UC Irvine
UC Irvine Previously Published Works

Title

Methods for modeling particle deposition as a function of age

Permalink

Journal

Respiratory Physiology & Neurobiology, 128(1)

ISSN

Authors

Phalen, Robert F
Oldham, Michael J

Publication Date

2001-10-01

DOI

Copyright Information

Peer reviewed

Methods for modeling particle deposition as a function of age

Robert F. Phalen *, Michael J. Oldham

Community and Environmental Medicine, Air Pollution Health Effects Laboratory, University of California, Irvine, CA 92697-1825, USA

Abstract

The purpose of this paper is to review the application of mathematical models of inhaled particle deposition to people of various ages. The basic considerations of aerosol physics, biological characteristics and model structure are presented along with limitations inherent in modern modeling techniques. Application of the models to children and senescent adults has been largely based on extrapolating anatomical and physiological data from young adults to match the changes observed during growth and aging. Sample results are included for total particle deposition and deposition in the bronchial and pulmonary regions. The models proposed provide particle deposition predictions that are consistent with the scant measurements available. The models discussed appear to be on firm theoretical grounds, but they are largely limited in application to simple aerosols and average individuals. Also, additional validation of the computational predictions is needed. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Airways; Particle deposition; Development, children, senescent adult; Mammals, humans; Model, particle deposition, airways

1. Introduction

The purpose of this paper is to examine the current mathematical methods used for estimating the deposition of particles inhaled by people of various ages. Historically, age-related aerosol deposition models were advanced in order to establish acceptable air concentrations of radionuclides for general populations (as opposed to workers) (Hofmann et al., 1979; Hofmann, 1982; R.G. Thomas and J.W. Healy, unpublished; Crawford, 1982; Crawford and Eckerman, 1983; ICRP, 1994; NCRP, 1997). Recently, interest in medicinal aerosols and particulate urban air pollutants have stimulated model developments (Xu and Yu, 1986; Yu and Xu, 1987; Ferron et al., 1989; Hofmann et al., 1989; Kim and Hu, 1998; Martonen and Zhang, 1993). Modern aerosol deposition models are elegant with respect to the aerosol physics involved, the quantitative specification of respiratory tract anatomy, and the application of modern computers. However, the many anatomi-

* Corresponding author. Tel: + 1-949-824-4758; fax: -1-949-824-4763.

E-mail address: rfphalen@uci.edu (R.F. Phalen).

cal simplifications currently used tend to restrict the results to representing group averages, rather than applying to individuals. Also, such factors as aerosol charge and hygroscopicity, unusual anatomical/physiological factors, and the complex nature of cyclic airflows in branching airways, are not well modeled. In addition, the paucity of clinical measurements of aerosol deposition in many age groups prevents broad validation of the model predictions. On the other hand, scientific progress in the area seems to be steady, solid and innovative. The complexity and limitations of inhaled particle deposition modeling are presented in recent treatments of the topic (ICRP, 1994; NCRP, 1997; Schulz et al., 2000).

2. Basic considerations

It is difficult to succinctly describe the complex subject of modeling the deposition of inhaled aerosols. Of necessity, such modeling is sophisticated with respect to both aerosol physics and physiological considerations. This section attempts to display many of the important factors involved and how such models are being applied to various age groups. For a more complete treatment of any topic, the cited references must be consulted.

Prior to calculating the deposition of inhaled aerosol particles, the probability that the particles actually enter the nose or mouth must be assessed. This probability, the inhalability (also aspiration efficiency) varies strongly with particle diameter, with the external wind speed and the direction at which the wind meets the face (orientation angle). The equation used for human inhalability (Appendix), which is averaged over all wind orientations, was obtained from experimental studies with mannequins (Ogden and Birkett, 1977; Vincent et al., 1990; Phalen et al., 1992). Inhalability considerations have been recently reviewed by Vincent (1999).

Once a particle has been inhaled, models of its deposition are based on an understanding of basic particle physics (Findeisen, 1935; Task Group on Lung Dynamics, 1966; Taulbee and Yu, 1975; Yeh and Schum, 1980; Heyder and Rudolf, 1984). The motion of simple aerosol particles (smooth, un-

changing, uncharged spheres) in air is largely well understood. For example, the deposition probability of such particles due to gravitational settling while passing through a cylindrical tube in which any contact of the particle with the wall causes deposition is given by the formula (NCRP, 1997):

$$\mathrm{Ps} = 1 - \exp\left[\frac{-4g\mathrm{C}\rho_p r_p^2 \mathrm{L}\cos\phi}{9\pi\mu\mathrm{R}\bar{v}}\right] \tag{1}$$

where Ps = sedimentation deposition probability, ρ_p = density of the particle (g/cm^3), ϕ = inclination of the tube to gravity ($\phi = 0$ degrees for horizontal tube), R = radius of the tube (cm), $\bar{v}$ = mean air flow velocity (cm/sec), g = acceleration due to gravity (cm/sec^2), C = Cunningham slip correction, r_p = radius of the particle (cm), μ = viscosity of the fluid (dyn sec/cm^2), and L = length of the tube (cm).

