yields varying deposition results, caused primarily by (i) different lung morphometries employed in their derivation, (ii) the choice of the central bifurcation zone geometry, and (iii) the assumption of specific flow profiles.

Keywords: Bronchial airway models, lung casts, particle deposition equations, experimental studies

Zusammenfassung

Die Berechnung der Deposition inhaliertes Teilchen mit verschiedenen Depositionsmodellen hängt sowohl von physikalischen und biologischen Faktoren, als auch von mathematischen Modellierungsmethoden ab. Die Validierung dieser Modelle erfolgt durch den Vergleich der berechneten Werte mit vergleichbaren experimentellen Daten. In dieser Studie wurden experimentelle Ergebnisse der Deposition in einzelnen Generationen in Luftwegsmodellen und Lungenabgüssen mit den Berechnungen mit dem stochastischen Depositionsmodell IDEAL verglichen. Weiters wurde die Abhängigkeit der Luftwegsdeposition von

verschiedenen analytischen Formeln für die drei wichtigsten Depositionsmechanismen, nämlich Diffusion, Impaktion und Sedimentation, untersucht. Zusammenfassend kann gesagt werden, dass strukturelle Unterschiede in der Lugenmorphologie verschiedener Personen die Hauptursache für die beobachtete Variabilität in den einzelnen Generationen sind. Weiters führt die Verwendung verschiedener Depositionsformeln zu unterschiedlichen Depositionsergebnissen. Die wichtigsten Faktoren dafür sind (i) die spezifische Lungengeometrie bei ihrer theoretischen Ableitung, (ii) die Wahl der Geometrie von Luftwegsverzweigungen, und (iii) die Annahme spezifischer Strömungsprofile.

Schlüsselwörter: Bronchiale Luftwegsmodelle, Lungenabgüsse, Depositionsgleichungen, experimentelle Studien

1. Introduction

Various modeling techniques have been applied to predict particle deposition fractions throughout bronchial and alveolar airway generations. However, deposition fractions predicted by different deposition models vary with respect to physical (fluid dynamics of the inhaled air) and biological (lung morphology and respiratory physiology) factors as well as mathematical modeling techniques. Therefore, it is necessary to validate simulated deposition fractions with experimental data for specified aerosol parameters at defined flow rates.

Three-dimensional (3D) radionuclide imaging provides detailed information on the distribution of inhaled aerosol within lung airways. Analysis of the data can provide estimates of the deposition per airway generation. FLEMING et al. (1995, 2006) used the Single Photon Emission Computed Tomography [SPECT] and the Positron Emission Tomography [PET] techniques to assess the deposition among bronchial and pulmonary airways. KIM et al. (1996, 1999, 2005, 2006) determined regional and total deposition of inhaled particles in human lungs by the serial bolus delivery method. Similarly, experimental deposition data supplied by deposition studies in surrogate airway models or lung casts of upper bronchial airway generations (SCHLESINGER et al. 1982, GURMAN et al. 1984, COHEN et al. 1990, SMITH et al. 2001) are available for comparison purposes on the airway generation level.

Advantages of conducting *in vitro* aerosol deposition studies with replica casts and airway models include the accurate control of airflow rates, the ability to precisely measure deposition efficiencies, and the assessment of local deposition distributions and "hot spots". Therefore it is important to know the differences in deposition patterns between modeling and experiments in realistic airway castes to understand the apparent discrepancies in deposition fractions.

In a previous study, HOFMANN et al. (1998, 2002) investigated the effect of intersubject variability of airway dimensions in the thoracic region on total deposition fractions (TDF). In this paper we compare the experimental deposition measurements in different human lung airway casts with the stochastic modeling predictions using the Monte Carlo deposition code IDEAL (KOBLINGER & HOFMANN 1990, HOFMANN & KOBLINGER 1990) on the generation level (up to 7 generations). Lung geometries obtained from lung casts were implemented into the IDEAL code to study their effect on particle deposition. Secondly we investigate the effect of different deposition equations for diffusion, sedimentation and impaction on particles deposition.

2. Materials and Methods

In this study, deposition was calculated for the first 7 tracheobronchial (TB) airway generations (trachea = generation 1). Deposition fractions for inhaled unit density monodisperse particles with diameters of 0.04, 0.20 and 3 μm were calculated to cover diffusion, sedimentation and impaction regimes. Deposition was calculated for uniform inspiratory flow rates of 15 and 34 l min^{-1} , splitting symmetrically between the daughter airways. Deposition fractions are based upon the number of particles entering the first generation.

To investigate the effect of different deposition equations on deposition, several analytical equations derived for the major deposition mechanisms, i.e. diffusion, sedimentation and impaction, were implemented into the IDEAL code. These deposition equations, listed in the following sections, were used to determine the deposition fractions for each cast geometry and the stochastic lung geometry as well.

2.1 Experimental data of different lung casts

Several geometric lungs models of the human respiratory system have been employed to calculate the deposition of ambient aerosols (WEIBEL 1963, SOONG et al. 1979, YEH & SCHUM 1980, KOBLINGER & HOFMANN 1990) leading to a range of deposition fractions. Thus different casts were produced to obtain more reliable experimental information on deposition and hence dose distribution in the human lung. Unfortunately, such experimental data are limited to the upper bronchial airways due to technical limitations in cast production. The various cast measurement studies, which were implemented into IDEAL to study their effect on deposition, will be discussed below. The characteristic dimensions obtained from these studies are shown in Figure 1.

Cast prepared from autopsy specimens of the human TB tree for the study of particle deposition was developed by SCHLESINGER and LIPPMANN (1972) and SCHLESINGER et al. (1982), using a hollow silicon rubber cast (normal lung of a 54 y old woman). Deposition studies were carried out for coarse particles (2.5–8 μm).

The airways were assigned to generation numbers according to the lung model of WEIBEL (1963). The laryngeal jet was considered in these experiments to simulate the effect of the larynx on deposition in for the first few generations.

COHEN and ASGHARIAN (1990) carried out deposition experiments in replicate hollow casts of the upper airways of a 34 y old man TB tree using ultrafine particles ($<0.2 \mu\text{m}$) for a variable larynx. The casting process and replicate production in that study were carried out using the methods described by SCHLESINGER et al. (1982). The length and diameter of the airways were smaller than those of YEH and SCHUM (1980). The airways were assigned again to generation numbers according to WEIBEL'S (1963) model.

