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Modeling regional deposited dose of submicron aerosol particles

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HIGHLIGHTS

- Modeling can accurately estimate deposited dose of aerosol particles in the respiratory system.
- Hygroscopicity of inhaled particles is an important factor in calculations of deposited dose.
- Most likely, adult males receive higher deposited dose than adult females.
- The pulmonary/alveolar region received the largest fraction of the deposited dose.
- The deposited dose received on workdays is high because the exposure level is high.

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ABSTRACT

We developed a simple model to calculate the regional deposited dose of submicron aerosol particles in the respiratory system. This model incorporates measured outdoor and modeled indoor particle number size distributions, detailed activity patterns of three age groups (teens, adults, and the elderly), semi-empirical estimation of the regional deposition fraction, hygroscopic properties of urban aerosols, and reported breathing minute volumes. We calculated the total and regional deposited dose based on three concentration metrics: particle number (PN), mass (PM), and surface area (PSA). The 24-h total deposited dose of fine particles in adult males was around 40 μg (57 × 109 particles, 8 × 102 mm^2) and 41 μg (40 × 109 particles, 8 × 102 mm^2) on workdays and weekends, respectively. The total and regional 24-h deposited dose based on any of the metrics was at most 1.5 times higher in males than in females. The deposited dose values in the other age groups were slightly different than in adults. Regardless of the particle size fraction or the deposited dose metric, the pulmonary/alveolar region received the largest fraction of the deposited dose. These values represent the lowest estimate of the deposited dose and they are expected to be higher in real-life conditions after considering indoor sources of aerosol particles and spatial variability of outdoor aerosols. This model can be extended to youngsters (<12 years old) after gaining accurate information about the deposition fraction inside their respiratory system and their breathing pattern. This investigation is foreseen to bridge the gap between exposure and response in epidemiological studies.

1. Introduction

Air pollution can be in the form of gas phase or particulate matter that exists with sufficient amounts in the atmosphere leading to environmental impacts and health effects, which have been directly linked to the so called "deposited dose" (e.g. Anderson, 2009; Dockery et al., 2005; Lohmann and Feichter, 2005; Pope et al., 2002; Haywood and Boucher, 2000; Künzli et al., 2000; Jones, 1999).

The deposited dose can be measured by monitoring the inhaled and exhaled particle concentrations. This method can be also extended to get an empirical estimation for the deposition patterns of aerosol particles in the respiratory system. In practice, the regional dose in the respiratory system is very difficult to be addressed experimentally. Therefore, the regional dose is typically estimated by means of mathematical models; the most widely available are the International Commission on Radiological Protection model (ICRP) and the multiple path particle dosimetry model (MPPD). To calculate the deposited dose with such models requires the exposure time and level, breathing characteristics, respiratory parameters, anatomy of the lungs, and physical–chemical properties of inhaled particles. Typically, the

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exposure is better understood than respiratory parameters, anatomy, and particle characteristics. The latter three factors influence the deposited dose substantially. For instance the deposited dose of ultrafine particles (UFP, diameter <0.1 μm) increases 4–5 times during exercise as a result of high volumes of breathed air (Löndahl et al., 2007; Daigle et al., 2003). The deposited dose may be altered in people with lung disease (Löndahl et al., 2012; Chalupa et al., 2004; Anderson et al., 1990). The physical–chemical properties of inhaled particles could increase the deposited dose, when estimated by particle number or surface area, by at least 16-fold even at the same mass concentrations (Löndahl et al., 2009).

However, the deposited dose has been often reported in terms of deposited amounts of particulate mass. Particle surface area or number concentration, chemical composition, physical properties, and toxicity of inhaled particles might also be important issues in risk analysis and health effects (e.g. Osunsanya et al., 2001; Seaton et al., 1995). Therefore, we should gain more understanding about the deposited dose based on particle surface area and number concentration besides particulate mass concentration (e.g. Oberdörster et al., 2004; Annals of the International Commission on Radiological Protection, ICRP, 1994). Furthermore, models of deposited dose are mostly based on particulate mass measures for exposure and they are typically valid for spherical hydrophobic particles. In the real world, particles are usually irregular in shape and hygroscopic. Being hygroscopic implies that the particle grows in size by absorbing water when exposed to a humid environment such as that inside the respiratory system. This would alter the deposited dose calculations because the deposition of aerosol particles depends on the particle size. For instance, a hydrophobic 0.1 μm particle may have 2–4 times higher deposition probability compared to a hygroscopic particle (Löndahl et al., 2007). Therefore, the actual particle size inside the respiratory system is a vital parameter in order to obtain a proper estimate for the deposited dose.