Similar equations are available for other mechanisms that produce the deposition of particles in various regions of the respiratory tract (Appendix). For the bronchial region the mechanisms of particle diffusion to the wall of a cylinder, sedimentation to the cylinder floor, and impaction on the wall at a bend in a tube are used for computations (ICRP, 1994; NCRP, 1997). These equations define the input information required to perform particle deposition calculations in the respiratory tract. This mechanistic theoretical approach works well when the anatomy can be adequately represented by simple shapes, for example by a linked set of bent and straight tubes. It is usually assumed that bronchial tubes and their bifurcations can be so represented. For those structures not reducible to such tubes (the nose for example), semi-empirical equations arrived at by fitting logical mathematical functions to human clinical or model-acquired data are usually employed (Cheng et al., 1988; Stahlhofen et al., 1989; ICRP, 1994; Yeh et al., 1996; NCRP, 1997). The airflow assumptions, which include either laminar plug flow, laminar parabolic flow, or turbulent flow within any given region, are also simplifications.

The deposition equations themselves actually define (and guide the acquiring of) the physical, anatomical and physiological measurements that

are required for computing particle deposition. For Eq. (1), airway length, radius, inclination to gravity and average throughput air velocity must be known. For the aerosol particles, Eq. (1) requires the density, radius and a slip correction for small particles. Environmental parameters needed include the gravitational acceleration and the air viscosity, which weakly depends on composition, temperature and humidity of the air. For impaction-produced aerosol deposition, the tube bend angle (as a surrogate for branch angle) is also required, and for diffusion the aerosol particle diffusion coefficient must be specified. For non-spherical particles, equivalent (aerodynamic or diffusional) diameters are used. For evaporating or growing particles both the particle diameters and densities may change during passage through the airway lumens, which adds complexity to the calculations (Ferron et al., 1989; Martonen and Zhang, 1993).

The needed airway anatomical data are not easy to acquire. Sensitivity calculations of the effect of errors in airway sizes on particle deposition indicate that as little as a 10% error in airway size information can produce significant errors in calculated particle doses (Phalen et al., 1990). Measurements from radiographs, tissue sections, tomographic scans, replica casts, pulmonary function tests, and aerosol bolus inhalation experiments have all been used to define airway dimensions, and each method has its limitations. Because morphometric data are sparse, interpolations, extrapolations and scaling principles have been used to derive information as functions of age and body size. It must be noted that after the early period of lung development, age per se often has less to do with airway sizes and breathing patterns than does body size; thus body size (represented by height or mass) is important for making estimates of nasal, oral and tracheobronchial airway size and ventilation along with age. The alveolar region must be scaled as a function of age in the postnatal development period. Similarly, gender per se is expected to have less of an influence on airway sizes and airflows than does body size; an exception may be the larynx (Pritchard et al., 1986). Clinical measurements indicate that women tend to have greater

bronchial aerosol deposition efficiencies for many particles, but additional research is needed (Kim and Hu, 1998).

The postnatal growth of human airways is not well understood quantitatively. Morphometric measurements on 20 in-situ casts for children aged 11 days to 21 years were used to construct airway length and diameter predictions as linear functions of body height (Phalen et al., 1985). The relationships proposed were:

$$L_n = a_n H + b_n \qquad (2)$$

$$D_n = c_n H + d_n \qquad (3)$$

where L_n = the average length in cm of a generation n airway ($n = 1$ for trachea), D_n = the average diameter in cm of a generation n airway, H = body height (cm), and, a_n, b_n, c_n, d_n are constants that change with airway generation.

The airway constants are provided in Table 1, and Table 2 gives age-related data that are useful for scaling particle deposition models. Figs. 1 and 2 depict growth of the tracheobronchial airways (Eq. (2) and Eq. (3)). Table 2 also provides average tracheobronchial dead space values because dead space variations will influence airway sizes and the inhaled aerosol deposition pattern.

Table 1
Constants used to calculate airway dimensions for people of different heights using Eq. (2) and Eq. (3).

