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Regional lung deposition of aged and diluted sidestream tobacco smoke

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Abstract. Since aged and diluted smoke particles are in general smaller and more stable than mainstream tobacco smoke, it should be possible to model their deposition on the basis of their measured particle diameters. However in practice, measured deposition values are consistently greater than those predicted by deposition models. Thus the primary objective of this study was to compare theoretical predictions obtained by the Monte Carlo code IDEAL with two human deposition studies to attempt to reconcile these differences. In the first study, male and female volunteers inhaled aged and diluted sidestream tobacco smoke at two steady-state concentrations under normal tidal breathing conditions. In the second study, male volunteers inhaled aged and diluted sidestream smoke labelled with ^{212}Pb to fixed inhalation patterns. Median particle diameters in the two studies were 125 nm (CMD) and 210 nm (AMD), respectively. Experimental data on total deposition were consistently higher than the corresponding theoretical predictions, exhibiting significant inter-subject variations. However, measured and calculated regional deposition data are quite similar to each other, except for the extra-thoracic region. This discrepancy suggests that either the initial particle diameter decreases upon inspiration and/or additional deposition mechanisms are operating in the case of tobacco smoke particles.

1. Introduction

Despite widespread prevalence of tobacco smoking in the population, very few studies of the total and regional deposition of smoke particles in the lung have been reported, either for mainstream (active) or environmental (passive) tobacco smoke. A recent review [1] has summarised experimental retention efficiency data and shown efficiencies of 60-80% for mainstream smoke, but 10-40% for environmental tobacco smoke (or aged and diluted sidestream smoke). These differences may arise from differences in particle diameter and chemistry, but may also be influenced by normal inhalation versus smoking behaviour [2].

Aged and diluted sidestream smoke particles are in general smaller and more stable than mainstream tobacco smoke. On dilution, coagulation is no longer significant, a significant mass fraction of the particles evaporates, and little hygroscopic growth potential is observed. Thus it should be possible to model deposition behaviour of these smoke particles on the basis of their measured diameter. However in practice, measured deposition values are greater than those predicted by the model for the controlled breathing conditions used experimentally [3].

2. Model description

Deposition of inhaled cigarette smoke was computed by an updated version of the stochastic Lagrangian transport and deposition model IDEAL, which was originally developed by Koblinger and Hofmann [4] and Hofmann and Koblinger [5]. In this computational model, geometric airway parameters, such as diameters, lengths, branching and gravity angles are randomly selected from probability density distributions and correlations among some of these parameters, derived from published morphometric data. The random walk of single particles, inhaled at randomly selected times during inhalation, through the stochastic, asymmetric lung structure on inspiration and expiration is simulated by Monte Carlo methods. Particle deposition in single airways is calculated by using analytical equations in straight and bent tubes for the physical deposition mechanisms affecting submicron particle deposition, such as Brownian motion or inertial impaction. Hence deposition of an individual particle is based on the average deposition behaviour of many particles.

To demonstrate the validity of the stochastic deposition model for ultrafine particles, predicted total deposition values were compared in Figure 1 with the experimental data of Heyder et al. [6] and Schiller et al. [7] for monodisperse spherical particles under oral breathing conditions. Considering the effect of inter-subject variability on lung deposition, excellent agreement between experimental data and theoretical predictions was obtained.

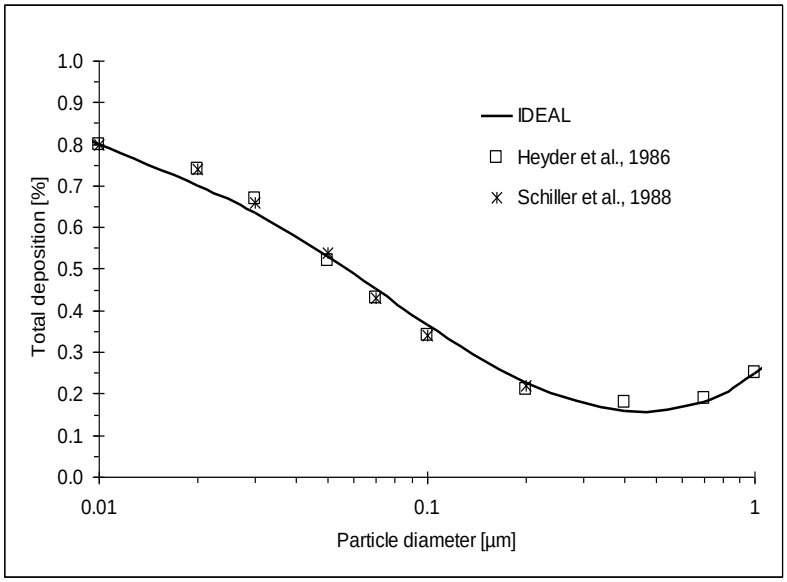

Figure 1. Comparison of theoretical predictions of total deposition with experimental data in human test subjects for a flow rate of 250 ml.s^{-1}, a tidal volume of 1000 ml, and a breathing frequency of 7.5 min^{-1} [6,7] under oral breathing conditions.