A silicon rubber cast of the respiratory tract was made by YAMADA et al. (1994) for a normal human adult. The model consisted of the trachea and the main bronchi with branching generations from 4 to 10 and each individual airway segment was assigned a unique binary identification number using the system designed by RAABE et al. (1976). This study was conducted for ultrafine particles below $0.1 \mu\text{m}$ where diffusion is the dominant deposition mechanism.

Replicate casts of the larynx and five to eight generations of a 23 y old male human TB tree, obtained by autopsy, were produced by SMITH et al. (2001). The production mold for this cast was made of silicone rubber. A light coat of oil was applied to the interior of the models to simulate the mucous lining of the TB tree. The individual airways were identified using the numbering scheme proposed by RAABE et al. (1976). That study was conducted to determine the deposition patterns of nanometer-sized particles in the TB airways. The results obtained by SMITH et al. (2001) verified the experimental findings of COHEN and ASGHARIAN (1990), showing higher diffusional deposition in cylindrical tubes predicted by theory.

The anatomical data (airways dimensions and branching angles) of the above mentioned casts were employed for the calculation of deposition fractions for both ultrafine and fine particles at flow rate of 15 and 34 l min^{-1} .

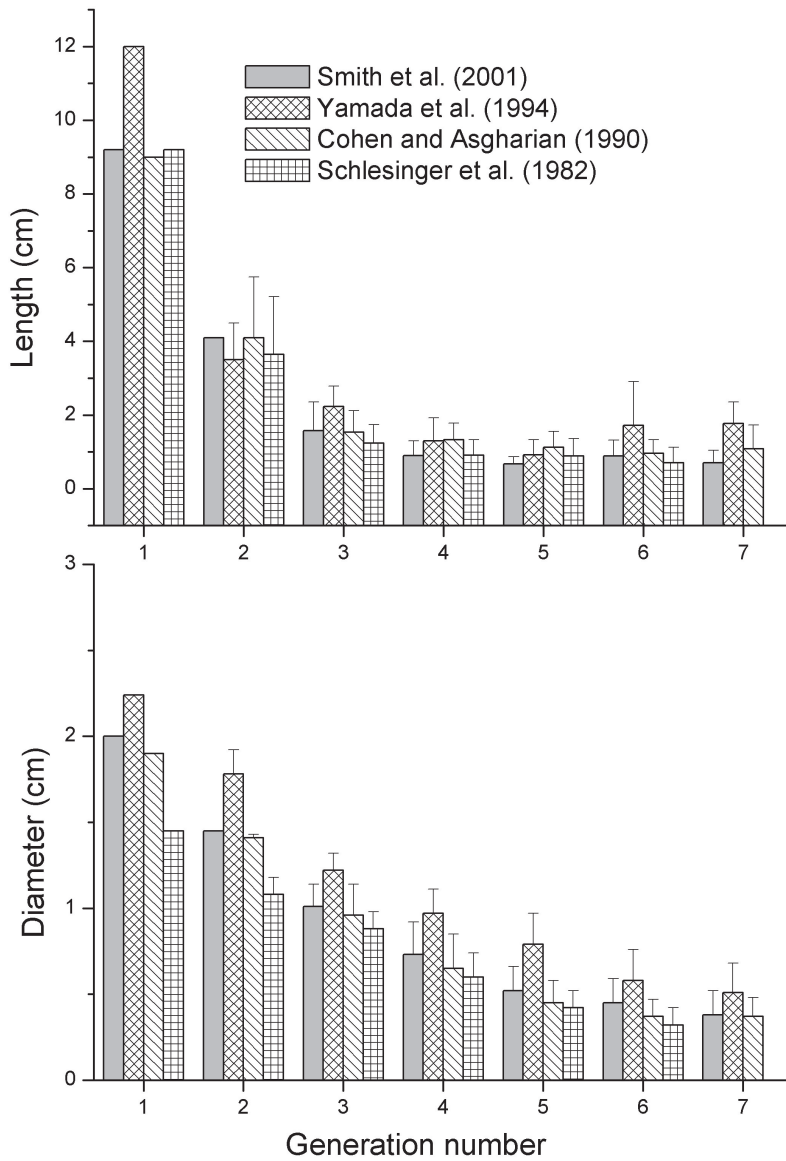


Figure 1: Characteristic dimensions (mean \pm SD), i.e. lengths and diameters, of the first 7 airway generations of different tracheobronchial casts.

2.2 Application of different deposition equations

Three basic deposition mechanisms, i.e. Brownian motion, impaction and sedimentation, play a major role in the TB region. For particles with diameters $d_p \leq 0.5 \mu\text{m}$, deposition in the TB region is predominantly caused by the diffusion mechanism, while for particle sizes $d_p > 0.5 \mu\text{m}$, deposition is caused primarily by both impaction and sedimentation. Various deposition equations have been derived by a number of scientists for the estimation of deposition fractions in the TB region. The following equations were employed in this study.

2.2.1 Deposition by diffusion

Equation formulated by YEH and SCHUM (1980)

For laminar flow conditions YEH and SCHUM (1980) derived the following deposition equation:

$$\eta_d = 1 - 0.819e^{-7.315x} - 0.0976e^{-44.61x} - 0.0325e^{-114x} - 0.0509e^{-79.3x^{2/3}} \quad [1]$$

where $x = LD / 2R^2\bar{v}$, R (cm) is the radius of airway tube, \bar{v} (cm/s) is mean flow velocity and L (cm) is length of airway tube, and D is the particle diffusion coefficient.

Equation formulated by COHEN and ASGHARIAN (1990)

For a replica cast of the upper bronchial airways, Cohen and Asgharian (1990) derived the following empirical equation for enhanced diffusion deposition of ultrafine particles in the turbulent region due to the branching of airways as follows:

$$\eta_d = 2.965\Delta^{0.568} \quad [2]$$

where $\Delta = \pi lD / 4Q$; l is the airway length, D the diffusion coefficient, and Q is the flow rate measured in ml s^{-1} .

Equation formulated by INGHAM (1991)

INGHAM (1991) derived the following equation theoretically for the deposition efficiency in the human airways for laminar flow conditions based on theoretical considerations:

$$\eta_d = 4.458\Delta^{0.55} Sc^{-0.111} \quad [3]$$

Where Sc is the Schmidt number, which includes the airway radius R and the kinematic viscosity, ν .