	Airway length		Airway diameter	
n	a_n	b_n	c_n	d_n
1	0.0500	0.150	0.010	0.0690
2	0.0180	0.679	0.0069	0.0886
3	0.0070	0.246	0.0046	0.0982
4	0.0053	0.124	0.0033	0.0937
5	0.0035	0.196	0.0017	0.0999
6	0.0033	0.113	0.0014	0.0711
7	0.0022	0.112	0.0012	0.0541
8	0.0013	0.133	0.0007	0.0496
9	0.0008	0.152	0.0004	0.0499
10	0.0009	0.130	0.0003	0.0488
11	0.0007	0.129	0.0002	0.0479
12	0.0006	0.127	0.0001	0.0461
13	0.0005	0.125	0.00009	0.0452
14	0.0004	0.123	0.00006	0.0440
15	0.0003	0.121	0.00004	0.0429
16	0.0002	0.120	0.00002	0.0419

Table 2
Age and body size relationships for United States children as used in respiratory tract models

Age (y)	Height (cm)	Body mass (kg)	TB dead space volume (cm^3)
2	88	10	21
4	104	16.4	31
6	115	22	39
8	127	27	49
10	138	34	59
12	150	43	68
14	162	54	85
16	170	63	95
18	175	70	101

Tracheobronchial (TB) dead-space volume is the difference between total dead space and airway (mouth, pharynx, larynx) volume. (NCRP, 1997).

Once the aerosol, anatomical, airflow and environmental parameters have been defined, the aerosol deposition probability calculations can be initiated. For this process, any initial inhaled particle concentration may be used, but for convenience, usually 1.000 particle per unit volume of air is assumed. This number is decreased at the entrance to each airway structure by subtracting the deposition in all of the preceding airways. Following inspiration, a breath-hold period in which sedimentation and diffusion (but not im-

Fig. 1. Modeled human bronchial airway changes in length as based on fitted linear equations for measurements of 21 casts of lungs of American children. Numbers below lines indicate airway generations (some not numbered), (Phalen et al., 1985; NCRP, 1997).
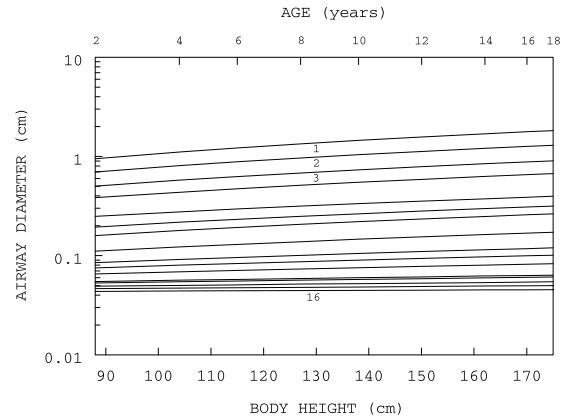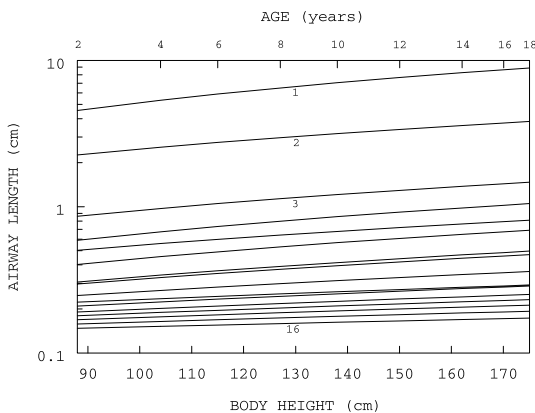

Fig. 2. Modeled human bronchial airway changes in diameter as based on fitted linear equations for measurements of 21 casts of lungs of American children. Numbers below lines indicate airway generations (some not numbered), (Phalen et al., 1985; NCRP, 1997).

paction) produces additional deposition may be assumed. Usually, inspiration is immediately followed by expiration, in which all three deposition mechanisms act on the remaining particles as they pass through the anatomical structures in reverse order. Complexities in the calculations include the effects of dead space, residual air in the lungs and air mixing due to asymmetric in/out airflows within the branchings of the respiratory tract. The approach just described is called 'deterministic', although sometimes a Monte-Carlo computational method is used that follows individual particles through a statistically-obtained pathway through the respiratory tract (Koblinger and Hofmann, 1990; Anjilvel and Asgharian, 1995). Table 3 presents sample calculations for predicted bronchial and pulmonary deposition of seven particle sizes in children and adults for two different dead space assumptions. The large dead space could represent either individual variation or a loss of bronchial muscle tone, as may occur in advanced age. These computations are reproduced from Schum et al. (1991). Other similar modeling results have been published (Hofmann, 1982; Yu and Xu, 1987; Martonen and Zhang, 1993; ICRP, 1994).

Many factors, that may or may not be significant, are usually ignored in the particle deposition

models. One study indicated that older children (8–16 years old) exhibited more oral breathing at rest than did adults, who had mainly nasal breathing (Becquemin et al., 1999). The effect of heart motion on airway dimensions and airflows, the deviation of tracheobronchial airways from smooth right circular cylinders, and the shapes of bifurcations at airway branching points are other potentially-important factors that are not usually modeled.

Available models of particle deposition are varied and difficult to compare. The following ten criteria are suggested for comparing and evaluating computational models used for predicting the deposition of inhaled aerosol particles.

