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Indoor aerosol modeling for assessment of exposure and respiratory tract deposited dose

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HIGHLIGHTS

- Indoor Aerosol Models (IAM) have the potential to replace indoor measurements.
- In exposure assessment, IAM can be coupled with urban air quality and inhaled dose models.
- Exposure to outdoor aerosols also occurs indoors.
- Inclusion of indoor sources in IAM is more realistic for accurate exposure assessment.

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ABSTRACT

Air pollution is one of the major environmental problems that influence people's health. Exposure to harmful particulate matter (PM) occurs both outdoors and indoors, but while people spend most of their time indoors, the indoor exposures tend to dominate. Moreover, higher PM concentrations due to indoor sources and tightness of indoor environments may substantially add to the outdoor originating exposures. Empirical and real-time assessment of human exposure is often impossible; therefore, indoor aerosol modeling (IAM) can be used as a superior method in exposure and health effects studies. This paper presents a simple approach in combining available aerosol-based modeling techniques to evaluate the real-time exposure and respiratory tract deposited dose based on particle size. Our simple approach consists of outdoor aerosol data base, IAM simulations, time-activity pattern data-base, physical –chemical properties of inhaled aerosols, and semi-empirical deposition fraction of aerosols in the respiratory tract. These modeling techniques allow the characterization of regional deposited dose in any metric: particle mass, particle number, and surface area. The first part of this presentation reviews recent advances in simple mass-balance based modeling methods that are needed in analyzing the health relevance of indoor exposures. The second part illustrates the use of IAM in the calculations of exposure and deposited dose. Contrary to previous methods, the approach presented is a real-time approach and it goes beyond the exposure assessment to provide the required information for the health risk assessment, which is the respiratory tract deposited dose. This simplified approach is foreseen to support epidemiological studies focusing on exposures originating from both indoor and outdoor sources.

1. Introduction

The first step for assessing the health effects of inhaled aerosol particles is based on the evaluation of the human exposure levels (e.g. Nethery et al., 2008; Gerharz and Pebesma, 2013). The next step to deepen the understanding is to calculate the deposited dose in the respiratory tract (e.g. Löndahl et al., 2007). Recently, Hänninen et al. (2014) highlighted the dominating role of

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particulate matter (PM) effects against eight other environmental stressors in six European countries. PM mass concentration of outdoor atmospheric aerosols has been identified as a health relevant metric originally in the Harvard Six Cities study and followed by the American Cancer Society study and a large number of follow-up studies (e.g. Pope and Dockery, 2006). The effects are seen to occur at relatively low particle mass concentrations; and therefore, it has been suggested that the toxicity of inhaled particles, especially for ultrafine particles (UFP, diameter < 0.1 μm), can be also due to their number or surface area concentrations (e.g. Osunsanya et al., 2001). Therefore, other aerosol metrics should be adopted besides PM mass concentrations in health risk assessments.

The deposited dose of atmospheric aerosols in the human respiratory tract is measured by monitoring the inhaled and exhaled particle concentrations. This provides an empirical estimation for the total deposition pattern of aerosol particles in the respiratory system. Due to experimental limitations, the regional dose in the respiratory system is typically estimated by means of mathematical models. The most widely available are the International Commission on Radiological Protection model (ICRP, 1994) and the Multiple Path Particle Dosimetry model (MPPD, Chemical Industry Institute of Toxicology, Research Triangle Park, NC).

Exposure to harmful aerosol particles occurs both indoors and outdoors. While being indoors people are exposed to a mixture of particles that are either from outdoor origin or produced indoors (Kaur et al., 2007). Besides the outdoor air, indoor aerosol particles are also produced indoors due to a vast range of inhabitants' activities, which emit high quantities of aerosol particles (secondary and primary) and also vapors, which are involved in the dynamics and chemical reactions of indoor aerosol particles. The most common indoor sources are produced during combustion processes, operation of electric appliances, computer equipment, etc, (e.g. Abdullahi et al., 2013; Wu et al., 2012; Glytsos et al., 2010; Sjaastad and Svendsen, 2008; Lazaridis et al., 2006; Abt et al., 2000; Hetland et al., 2000). There are also many poorly understood emerging sources that introduce new exposure aspects indoors such as electronic cigarettes, decorative ethanol fireplaces, zeolites from washing powders, and household products containing nanoparticles (Schripp et al., 2014, 2013; Quadros and Marr, 2011; Gudmundsson et al., 2007).