Equation formulated by YU and COHEN (1994)

YU and COHEN (1994) derived an expression for the deposition efficiency of the form given in equation 3 on the basis of their experiments:

$$\eta_{Dth} = a Re^b Sc^c \left(\frac{l}{R}\right)^d = a \left(\frac{2\dot{V}}{R\pi v}\right) \left(\frac{v}{D}\right)^c \left(\frac{l}{R}\right)^d \quad [4]$$

where Re is Reynolds number. The best fitted values of constants a , b , c and d to the experimental data found by Yu and Cohen (1994) are:

$$a = 1.2027, \quad b = -0.6067, \quad c = -0.5108, \quad d = 0.50081$$

In the trachea, the deposition data measured were substantially higher than the bronchial data due to the effect of the laryngeal jet. Thus for tracheal deposition, the following enhanced values of constants were used:

$$a = 20630, \quad b = -2.2004, \quad c = -0.2339, \quad d = 1.0$$

Equation formulated by MARTONEN et al. (1996)

MARTONEN et al. (1996) solved the momentum and concentration equations analytically using a scaling technique to develop a theoretical model for particle diffusion for developing flows within airways. The effect of the curvature of the tube has been considered when deriving the equation which has improved accuracy of the model. The equation is of the form:

$$\eta_D = 3.89 \Delta^{1/2} Sc^{-1/6} \quad [5]$$

where Δ is the dimensionless diffusion parameter defined as $\Delta = DL/4UR^2$ where U is the average inlet velocity, and L is the developing velocity profile length.

Equation formulated by BRODAY (2004)

BRODAY (2004) developed an expression for the average diffusive flux toward the airway wall based on similarity solutions for both the velocity and concentration fields in the respective boundary layers that develop adjacent to the surface of a plane wedge. The expression for the deposition efficiency compares favorably to those obtained by rigorous computational fluid dynamics simulations and account for different branching angles, airflow rates, and particle sizes.

$$\eta_D = 1.6 Re^{-1/2} \left(\frac{2R_0}{l}\right)^{-1} Sc^{-2/3} \quad [6]$$

where R_0/l is the ratio of the radius of the parent tube to the length of the daughter tube.

2.2.2 Deposition by Impaction

Equation formulated by JOHNSTON and SCHROTER (1979)

JOHNSTON and SCHROTER (1979) derived the following formula for impaction deposition probability calculations:

$$P(I) = 8.5 \times 10^3 \rho \operatorname{Re}' \left(\frac{d_p}{2R} \right)^{2.5} \sin^3 \theta \quad [7]$$

where Re' is the parent airway Reynolds number, d_p is the particle diameter, ρ is the particle density, R is the airway radius and θ is the airways branching angle in radians.

Equation formulated by YEH and SCHUM (1980)

YEH and SCHUM (1980) derived the following impaction deposition equation:

$$P(I) = 1 - \frac{2}{\pi} \cos^{-1}(\theta St) + \frac{1}{\pi} \sin \left[2 \cos^{-1}(\theta St) \right] \quad \text{for } \theta St < 1 \quad [8]$$

$$P_1 = 1 \quad \theta St \geq 1$$

where St the Stokes number.

Equation formulated by MARTONEN et al. (1985)

The equation for the impaction deposition probability derived by MARTONEN et al. (1985) for laminar flow is as follows:

$$P(I) = \frac{2}{\pi} \left[e \left(1 - e^2 \right)^{1/2} + \arcsin(e) \right] \quad [9]$$

while for turbulent flow it is:

$$P(I) = 1 - \exp \left\{ \frac{-4e}{\pi} \right\} \quad [10]$$

with $e = \theta \tau U / 2R$, where U is the mean air velocity, R the airway radius, and $\tau = mC / 3\pi\mu D$ the particle relaxation time, where C is the particle slip correction factor, μ is the air absolute viscosity, and D is the particle diffusion coefficient.

Equation formulated by GAWRONSKI and SZEWCZYK (1986)

GAWRONSKI and SZEWCZYK (1986), using concept of stopping distance derived the following equation for bent tubes for inertial impaction deposition:

$$P(I) = \frac{16}{3\pi} \phi \cdot St \left[2 - \left(\frac{4}{3} \phi \cdot St \right)^{1/2} \right] \quad [11]$$

where $\phi = 2(R/R_0)^2 \sin \theta$, θ is the branching angle, R is the radius of the daughter branch, and R_0 is the radius of the parent branch.

Equation formulated by ZHANG *et al.* (1997)

ZHANG *et al.* (1997) derived the following deposition equation for cylindrical tubes by impaction:

$$\begin{aligned} P(I) &= 0.000654 \exp(55.7Stk^{0.954}) Re^{1/3} \sin \theta && \text{for } Stk < 0.4 \\ &= [0.19 - 0.193 \exp(-9.5Stk^{1.565})] Re^{1/3} \sin \theta && \text{for } Stk \geq 0.04 \end{aligned} \quad [12]$$

for parabolic flow, and

$$\begin{aligned} P(I) &= 0.000425 \exp(22.7Stk^{0.832}) Re^{1/3} \sin \theta && \text{for } Stk < 0.07 \\ &= [0.19 - 0.194 \exp(-3.28Stk^{1.585})] Re^{1/3} \sin \theta && \text{for } Stk \geq 0.07 \end{aligned} \quad [13]$$

for uniform inflow.

2.2.3 Deposition by Sedimentation

Equation formulated by PICH (1972)

For fully developed laminar flow in horizontal tubes, PICH (1972) proposed the following sedimentation deposition equation:

$$P(S) = \frac{2}{\pi} \left[2\varepsilon \sqrt{1 - \varepsilon^{2/3}} - \varepsilon^{1/3} \sqrt{1 - \varepsilon^{2/3}} + \arcsin(\varepsilon^{1/3}) \right] \quad [14]$$

where $\varepsilon = 3v_s l / 8RU$, v_s the particle settling velocity, l the tube length, U the average flow velocity, and R the tube radius. For inclined tubes, with $\frac{v_s}{u} \sin \phi \ll 1$, the deposition efficiency can be calculated using above formula with $\varepsilon = \frac{3v_s L}{8rU} \cos \phi$, where ϕ is the gravity angle.