1. Type of model: Is the model deterministic, stochastic, computational fluid dynamic, empirical, semi-empirical, etc.?
2. Aerosol physics: What aerosol deposition mechanisms are included: sedimentation, diffusion, impaction, interception, electrostatic attraction, etc.? Are fluid dynamic factors such as non-axial and turbulent flows included?

Table 3
Estimated thoracic deposition efficiencies in the adult and 2-year old child tracheobronchial anatomical model of Phalen et al. (1985) scaled to dead space volumes of 20 cm^3 and 40 cm^3 for a low level of physical activity

	Particle aerodynamic diameter (μm)						
	0.1	0.25	0.50	1.0	2.5	5.0	10.0
Low Activity: 20-year old adult (Minute ventilation 10.0 l/min)							
Pulmonary deposition efficiency	0.22	0.13	0.08	0.10	0.35	0.40	0.08
Bronchial inhalation efficiency							
100 cm^3 dead space	0.059	0.031	0.024	0.031	0.098	0.310	0.771
200 cm^3 dead space	0.059	0.030	0.024	0.029	0.090	0.284	0.740
Bronchial exhalation efficiency							
100 cm^3 dead space	0.043	0.024	0.020	0.020	0.032	0.051	0.080
200 cm^3 dead space	0.042	0.025	0.020	0.023	0.042	0.075	0.120
Total bronchial efficiency							
100 cm^3 dead space	0.102	0.055	0.044	0.051	0.130	0.361	0.851
200 cm^3 dead space	0.101	0.055	0.044	0.052	0.132	0.359	0.860
Total deposition efficiency							
100 cm^3 dead space	0.322	0.185	0.124	0.151	0.480	0.761	0.931
200 cm^3 dead space	0.321	0.185	0.125	0.152	0.482	0.759	0.940
Low activity: 2-year old (Minute ventilation 2.75 l/min)							
Pulmonary deposition efficiency	0.18	0.10	0.05	0.06	0.22	0.22	0.02
Bronchial inhalation efficiency							
20 cm^3 dead space	0.100	0.047	0.040	0.062	0.232	0.633	0.987
40 cm^3 dead space	0.100	0.048	0.037	0.048	0.168	0.491	0.953
Bronchial exhalation efficiency							
20 cm^3 dead space	0.072	0.039	0.029	0.029	0.048	0.040	0.000
40 cm^3 dead space	0.072	0.040	0.031	0.034	0.071	0.102	0.023
Total bronchial efficiency							
20 cm^3 dead space	0.172	0.086	0.069	0.091	0.280	0.673	0.987
40 cm^3 dead space	0.172	0.088	0.068	0.082	0.239	0.593	0.976
Total deposition efficiency							
20 cm^3 dead space	0.352	0.186	0.119	0.151	0.500	0.893	1.007
40 cm^3 dead space	0.352	0.188	0.118	0.142	0.459	0.813	0.996

Adapted from Schum et al. (1991).

3. Non-ideal aerosols: In addition to ideal smooth spherical particles, what aerosols can be modeled: hygroscopic, volatile, charged, polydisperse, heterodisperse, fibrous, etc.?

4. Anatomy/Physiology: How completely and accurately are the anatomical features of the respiratory tract modeled? How accurately are breathing patterns, airflows and air mixing phenomena represented?

5. Anatomical detail: To what extent are anatomical details such as bifurcation shapes, local airway constrictions, asymmetric branching, surface roughness and dimensional changes during respiration captured?

6. Output: What results may be obtained: total deposition, regional deposition, lobar deposition, specific airway deposition, deposition per unit surface area and local deposition in small regions?

7. Extrapolation: Can the model be used to compare species, body sizes, ages, genders, disease states, and unique individuals?

8. Limitations: Are the limitations of the model with respect to modeled particle and biological parameters known and explicitly stated?

9. Validity: Have the results been compared to aerosol deposition data in living subjects or surrogate models?

10. Documentation and ease of use: How well documented is the model? Does the documentation provide the user with an understanding of the scientific basis, applicability, computational methods, limitations and implementation of the model? How easy is the model to use, with respect to availability, cost, installation, and user training/qualifications?

3. Models proposed

Several investigators have proposed aerosol deposition models that account for age-related factors. The initial efforts to mathematically model aerosol deposition in children followed the publication of the ICRP Task Group on Lung Dynamics Model (Task Group on Lung Dynamics, 1966). The ICRP-66 model organized the adult respiratory system into logical regions, selected useful mathematical equations for the major deposition mechanisms, provided realistic aerosol deposition results, and it was well-documented and easy to apply. In this model, semi-empirical equations were applied to particle deposition in the nose, and no provision was made for scaling to children. Pioneering work on adopting these computational methods to children was motivated by radiation protection considerations — from nuclear weapon or accident fallout, natural radon in homes, and other natural and anthropogenic sources (Hofmann et al., 1979; Crawford, 1982; Hofmann, 1982; Crawford and Eckerman, 1983). More recent modeling efforts were stimulated by an interest in other environmental contaminants including combustion products as well as inhaled medications (Phalen et al., 1985; Xu and Yu, 1986; Yu and Xu, 1987; Ferron et al., 1989; Martonen and Zhang, 1993).