In this work we developed a simple model to calculate the regional deposition of submicron aerosol particles in subjects older than 12 years classified into three age groups: teens, adults, and the elderly. Our calculations were based on measured and simulated particle number size distribution and we assumed spherical particles with unit density to calculate the deposited dose for three concentration metrics: particle number (PN), particle mass (PM), and particle surface area (PSA). This model incorporates the hygroscopic properties of urban aerosol particles reported by Massling et al. (2005). We described the deposition patterns of submicron aerosol particles inside the respiratory system by merging the reported results from both the ICRP and MPPD with experimental observations by Löndahl et al. (2007). We applied this model for a population group (teens, adults, and the elderly; males and females) that included school students, teachers, and their families with their activity patterns reported by Hussein et al. (2012a).

2. Materials and Methods

Mathematically, the deposited dose of a certain particle size-fraction (D_{p1}–D_{p2}) based on particle number could be described as

$$\mathrm{Dose}_{PN} = \int_{t1}^{t2}\int_{D_{p1}}^{D_{p2}} V_E \cdot DF \cdot n_N^0 \cdot d\log D_p \cdot dt \quad (1)$$

where VE [cm^3/min] is the minute ventilation (or so called volume of air breathed), DF [−−] is the deposition fraction of aerosol particles in the respiratory system, and $n_N{}^0 = dN/d\log(D_p)$ [particles/cm^3] is the lognormal particle number size distribution. Both DF and $n_N{}^0$ are functions of $\log(D_p)$ where D_p is the particle diameter. The integrals are evaluated during an exposure time period $\Delta t = t_2 - t_1$ based on half-hourly time resolution and 36-bins of submicron particle diameter.

Similarly, the deposited dose based on other metrics (denoted by f) can be extended from Eq. (1)

$$\mathrm{Dose}_f = \int_{t1}^{t2}\int_{D_{p1}}^{D_{p2}} V_E \cdot DF \cdot n_N^0 \cdot f \cdot d\log D_p \cdot dt \quad (2)$$

where f is a dose metric such as particle surface area (πD_p^2) or particle mass $\left(\frac{\pi}{6} D_p^3 \rho_p\right)$.

Evaluation of Eq. ((1) or (2)) requires the following:

1. Activity pattern conducted by a certain age group.
2. Minute ventilation (V_E).
3. Size-dependent deposition fraction of aerosol particles (DF) in the respiratory system.
4. Particle number size distribution ($n_N{}^0$) contained in the air breathed.
5. Hygroscopic properties of aerosol particles.

Therefore, the deposited dose calculation consisted of several parts: adoption of minute ventilation values from the literature, derivation of regional deposition patterns of aerosol particles inside the respiratory system, processing of outdoor particle number size distributions taken from routine measurements at an urban background site, model simulations of indoor particle number size distributions inside an average size classroom and a typical Finnish apartment, parameterization of the hygroscopic properties of aerosol particles, and utilization of activity patterns.

2.1. Activity Patterns

We distinguished subjects into three age categories: teens (12–18 years), adults (18–63 years), and the elderly (older than 63 years). We then utilized the daily activity pattern results reported by Hussein et al. (2012a) for school students and their families in Helsinki (Table 1 and Fig. 1). The questionnaire was conducted during three periods in year 2009: period I (January 31–February 8), period II (March 21–29), and period III (May 16–24). The subjects reported their activities and residence place with half-hourly time resolution. The questionnaire included three main categories for the type of residence: indoor, outdoor, and transportation. The indoor category included five subcategories: home, kindergarten/school, work, shops, and others. The outdoor category included four subcategories: work, city, nature, and others. We counted the time spent at home to be either sleeping or sitting/standing, at work to be sitting/standing, outdoors and other indoor environments to be walking, and being in transportation as sitting or standing.

Table 1
Residence time (hours) based on gender and age according to the activity pattern diary by Hussein et al. (2012a).

Gender	Age group [years]			Indoor			Outdoor	Traffic
				Home	School work	Shops others		
Females	Teens	12–17	Weekends	17.7	–	4.0	1.6	0.7
			Workdays	16.2	4.9	1.2	1.4	0.4
	Adults	18–63	Weekends	17.6	0.6	3.2	1.8	0.8
			Workdays	14.7	5.5	1.7	1.0	1.1
	Elderly	>63	Weekends	19.4	–	2.9	1.2	0.4
			Workdays	19.2	0.5	2.9	0.8	0.6
Males	Teens	12–17	Weekends	16.7	–	4.1	2.5	0.8
			Workdays	15.1	4.5	1.6	2.3	0.6
	Adults	18–63	Weekends	16.4	0.3	3.9	2.3	1.1
			Workdays	12.8	5.5	2.5	1.3	1.9
	Elderly	>63	Weekends	17.4	0.1	3.9	1.6	1.0
			Workdays	19.4	0.1	2.4	1.2	0.8