Human exposure can be measured in real-time by accompanying portable instruments to the subject and recording the air pollutants concentrations at the breathing zone (e.g. Broich et al., 2012). However, this is a big burden on the subjects, especially when they are elderly or children, and it is sometimes annoying, disturbing, and stressful to keep and carry instruments while moving around. An alternative method is to setup monitoring networks to record the exposure levels in space and to combine that with detailed information on residence location and time of subjects; i.e. time–activity patterns (e.g. Buonanno et al., 2014; Hussein et al., 2012a; Freeman and Tejada, 2002). But establishing and maintaining monitoring networks can be cumbersome and not always possible. Therefore, modeling of air pollution (both indoors and outdoors) and modeling of the respiratory tract deposited dose with combination of time-activity pattern diaries can serve as a useful alternative approach (e.g. Hussein et al., 2013). This approach is also valuable to predict the health effects in advance by means of air quality forecast models, which have become more available now days.

The main objective of the current article is to present a simple approach in combining available aerosol-based modeling techniques to evaluate the exposure and regional deposited dose in the human respiratory tract. This approach consists of outdoor aerosol data base (either measured or modeled), indoor aerosol model (IAM) simulations to generate indoor aerosol data-bases, time–activity pattern data-base, physical–chemical properties of inhaled aerosols, and semi-empirical deposition fraction of aerosols in the respiratory system. We first briefly describe the basic principles of IAM and their general application. Then we illustrate the use of IAM in the calculations of exposure and deposited dose. This simplified approach is foreseen suitable for supporting exposure assessment in epidemiological studies focusing on indoor exposures, originating from both indoor and outdoor sources. Contrary to previous methods, the approach presented in this article goes beyond the exposure assessment by estimating the respiratory tract deposited dose, which is needed for health risk assessment.

2. Exposure and deposited dose calculation

A key link to relate indoor air quality to biological response is the deposited dose (Fig. 1), here defined as the amount of aerosol deposited in the respiratory tract during breathing. As suggested by Hussein et al. (2013), the deposited dose can be expressed as

$$\text{Deposited Dose}_f = \int_{t1}^{t2} \int_{D_{p1}}^{D_{p2}} V_E \cdot DF \cdot n_N^0 \cdot f \cdot d \log D_p \cdot \mathrm{d}t \qquad (1)$$

where V_E is the minute ventilation (or breathing rate: volume of air breathed per time), DF is the deposition fraction of aerosol particles in the respiratory system, and $n_N^0 = dN/d\log(D_p)$ 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. f is a dose metric such as particle surface area (πD_p^2) or particle mass $\left(\frac{\pi}{6} D_p^3 \rho_p\right)$, where ρ_p is the particle density. The double integral is evaluated for an exposure time period $\Delta t = t_2 - t_1$ based on any selected time resolution.

The minute ventilation (V_E) depends on the body size of the subject (e.g. Bennett and Zeman, 2004). It also depends on the activity and status of the subject (e.g. Holmes, 1994; ICRP, 1994). The deposition fraction (DF) is different for different parts of the respiratory system (head/throat, tracheobronchial, and pulmonary/alveolar). It is also dependent on the physiology, status, and activity of the subject (Löndahl et al., 2007; ICRP, 1994; MPPD).

An important issue to be taken into account is the physical–chemical properties of inhaled particles. For instance, the DF curves are usually reported for hydrophobic particles (ICRP, 1994); but in reality ambient particles usually are hygroscopic to some extent (Swietlicki et al., 2008). This affects the size of the particles while being inside the respiratory system at relative humidity around 99.5% (e.g. Asgharin, 2004) and consequently also the deposition probability (DF).

Several data-bases of outdoor aerosol particle concentrations are available and easily accessible, especially at urban background locations (e.g. Chow et al., 2002). However, data-bases of indoor aerosol particles are not usually available. Therefore, an IAM is expected to have a key role in exposure studies as an alternative to actual indoor aerosol measurements.