Major inhaled particle dosimetry modeling updates were recently published by the International Commission on Radiological Protection (ICRP, 1994) and the National Council on Radiation Protection and Measurements (NCRP, 1997). In both of these models, improvements were made for the deposition of particles in the nasal and oral airways, and children were included. The lung growth data for both models was based on measurements of replica casts of 21 children's lungs (Phalen et al., 1985) as shown in Tables 1 and 2.

4. Results

For children, the particle deposition models consistently predict greater tracheobronchial aerosol deposition and lesser pulmonary deposition than is calculated for adults (Phalen et al., 1985; Yu and Xu, 1987; Hofmann et al., 1989; Martonen and Zhang, 1993). Sample predictions are shown in Table 3 for the 2-year old and 20-year old. The main differences are due to the smaller airways as a result of smaller body size, but other factors are also important (Bennett et al., 1996). For example, the specific ventilation (ventilation volume/body mass) is increased as body mass is
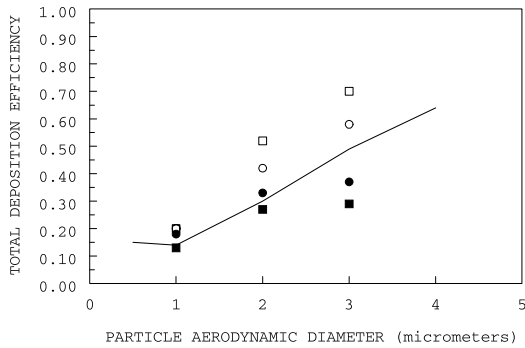
Fig. 3. Comparison of theoretical total deposition efficiency for an 8.2-year old (solid line) using the theory of Martonen and Zhang (1993), and experimental data from Roy et al. (1986) (a group of eight children of 7.4 years average age and a group of nine children of 11.3 years average age, solid circles and squares, respectively) and Schiller-Scotland et al. (1992) (a group of six children of 5.3 years average age and a group of 23 children of 10.6 years average age, open circles and squares, respectively). Although the model does not use the same ages as did the experimental investigations, the average ages match relatively well.

decreased (Guyton, 1947; Phalen et al., 1992). The general agreement between theoretical particle deposition predictions and clinical measurements in adults has been well documented (ICRP, 1994; Yeh et al., 1996; NCRP, 1997). The agreement is good for group averages, but individual differences are large (Bennett and Smaldone, 1987). For children, very few clinical aerosol deposition measurements have been performed (Roy et al., 1986; Schiller-Scotland et al., 1992; Bennett et al., 1996). These clinical measurements can be compared to theoretical computations on a similar-age case by Martonen and Zhang (1993). As shown in Fig. 3, the general agreement of these measurements with theory is encouraging. However, good direct comparisons of predictions and clinical measurements for individuals are needed.

Although considerable scientific progress has been made on modeling aerosol deposition in children, similar progress has not been seen on behalf of the elderly. An initial modeling effort used the age-related increase in anatomic dead space in aging adults to estimate tracheobronchial airway dimensions (Schum et al., 1991). The predicted effect of this airway enlargement was to decrease the inspiratory bronchial deposition of

inhaled particles larger than about 0.5 μm (Table 3). As expected, larger airways would be less efficient than smaller airways at trapping inhaled particles by impaction, provided the airflows are unchanged.

5. Discussion

Modeling aerosol deposition efficiencies as a function of age is an area undergoing steady development. At this time, the approach used for adults appears to be valid for children in that the predictions and scant clinical data show similar trends in comparison to data from adults. Improvements are needed in several areas. Better ways of defining the appropriate airway shapes and dimensions, especially for individuals, are needed. Improvements in modeling the deposition of non-ideal aerosols are also required. Non-ideal aerosols include those that are hygroscopic, have significant charge, are volatile or have complex shapes. Additional research is needed on incorporating the complexities of airflow into the models, as current assumptions are highly simplified. In this regard, computational fluid dynamics (CFD) approaches may be important. Although CFD has only recently been applied to understanding the deposition of inhaled aerosols (Gradon and Orlicki, 1990), early results are encouraging (Ferron and Edwards, 1996; Hofmann, 1996; Oldham et al., 2000).

The effects of adult aging-related phenomena on inhaled aerosol deposition have not been well quantified, or even fully delineated. Increases in dead space, enlargement of distal airways, the cumulative effects of wear and tear, chronic disease related effects, changes in tissue elasticity and other factors may be significant. Modelers have neither placed much emphasis nor made major progress in modeling particle deposition in aging lungs.