3. Results

In the current paper, data from two earlier human deposition studies with additional regional and inhalation information have been re-analysed to attempt to reconcile the observed differences between experimental data and modelling predictions.

3.1. Exhale capture study

In the first study [7], ten non-smoking male and ten female subjects inhaled aged and diluted sidestream tobacco smoke via an oro-nasal mask at two steady-state concentrations (termed high and low, on average, 980$\pm$140 and 150$\pm$60 µg.m^{-3} respectively) over a period of 60 minutes with exhale

capture to a vacuum-assisted filter pack. Particle diameter was measured using a quartz crystal microbalance (MMD = 140 nm, GSD = 2.5) and a Las-X spectrometer (CMD = 125 nm, GSD = 1.5). Retention efficiency for UVPM (UV absorbance at 325 nm [9]), solanesol [10] and nicotine was carried out with retention approximately 40 ± 20% for the two particulate markers and 80 ± 20% for the vapour phase nicotine. Inhalation patterns for both genders showed average depths of 17 ± 6% of FVC, implying normal tidal breathing was approached during the exposure. Average breathing patterns measured were 7.5 x 0.94 $l.min^{-1}$ (male), and 9.4 x 0.63 $l.min^{-1}$ (female).

Table 1. Comparison of measured total deposition (retention) data with modelling predictions.

Condition	Male retention (%)		Female retention (%)	
	exp	mod	exp	mod
UVPM high	41 ± 14	28	17 ± 10	26
UVPM low	36 ± 20	30	-	-
Solanesol high	40 ± 20	28	27 ± 14	22

While theoretical predictions were consistently lower than the corresponding experimental data, as shown in Table 1, they still fall within the range of the reported standard deviations.

Since high inter-subject variations were observed in the experiments for both men and women for all three markers, the individual exposure data were used to compute individual deposition data for both male (Figure 2) and female (Figure 3) volunteers. While measured total deposition in the male subjects is consistently higher than the corresponding computed values, agreement is obtained for the average of the female subjects. A number of low UVPM values were unavailable for the females as the exhaled amount was below the limit of quantification.

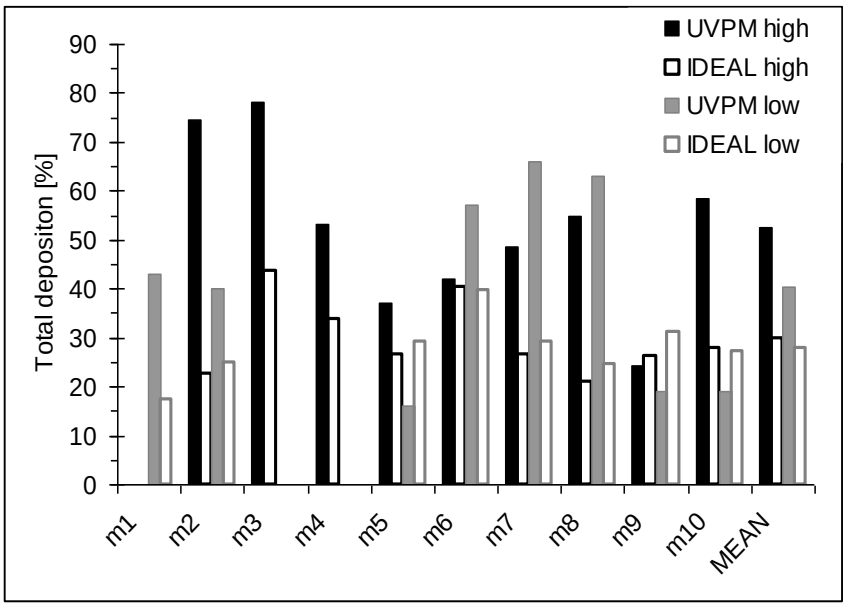

Figure 2. Comparison of measured total UVPM deposition (retention) data with modelling predictions for male volunteers for high and low concentrations.