Equation formulated by YU et al. (1977)

YU et al. (1977) derived an equation to calculate deposition in a horizontal circular channel for laminar uniform flow by solving the governing equation for simultaneous sedimentation and diffusion. For negligible diffusion, the deposition efficiency equation reduces to:

$$P(S) = \frac{2}{\pi} \left[\text{Sin}^{-1} \left(\frac{4}{3} \right) \varepsilon - \frac{4}{3} \varepsilon \sqrt{1 - \left(\frac{4}{3} \varepsilon \right)^2} \right] \quad [15]$$

Equation formulated by YEH and SCHUM (1980)

Deposition by sedimentation, formulated by YEH and SCHUM (1980), is given as:

$$P(S) = 1 - \exp \left[\frac{-4gC\rho_p r_p^2 L \cos \phi}{9\pi\mu R \bar{v}} \right] \quad [16]$$

where g is the acceleration of gravity, ϕ is the angle relative to gravity, ρ_p is the density of the particle, C is the Cunningham slip correction factor, r_p is the particle radius and, μ is the viscosity of the fluid.

Equation formulated by MARTONEN et al. (1985)

MARTONEN et al. (1985) formulated the following equation for sedimentation deposition probability during laminar flow:

$$P(S) = \frac{2}{\pi} \left[e(1 - e^2)^{1/2} + \arcsin(e) \right] \quad [17]$$

with $e = tV \cos \phi / 2R$, where t is the residence time in the respective airway generation, and v_s is the particle terminal settling velocity.

For turbulent flow the sedimentation deposition probability with gravitational constant g is:

$$P(S) = 1 - \exp \left\{ \frac{-2\tau g t \cos \phi}{\pi R} \right\} \quad [18]$$

where g is the gravitational constant.

3. Results and Discussion

3.1 Deposition fractions for different cast geometries

The comparison of mean deposition fractions in each of the first 6–7 generations including the trachea is shown in Figure 2. Deposition calculations were performed for 0.2 μm size particles at a low rate of 15 l min^{-1} and for 3 μm particle size at a flow rate of 34 l min^{-1} . Significant differences can be observed for both particle sizes and flow rates due to the variability of the dimensions of airways. While deposition is higher for smaller cross-section areas of the generations, average deposition fractions are compensated by their smaller surface areas in each generation, i.e. the larger the surface area of a particular generation, the lower will be the average deposition fraction. Variations observed in the morphometric parameters of up to 45% lead to corresponding variations in deposition of up to 14% for 0.2 μm size particles and up to 40% for 3 μm size particles. Due to the consideration of the laryngeal jet during calculations, deposition is increased in the first few generations. However, as the flow starts to become laminar, this enhanced deposition is reduced especially for large particles, where impaction deposition is dominant. The trachea is considered here as the first generation. Hence due to the absence of a bifurcation in the first generation, deposition fractions are lower as compared to the second generation.

The stochastic model predicts a lower deposition fraction in generations 2 and 3 for 0.2 μm size particles, and a consistently lower deposition fraction in all 7 generations for 3 μm size particles as compared to other lung models, primarily due to its stochastic nature. Since airway diameters and lengths in each study refer to individual persons, they display an inherent biological variability. The application of different casting and measurement techniques in these studies may have added an additional systematic variability to the observed intersubject variations. Hence structural differences of lung morphologies among different individuals seem to be largely responsible for the variability in particle deposition.

3.2 Effect of different deposition equations on generational deposition

3.2.1 Diffusion

Diffusion in the respiratory tract typically occurs for particles less than 0.1 μm in diameter, due to their small mass relative to that of air molecules and the higher mobility compared to larger particles (HINDS, 1999). A number of diffusion equations (1-6) as listed in the previous section were employed to investigate their effect on particle deposition with a variety of TB airways cast geometries for 0.04 μm particles and a flow rate of 18 l min^{-1} . The flow conditions considered for the derivation of diffusion equations largely affect the deposition fractions. Increased

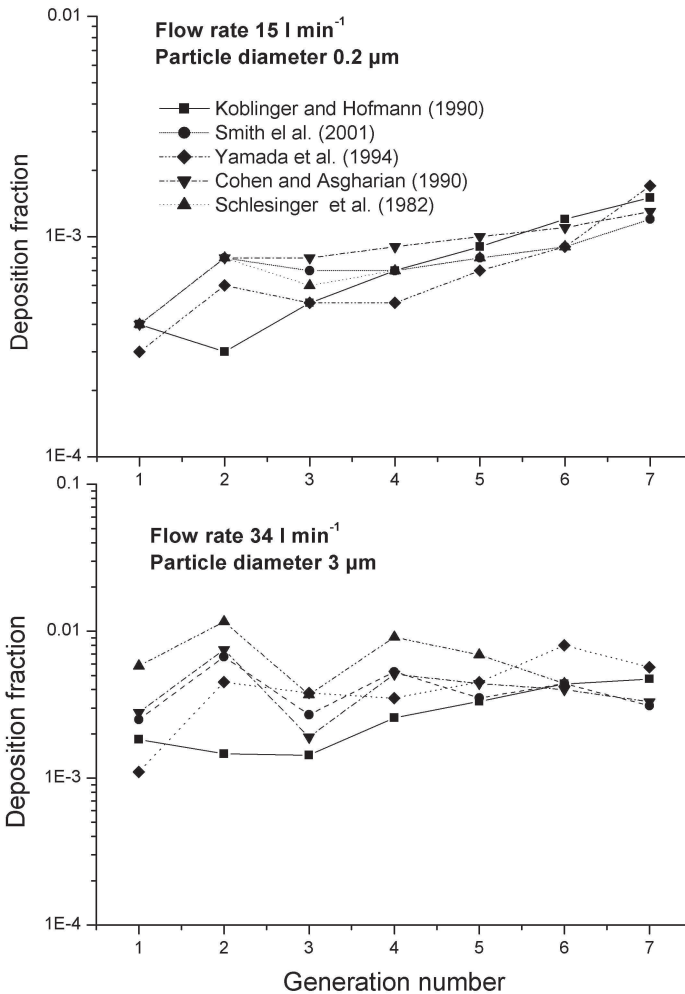


Figure 2: Deposition of particles in the first 7 tracheobronchial (TB) generations for two different particle sizes and flow rates, using different cast geometries.

deposition occurs for turbulent flow as compared to laminar flow conditions. In upper airway generations, normally turbulent and developing flow conditions can be found. The assumption of specific flow conditions further enhances the variation in deposition calculations for each deposition formula. These flow conditions become even more complicated in airway bifurcation zones, where airway branching takes place and hence results in the formation of secondary flows (HOFMANN et al. 2003). Similarly, the lengths and diameters of the airways measured in each cast

study also influence the deposition fractions. The deposition equations produce almost similar deposition patterns in the first 7 generations except for the COHEN and ASGHARIAN (1990) equation, which considers the turbulence in upper airway generations and hence higher deposition efficiency (Figure 3).