What can be said in conclusion? First, current aerosol deposition models that are being applied to various age groups appear to have solid mechanistic foundations, but they still do not include all of the potentially relevant aerosol phenomena. Second, the important anatomical data for the

airways of healthy American children and healthy adults are largely known, but many gaps in data for other populations remain. Third, the models do not deal with individual variations well; the use of body size as well as age as a descriptor helps, but is inadequate in some cases. Fourth, the modeling efforts are proceeding in a logical manner, with computational fluid dynamic approaches now emerging, and the results obtained thus far are consistent with the scant available data from human clinical and bench-top surrogate model studies.

Acknowledgements

Appendix A. Equations for calculating inhaled particle deposition

When computing particle deposition in the respiratory tract it is customary to first calculate the inhalability (aspiration efficiency), which depends on particle size, wind speed, and wind direction in relation to the facing direction of the head (Ogden and Birkett, 1977; Vincent et al., 1990; Vincent, 1999). Wind-tunnel data with various sizes of mannequins indicate that one relationship may be used for all body sizes (Phalen et al., 1992). Next, deposition in the airways of the head must be calculated for nasal and oral breathing, for inhalation and exhalation and for two mechanisms, diffusion and impaction. These equations, used for all ages and body sizes, separately calculate deposition due to diffusion and due to impaction (NCRP, 1997). For the tracheobronchial and pulmonary regions, three equations are used for the diffusion mechanism (one for laminar flow and one for turbulent flow, and one for a pause in the breathing cycle), two equations are used for the sedimentation mechanism (one during airflow and one for a pause) and two equations are used for the impaction mechanism (depending on the Stokes' number). For various ages or body sizes, the airway dimensions and airflow rates must be scaled. Minor variations in the equations exist. The equations given here, except for inhalability, are those adopted by the NCRP (1997). The units used are those from the original sources.

A. Inhalability (averaged over all wind directions in relation to the direction facing)

$$I = 0.5(1 + \exp(-0.06d_{ae})) + pU^q\exp(rd_{ae})$$

where I = probability that a particle will be inhaled, d_{ae} = particle aerodynaimc diameter (μm), U = wind speed (m/sec), U = wind speed (m/sec), $p = 1.04 \times 10^{-5}$, q = 2.757, and r = 0.0540.

B. Nasal-Oral-Pharyngeal-Laryngeal Region
   1. Diffusion
      a. Nasal Breathing
         Inhalation

$$N_i = 1 - \exp(-18.2D^{1/2}Q^{-1/8})$$

Exhalation

$N_e = 1 - \exp(-21.3 D^{1/2} Q^{-1/8})$

b. Oral Breathing

Inhalation

$O_i = 1 - \exp(-14.6 D^{1/2} Q^{-1/8})$

Exhalation

$O_e = 1 - \exp(-12.1 D^{1/2} Q^{-1/8})$

where N = probability of deposition in entire region during nasal breathing, O = probability of deposition in entire region during oral breathing, i = inhalation, e = exhalation, Q = average airflow rate during inspiration or expiration in $cm^3\ sec^{-1}$ and D = diffusion coefficient of the particles in $cm^2\ sec^{-1}$.

2. Impaction

a. Nasal Breathing

Inhalation

$N_i = 1[1 + (\rho d^2 Q / 4{,}600)^{-0.94}]^{-1}$

Exhalation

$N_e = 1[1 + (\rho d^2 Q / 2{,}300)^{-1.01}]^{-1}$

b. Oral Breathing

Inhalation

$O_i = 1[1 + (\rho d^2 Q / 30{,}000)^{-1.37}]^{-1}$

Exhalation

$O_e = O_i$ (if there is no other information)

where d = particle geometric diameter (cm) and, ρ = particle density in $g\ cm^{-3}$.

C. Tracheobronchial and Pulmonary Region

1. Deposition by Diffusion

a. For laminar flow

$$P_D = 1 - 0819\ e^{-7.315x} - 0.0976\ e^{-44.61x} - 0.0325\ e^{-114x} - 0.0509\ e^{-79.31x^{2/3}}$$

where P_D = diffusion deposition probability, D = diffusion coefficient of particles ($cm^2\ sec^{-1}$), R = radius of tube or airway (cm), $\bar{v}$ = mean flow velocity ($cm\ sec^{-1}$), L = length of tube or airway segment (cm) and $x = LD/2R^2\bar{v}$.

b. For turbulent flow

$$P_D = 2\frac{\sqrt{Dt}}{R}\left(1 - 2\frac{\sqrt{Dt}}{9R} + \cdots\right) = 2.828x^{1/2}(1 - 0.314x^{1/2} + \cdots)$$

where t = time for flow to pass through the tube or airway segment = $L/\bar{v}$ (sec).

c. For a pause

$$P_D = 1 - \exp(-5.784 KTCt'/6\pi\mu r_p R^2)$$

where t' = pause time (sec), K = Bolzmann constant, 1.38×10^{-16} dyn cm K^{-1}, T = temperature (K), C = Cunningham slip correction factor, r_p = radius of the particle (cm) and μ = viscosity of fluid in g cm^{-1} sec^{-1} (dyn sec cm^{-2})

Effects of entrance configurations (Yeh, 1974)

$$f_e = 1 + C_1(2R/L) \text{ for } L/R > 10$$

where f_e = factor for correcting the effect of entrance configuration, $C_1 = (2\theta/\pi)(13 - 12\theta/\pi)$, θ = bend angle or branching angle (in radians).