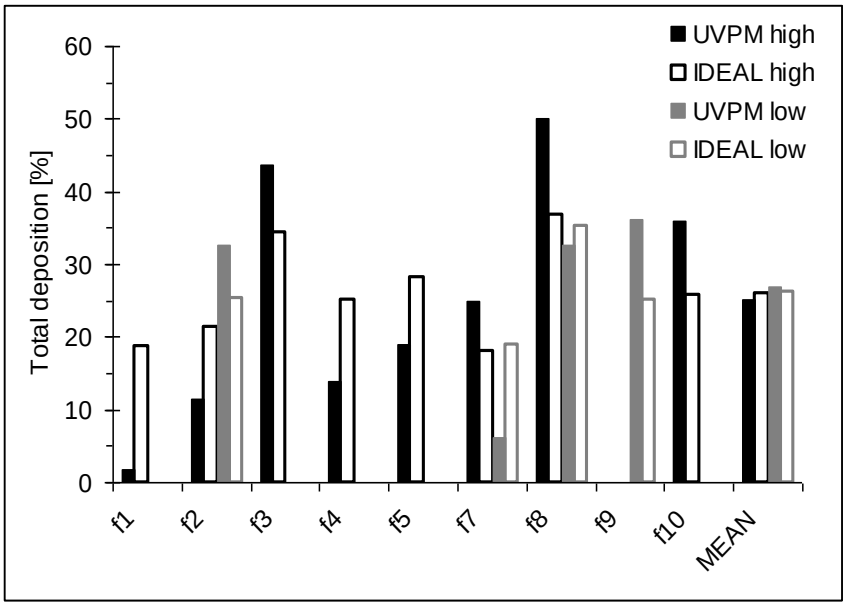

Figure 3. Comparison of measured total UVPM deposition (retention) data with modelling predictions for female volunteers for high and low concentrations.

3.2. Radiotracer study

In the second study [11], nine non-smoking male volunteers inhaled aged and diluted sidestream smoke labeled with ^{212}Pb [12] to fixed inhalation patterns. This smoke was aged for 15 minutes to meet radiological protection needs. Particle diameters were measured using a quartz crystal microbalance (MMD = 180 nm, GSD = 1.5) and a Delron low pressure impactor (AMD = 210 nm, GSD = 1.4). The measured half-time of bronchial clearance ranged on average from 8 – 12 hours. Total deposition is shown in Table 2 and regional deposition patterns are listed in Table 3.

Table 2. Average measured and modelled total deposition for three different breathing patterns.

Breathing pattern	Measured retention (%)	Modelled retention (%)
Nose: 6 x 1.0 l.min^{-1}	54 ± 10	27
Mouth: 6 x 1.0 l.min^{-1}	43 ± 17	25
Mouth: 12 x 0.5 l.min^{-1}	22 ± 8	14

Experimental data on total deposition for the different breathing patterns are consistently higher than the corresponding theoretical predictions. However, measured and calculated regional deposition data are quite similar proportionally to each other, except for the extra-thoracic region. This suggests

that the same factors, such as size reduction upon inhalation or additional deposition mechanisms affect deposition in all regions of the respiratory tract.

Table 3. Average measured and modelled regional deposition for three different breathing patterns.

Regional deposition	Measured rentention (%)	Modelled retention (%)
Extrathoracic	7 – 11	1 – 9
Bronchial	18 – 22	21 – 30
Alveolar	67 – 73	68 – 76

4. Conclusions

In both studies analysed in this paper, experimental data on total deposition are generally higher than the corresponding theoretical predictions. These findings are consistent with the experimental results of Morawska et al. [3], who observed similar differences. Since model predictions exhibit excellent agreement with experimental data for inert spherical particles [6,7], these differences may be attributed to either changes in particle diameter when entering the warm and humid atmosphere of the human lung, e.g. evaporation of volatile compounds or condensation-induced restructuring, and/or to additional deposition mechanisms which operate specifically for tobacco smoke particles, e.g. electrical charge effects, chain aggregation or cloud behaviour [13]. For ultrafine particles, Brownian motion is the dominating physical deposition mechanism, increasing deposition with decreasing particle diameter. Thus the experimental data suggest aerodynamic behaviour more consistent with smaller particles. In contrast, measured and calculated regional deposition data are quite similar to each other, indicating that the above mechanisms affect deposition in all regions of the respiratory tract.

Further work will seek to visualise sidestream smoke under similar and ageing conditions with electron microscopy and mobility measurements to determine the plausibility of shape factors, aggregation and charge.

Ethical Considerations

This work involved a re-analysis of data from two volunteer studies conducted by one of the current authors whilst at AEA Technology. Details of the procedures for ethical oversight for the original studies are contained in references [8,9].

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