The results obtained by COHEN and ASGHARIAN (1990) for 0.04 μm particle sizes at a flow rate of 18 l min^{-1} are in relatively close agreement with the deposition calculations with the YU and COHEN (1994) equation. The equations of YEH and SCHUM (1980) produce the highest total deposition fractions in the thoracic region (see Figure 6). Whereas the BRODAY (2004) equation, in which a wedge shaped bifurcation is considered, with average diffusive flux and laminar flow conditions produce minimum total deposition, i.e. almost 50% percent of the deposition predicted by YEH and SCHUM (1980). The INGHAM (1991) equation, which considers fully developed laminar flow, produces intermediate deposition fractions.

3.2.2 Impaction

Inertial impaction occurs when airborne particles possess enough momentum to keep its trajectory despite changes in the direction of the air stream, consequently colliding with the walls of the airways. The dimensionless Stokes number (Stk) controls the probability of particle deposition in the airways by impaction. The higher the Stokes number, the higher will be the probability of particle deposition by inertial impaction. Therefore, considering the bifurcation geometry of the lungs, large particles travelling through the airways at high airflow velocity are more likely to impact in the proximal portion of the respiratory tract (upper airways) (ZENG et al., 2001). The impaction deposition for various lung geometries and deposition formulas was calculated for 3 μm size particles and a flow rate of 34 l min^{-1} (Figure 5). The GAWRONSKI and SZEWCZYK (1986) formula yields variable high deposition fractions in the upper airway generations in all cast geometries. However, the JOHNSTON and SCHROTER (1979) equation predicts the highest total lung deposition fraction (see Figure 6). The SCHLESINGER et al. (1982) cast geometry contains the smallest diameters for each generation and hence produces the highest deposition by impaction (Figure 4d). ZHANG et al. (1997) considered the Reynolds number with uniform flow in upper airway generations, thus producing relatively higher deposition fractions. However, the distinct high peak for the JOHNSTON and SCHROTER (1979) equation in distal generations is probably caused by the higher exponent for the daughter to parent diameter ratio (Figure 6). An overall close agreement was found between the deposition fraction obtained by YEH and SCHUM (1980) and MARTONEN (1985) equations.

The SCHLESINGER et al. (1982) airway geometry shows relatively higher deposition fractions in each generation due to deposition by impaction. A close agreement was found between the GURMAN et al. (1984) studies and the GAWRONSKI and SZEWCZYK (1986) formula for 3 μm particles at 34 l min^{-1} .

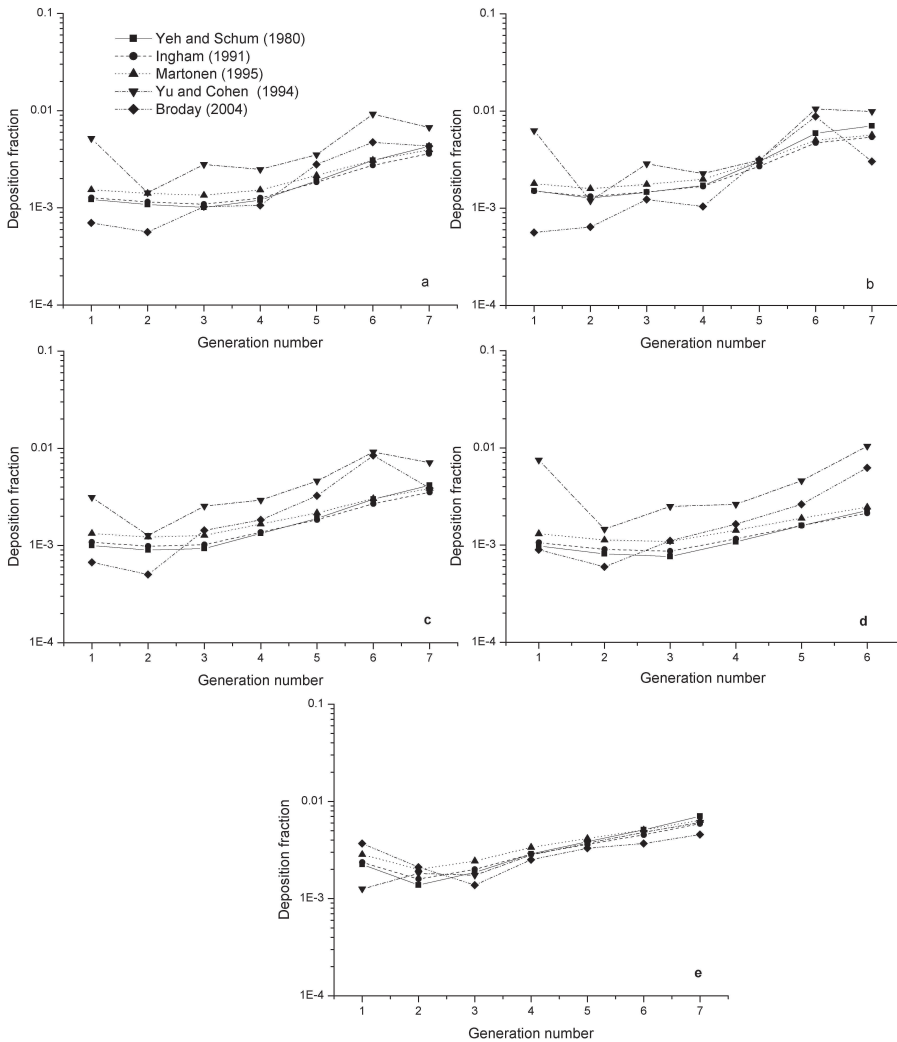


Figure 3: Inspiratory deposition fractions for inhalation of 0.04 μm size particles at a flow rate of 18 l min⁻¹. Deposition is calculated using different diffusion equations and lung cast geometries (a) SMITH et al. (2001), (b) YAMADA et al. (1994), (c) COHEN and ASGHARIAN (1990), (d) SCHLESINGER et al. (1982) in the first 6 generations, and (e) KOBLINGER and HOFMANN (1990).