The entrance corrected deposition probability is as follows.

$$P_D^E = 1 - (1 - P_D)^{f_e}$$

2. Deposition by Sedimentation

$$P_S = 1 - \exp\left[\frac{-4g C\rho_p r_p^2 L \cos\phi}{9\pi\mu R\bar{v}}\right]$$

where Ps = sedimentation deposition probability, g = acceleration due to gravity (cm sec^{-2}), ρ_p = density of the particle (g cm^{-3}), and ϕ = inclination angle relative to gravity ($\phi = 0$ degrees for horizontal tube).

For a pause, $L/\bar{v}$ is replaced by t' (the pause time) in sec.

3. Deposition by Inertial Impaction

$$P_1 = 1 - \frac{2}{\pi}\cos^{-1}(\theta St) + \frac{1}{\pi}\sin[2\cos^{-1}(\theta St)] \text{ for } \theta St < 1$$

$$P_i = 1 \text{ for } \theta St \geq 1$$

where P_i = impaction deposition probability, θ = bend angle or branching angle (in radians), and St = Stokes' numger = $C\rho_p r_p^2 \bar{v}/9\mu R$.

References

Anjilvel, S., Asgharian, B., 1995. A multiple-path model of particle deposition in the rat lung. Fund Appl. Toxicol. 28, 41–50.

Becquemin, M.M., Bertholon, J.F., Bouchikhi, A., Malarbet, J.L., Roy, M., 1999. Oronasal ventilation partitioning in adults and children: effect on aerosol deposition in airways. Radiat. Prot. Dosim. 81, 221–228.

Bennett, W.D., Smaldone, G.C., 1987. Human variation in the peripheral air-space deposition of inhaled particles. J. Appl. Physiol. 62, 1603–1610.

Bennett, W.D., Zeman, K.L., Kim, C.S., 1996. Variability of fine particle deposition in healthy adults: effect of age and gender. Am. J. Resp. Crit. Care Med. 153, 1641–1647.

Cheng, Y.S., Yamada, Y., Yeh, H.C., Swift, D.C., 1988. Diffusional deposition of ultrafine aerosols in a human nasal cast. J. Aerosol Sci. 19, 741–751.

Crawford, D.J., 1982. Identifying critical human subpopulations by age groups: radioactivity and the lung. Phys. Med. Biol. 27, 539–552.

Crawford, D.J., Eckerman, K.F., 1983. Modifications of the ICRP task group lung model to reflect size-dependence. Radiat. Prot. Dosim. 2, 209–220.

Ferron, G.A., Oberdörster, G., Henneberg, R., 1989. Estimation of the deposition of aerosolized drugs in the human respiratory tract due to hygroscopic growth. J. Aerosol Med. 2, 271–284.

Ferron, G.A., Edwards, D.A., 1996. Numerical simulation of air and particle transport in the conducting airways. J. Aerosol Med. 9, 303–316.

Findeisen, W., 1935. Über das absetzen kleiner, in der luft suspendierter teilchen in der menschlichen lunge bei der atmug. Pflügers Arch. 236, 367–379.

Gradon, L., Orlicki, D., 1990. Deposition of inhaled aerosol particles in a generation of the tracheobronchial tree. J. Aerosol Sci. 21, 3–19.

Guyton, A.C., 1947. Analysis of respiratory patterns in laboratory animals. Am. J. Physiol. 150, 78–83.

Heyder, J., Rudolf, G., 1984. Mathematical models of particle deposition in the human respiratory tract. J. Aerosol Sci. 15, 697–707.

Hofmann, W., Stainhäusler, F., Pohl, E., 1979. Dose calculations for the respiratory tract from inhaled natural radioactive nuclides as a function of age — I. Health Phys. 37, 517–532.

Hofmann, W., 1982. Dose calculations for the respiratory tract from inhaled natural radioactive nuclides as a function of age — II. Health Phys. 43, 31–44.

Hofmann, W., 1996. Lung morphometry and particle transport and deposition: overview of existing models. In: Marijnissen, J.C.M., Gradon, L. (Eds.), Aerosol Inhalation: Recent Research Frontiers. Kluwer Academic, Netherlands, pp. 91–102.