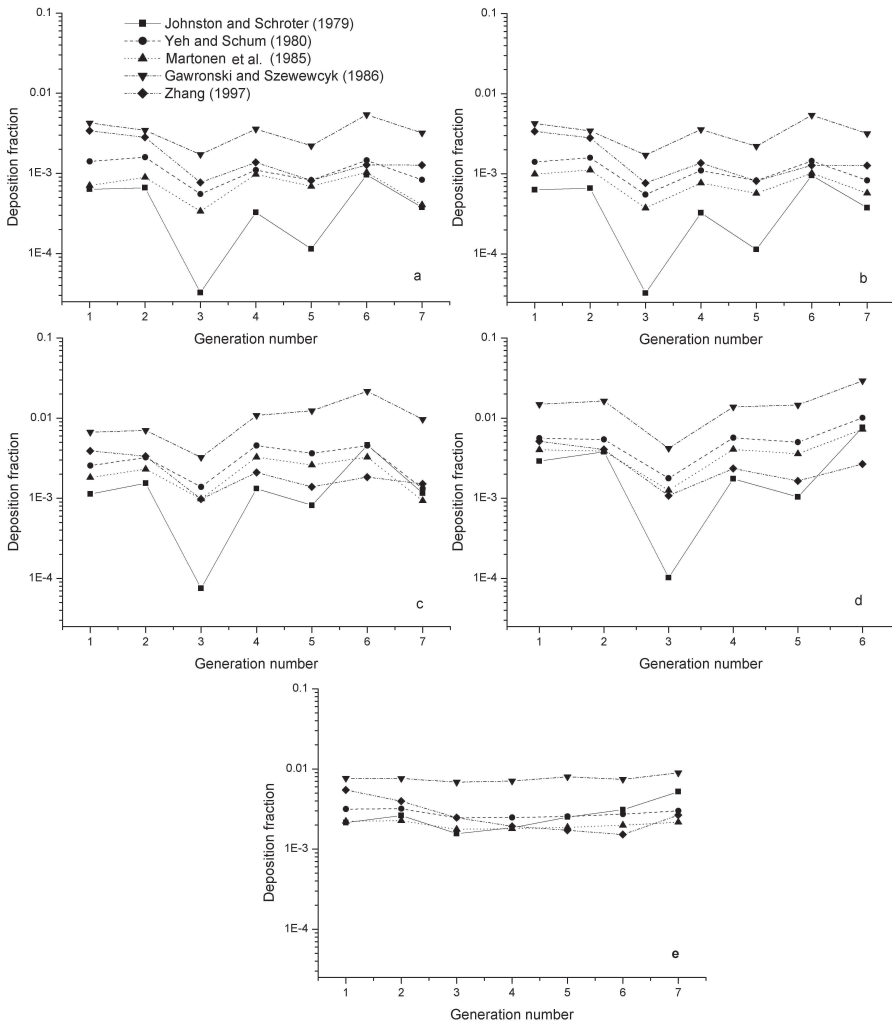


Figure 4: Inspiratory deposition fractions for inhalation of 3 µm particles at a flow rate of 34 l min⁻¹. Deposition is calculated by different impaction equations and lung casts geometries (a) SMITH et al. (2001), (b) YAMADA et al. (1994), (c) COHEN and ASGHARIAN (1990), (d) SCHLESINGER et al. (1982) in the first 6 generations, and (e) KOBLINGER and HOFMANN (1990).

3.2.3 Sedimentation

Sedimentation is a time-dependent process which occurs when gravitational force acts on a particle and causes it to gradually move out of the air stream line. If the weight of the particle is greater than the buoyant force exerted by the fluid on the particle, it will quit its original streamline path. As the particle settles, it experiences a drag from the fluid, causing it to quickly reach a terminal settling velocity. Sedimentation is the dominant mechanism for larger particles and low flow rates. Sedimentation is also dependent on the branching angle and the airway geometry. The sedimentation deposition for various lung geometries and deposition formulas was calculated for 3 μm particles at a flow rate of 34 l min^{-1} .

For the selected sedimentation equations, calculated deposition fractions exhibit an almost similar trend, primarily due to the constant branching angle employed in this study (see Figure 5). Branching angles for cast studies were not available for most of the studies. Similarly, all sedimentation deposition equations employed in this study were derived for laminar flow conditions, except for the YEH and SCHUM (1980) equation, which was derived for uniform flow. Deposition in all lung generations reveals that sedimentation deposition is dominant in distal generations of the TB tree, where airway diameters are smaller and flow rates are slower (Figure 6).

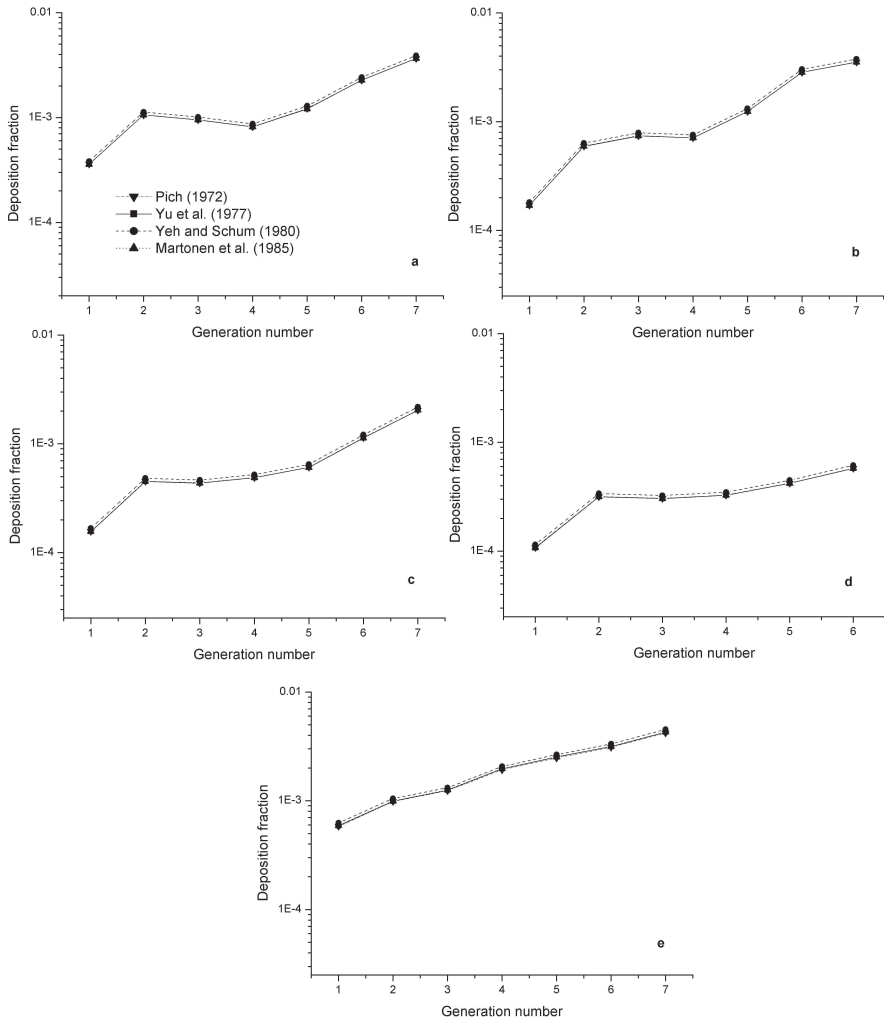


Figure 5: Inspiratory deposition fractions for inhalation of 3 μm particles at a flow rate of 34 l min⁻¹. Deposition is calculated by different sedimentation equations and lung cast geometries (a) SMITH et al. (2001), (b) YAMADA et al. (1994), (c) COHEN and ASGHARIAN (1990), (d) SCHLESINGER et al. (1982) in the first 6 generations, and (e) KOBLINGER and HOFMANN (1990).

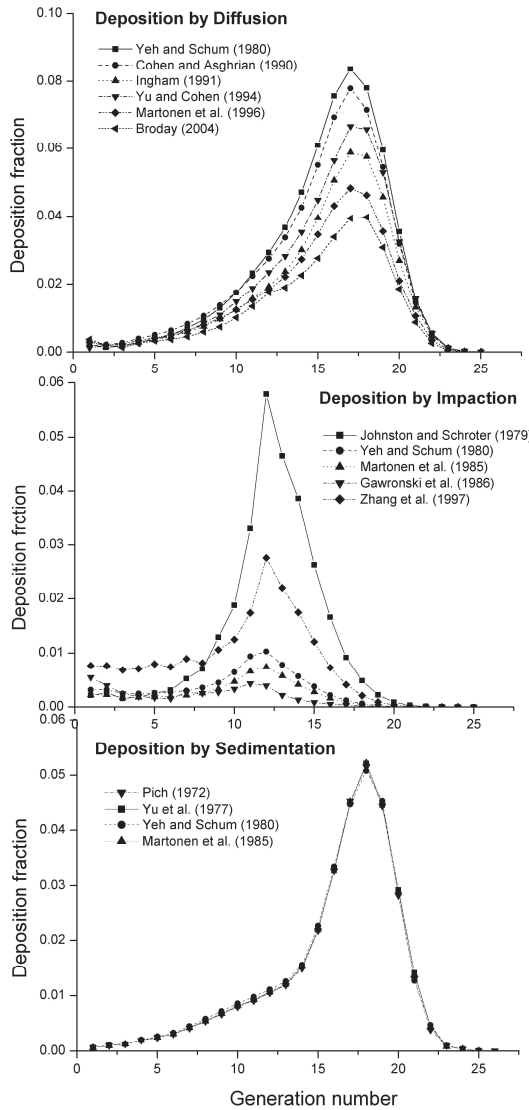


Figure 6: Inspiratory deposition fraction for the three major deposition mechanisms using different deposition equations and the stochastic lung geometry (KOBLLINGER and HOFMANN 1990). Deposition by diffusion is calculated for 0.2 μm size particle at flow rate of 15 l min^{-1} , whereas, deposition by impaction and sedimentation is calculated for 3 μm size particles at flow rate of 34 l min^{-1} .

4. Conclusion

Measured lung airway cast geometries with up to 7 generations obtained from four different experimental studies and deposition equations for the major deposition mechanisms derived by various scientists were employed in this study to compare their results with that of the stochastic deposition model IDEAL.

Deposition of 0.04, 0.2 and 3 μm particles was calculated for flow rates of 15, 18 and 34 l min^{-1} to investigate their effect on deposition. An overall close agreement among the deposition fractions for different cast geometries and the employed deposition equation was found. However, variability in deposition fractions using different cast geometries arises due to structural differences of lung morphologies, which were derived from different ethnic and age subjects. The variations in the deposition fractions by the application of different deposition equations were primarily caused by the lung morphometry employed in the derivation of the equations, the choice of the central bifurcation geometry (i.e. the branching angle and bifurcation shape), and the consideration of specific flow profiles (i.e. entrance effect). Up to 100% variation in deposition fractions by diffusion deposition and up to 300% variation in deposition fraction by impaction deposition could be observed. In contrast, different sedimentation equations produce almost similar deposition fractions.

The YU and COHEN (1994) diffusion deposition equation results were found in close agreement with the experimental data of COHEN and ASGHARIAN (1990). In addition, the GAWRONSKI and SZEWCZYK (1986) impaction deposition equation results were found in close agreement with the experimental studies of GURMAN et al. (1984).