Hofmann, W., Martonen, T.B., Graham, R.C., 1989. Predicted deposition of nonhygroscopic aerosols in the lung as a function of subject age. J. Aerosol Med. 2, 49–68.

ICRP, 1994. Human Respiratory Tract Model for Radiological Protection. Publication 66. Pergamon Press, New York.

Kim, C.S., Hu, S.-C., 1998. Regional deposition of inhaled particles in human lungs: comparison between men and women. J. Appl. Physiol. 84, 1834–1844.

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., Zhang, Z., 1993. Deposition of sulfate acid aerosols in the developing human lung. Inhal. Toxicol. 5, 165–187.

NCRP, 1997. Deposition, retention and dosimetry of inhaled radioactive substances. NCRP SC 57-2 Report. National Council on Radiation Protection and Measurements, Bethesda, MD.

Ogden, T.L., Birkett, J.L., 1977. The human head as a dust sampler. In: Walton, W.H. (Ed.), Inahled Particles IV. Pergamon Press, Oxford, pp. 93–105.

Oldham, M.J., Phalen, R.F., Heistracher, T., 2000. Computational fluid dynamic predictions and experimental results for particle deposition in an airway model. Aerosol Sci. Technol. 32, 61–71.

Phalen, R.F., Oldham, M.J., Beaucage, C.B., Crocker, T.T., Mortensen, J., 1985. Postnatal enlargement of human tracheobronchial airways and implications for particle deposition. Anat. Rec. 212, 368–380.

Phalen, R.F., Schum, G.M., Oldham, M.J., 1990. The sensitivity of an inhaled aerosol tracheobronchial deposition model to input parameters. J. Aerosol Med. 3, 271–282.

Phalen, R.F., Oldham, M.J., Dunn-Rankin, D., 1992. Inhaled particulate mass per unit body mass per unit time. Appl. Occup. Envir. Hygiene 7, 246–252.

Pritchard, J.N., Jefferies, J., Black, A., 1986. Sex differences in the regional deposition of inhaled particles in the 2.5-7.5 µm size range. J. Aerosol Sci. 17, 385–389.

Roy, M., Becquemin, M.H., Bonnefous, S., Bouchikhi, A., Patty, E., Lafuma, A., Perrier, J.C., 1986. Clinical study of inhaled aerosols total deposition in healthy adults and children. Presented at the Commission of the European Communities Symposium, Brazil.

Schiller-Scotland, C.F., Hlawa, R., Gebhart, J., Wönne, R., Heyder, J., 1992. Total deposition of aerosol particles in the respiratory tract of children during spontaneous and controlled mouth breathing. J. Aerosol Sci. 23 (Suppl. 1), S457–S460.

Schulz, H., Brand, P., Heyder, J., 2000. Particle deposition in the respiratory tract. In: Gehr, P.J., Heyder, J. (Eds.), Particle–Lung Interactions. Dekker, New York, pp. 229–290.

Schum, G.M., Phalen, R.F., Oldham, M.J., 1991. The effect of dead space on inhaled particle deposition. J. Aerosol Med. 4, 297–311.

Stahlhofen, W., Rudolf, G., James, A.C., 1989. Intercomparison of experimental regional aerosol deposition data. J. Aerosol Med. 2, 285–308.

Task Group on Lung Dynamics (Paul E. Morrow, Chairman), 1966. Deposition and retention models for internal dosimetry of the human respiratory tract. Health Phys. 12, 173–207.

Taulbee, D.M., Yu, C.P., 1975. A theory of aerosol deposition in the human respiratory tract. J. Appl. Physiol. 38, 77–85.

Vincent, J.H., Mark, D., Miller, B.G., Armbruster, L., Ogden, T.L., 1990. Aerosol inhalability at higher windspeeds. J. Aerosol Sci. 21, 577–586.

Vincent, J.H., 1999. Sampling criteria for the inhalable fraction. In: Vincent, J.H. (Ed.) Particle Size-selective Sampling for Particulate Air Contaminants. American Conference of Governmental Industrial Hygienists, Cincinnati, OH, pp. 51–72.

Xu, G.B., Yu, C.P., 1986. Effects of age on deposition of inhaled aerosols in the human lung. Aerosol Sci. Technol. 5, 349–357.

Yeh, H.C., 1974. Use of a heat transfer analogy for a mathematical model of respiratory tact deposition. Bull. Math. Biol. 36, 105–116.

Yeh, H.C., Schum, G.M., 1980. Models of human airways and their application to inhaled particle deposition. Bull. Math. Biol. 42, 461–480.

Yeh, H.C., Cuddihy, R.G., Phalen, R.F., Chang, I.Y., 1996. Comparisons of calculated respiratory tract deposition of particles based on the proposed NCRP model and the new ICRP66 model. Aerosol Sci. Technol. 25, 134–140.

Yu, C.P., Xu, G.B., 1987. Predicted deposition of diesel particles in young humans. J. Aerosol Sci. 18, 419–429.