Acknowledgments

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5. References

- BRODAY D.M. (2004): Deposition of ultrafine particles at carinal ridges of the upper bronchial airways. *Aerosol Sci. Technol.* 38:991–1000.
- COHEN B.S., ASGHARIAN B. (1990): Deposition of ultrafine particles in the upper airways: an empirical analysis, *J. Aerosol Sci.* 21:789–797.
- FLEMING J.S., NASSIM M., HASHISH A.H., BAILEY A.G., CONWAY J., HOLGATE S. HALSON P., MOORE E., MARTONEN T.B. (1995): Description of pulmonary deposition of radiolabeled aerosol by airway generation using a conceptual three-dimensional model of lung morphology, *J. Aerosol Med.* 8:341–356.
- FLEMING J.S., EPPS B.P., CONWAY J.H., MARTONEN T.B. (2005): Comparison of SPECT aerosol deposition data with a human respiratory tract model, *J. Aerosol Med.* 19:268–278.
- GAWRONSKI R., SZEWCZYK K.W. (1986): Inertial deposition of particles in the human branching airways. *J. Aerosol Sci.* 17:795–801.
- GURMAN J.L., LIPPMANN M., SCHLESINGER R.B. (1984): Particle deposition in replicate casts of the human upper TB tree under constant and cyclic inspiratory flow. I. Experimental. *Aerosol Sci. Technol.* 3, 245-252.
- HINDS W.C. (1999): Respiratory deposition. In: Hinds, W.C. (Ed.), *Aerosol technology: properties, behavior, and measurement of airborne particles*, 2nd ed., Wiley, New York.
- HOFMANN W., KOBLINGER L. (1990): Monte Carlo modeling of aerosol deposition in human lungs. Part II: Deposition fractions and their parameter variations. *J. Aerosol Sci.* 21:675–688.
- HOFMANN W., BERGMANN R., MENACHE M.G. (1998): The effect of intersubject variability in airway morphology on intersubject variations in particle deposition. *J. Aerosol Sci.* 29 (Suppl. 1): S943–S944.
- HOFMANN W., ASGHARIAN B., WINKLER-HEIL R. (2002): Modeling intersubject variability of particle deposition in human lungs. *J. Aerosol Sci.* 33:219–235.
- HOFMANN W., GOLSER R., BALASHAZY I. (2003): Inspiratory deposition efficiency of ultrafine particles in a human airway bifurcation model. *Aerosol Sci. Technol.* 37:988–994.
- INGHAM D.B. (1991): Diffusion of aerosol in the entrance region of a smooth symmetrical J. *Aerosol Sci.* 22:253–257.
- JOHNSTON J.R., SCHROTER R.C. (1979): Deposition of particles in model airways. *J. Appl. Physiol.* 47:947–953.
- KIM C.S., HU S.C., DEWITT P., GERRITY T.R. (1996): Assessment of regional deposition of inhaled particles in human lungs by serial bolus delivery method. *J. Appl. Physiol.* 81:2203–2213.

- KIM C.S., HU S. (1998): Regional Deposition of inhaled particles in human lungs: comparison between men and women. *J. Appl. Physiol.* 84:1834–1844.
- KIM C.S., JAKES P.A. (2005): Total lung deposition of ultrafine particles in elderly subjects during controlled breathing. *Inhal. Toxicol.* 17:387–399.
- KIM C.S., HU S.C. (2006): Total respiratory tract deposition of fine micrometer-sized particles in healthy adults: empirical equations for gender and breathing pattern. *J. Appl. Physiol.* 101:401–412.
- KOBLINGER L., HOFMANN W. (1990): Monte Carlo modeling of aerosol deposition in human lungs: Part I: Simulation of particle transport in a stochastic lung structure. *J. Aerosol Sci.* 21:661–674.
- MARTONEN T.B., ANDREW E.B., MILLER F.J. (1985): Ambient sulfate aerosol deposition in man: Modeling the influence of hygroscopicity. *Environ Health Perspect.* 27:139–150.
- MARTONEN T.B., ZHANG Z., YANG Y. (1996): Particle diffusion with entrance effect in a smooth-walled surface. *J. Aerosol Sci.* 27:139–150.
- PICH J. (1972): Theory of gravitational deposition of particles from laminar flow in channels. *J. Aerosol Sci.* 3:351–361.
- RAABE O.G., YEH H.C., SCHUM G.M., PHALENR. F. (1976): Tracheobronchial geometry: human, dog, rat, hamster. Report LF-53, Lovelace Foundation, Albuquerque, NM, USA.
- SCHLESINGER R.B., GURMAN J.L., LIPPMANN M. (1982): Particle deposition within bronchial airways: comparisons using constant and cyclic inspiratory flows. *Ann. occup. Hyg.* 26: 47-64.
- SCHLESINGER R.B., LIPPMANN M. (1972): Particle deposition in casts of the human upper tracheobronchial tree. *Am. Ind. Hyg. Assoc. J.* 33: 237-251.
- SMITH S., CHENG Y.S., YEH H.C. (2001): Deposition of ultrafine particles in human tracheobronchial airways of adults and children. *Aerosol Sci. Technol.* 35: 697–709.
- SOONG T.T., NICOLAIDES P., YU C.P., SOONG S.C. (1979): A statistical description of the human tracheobronchial tree geometry. *Respir. Physiol.* 37:161-172.
- WEIBEL E. R. (1963): *Morphometry of the Human Lung*. New York: Academic Press.
- YAMADA Y., KOIZUMI, A., FUKUDA S., INABA J., CHENG Y.S., YEH H.C. (1994): Deposition of ultrafine monodisperse particles in a human tracheobronchial cast. *Ann. Occup. Hyg.* 38:191-100.
- YEH H.C., SCHUM G.M. (1980): Models of human lung airways and their application to inhaled particle deposition. *Bull. Math. Biophys.* 42:461–480.
- YU C.P., LUI C.S., TAULBEE D.B. (1977): Simultaneous diffusion and sedimentation of aerosols in a horizontal cylinder. *J. Aerosol Sci.* 8:309–316.
- YU C.P., COHEN B.S. (1994): Tracheobronchial airway deposition of ultrafine particles. In: *Inhaled Particles VI*. *Ann. Occup. Hyg.* 38:83–89.
- ZHANG L., ASGHARIAN B., ANJILVEL S. (1997): Inertial deposition of particles in the human upper airway bifurcations. *Aerosol Sci. Technol.* 26:97–110.

ZENG X.M., MARTIN G.P., MARRIOTT C. (2001): Medicinal aerosols. In: Zeng, X.M., Martin, G.P., Marriott, C. (Eds.), Particulate Interactions in Dry Powder Formulations for Inhalation. Taylor & Francis, New York, NY, USA.

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