3. Indoor aerosol modeling – Mass-balance equation

Indoor aerosol models (IAM) have important applications. One of the most important applications is their utilization in exposure assessment to provide information about the real-time exposure level and deposited dose (e.g. Hussein et al., 2013). This is based on two facts. First, that exposure to outdoor particles also occurs indoors because they can easily penetrate indoors (e.g. Hänninen et al., 2013, 2011, 2004). Second, the urban population in developed countries spend most of their time indoors (e.g. Hussein et al.,

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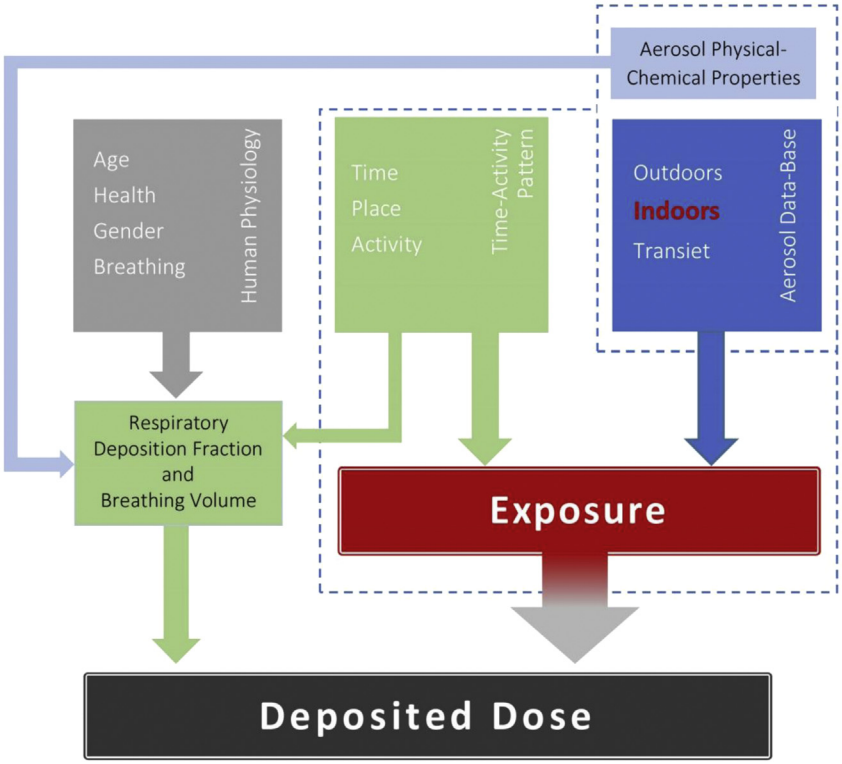

Fig. 1. A schematic diagram illustrating calculation of the respiratory tract deposited dose with an emphasis on the indoor aerosol data-base.

2012a; Schweizer et al., 2007; Klepeis et al., 2001; McCurdy et al., 2000). These two facts make the indoor aerosol processes a central modifier and determinant of the exposure level. Using an IAM and combining exposure assessment in a temporal-spatial basis can recover a missing insight into real-time personal exposure, which is needed for health effects assessment and epidemiology investigations.

The type and amount of aerosol particles present in indoor air are, in general, governed by the strength and type of sources, transformation processes, and fate of aerosol particles (Fig. 2). The concentrations of the transported particles from the outdoor air into the indoor air are affected by filtration and infiltration processes. The state and properties of the particles are also modified by the changes in the ambient conditions (temperature, relative humidity, etc.) between the indoor and outdoor environments. While indoors, the aerosol particles are either deposited onto indoor surfaces or removed from the indoor air via air cleaners or by ventilation. Aerosol particles also undergo complex processes through aerosol dynamics and chemical reactions that change their state, concentration, and physical–chemical properties. This dynamic behavior of indoor aerosols can be described by the mass-balance-equation (e.g. Hussein and Kulmala, 2008; Nazaroff, 2004). It is a first-order differential equation:

$$\frac{dI}{dt} = P\lambda O - (\lambda + \lambda_d)I + \mathrm{Re} + S + \left.\frac{dI}{dt}\right|_{\mathrm{others}} \quad (2)$$

where t is the time, I and O are the indoor and outdoor aerosol concentrations, respectively; P is the penetration factor of aerosol particles while being transported from the outdoor air into the indoor air, λ is the ventilation rate, λ_d is the deposition rate of aerosol particles onto available indoor surfaces, Re is the re-suspension rate of aerosol particles from indoor surfaces to become airborne again, S represents the emission rates due to indoor sources, and the last term is the change rate due to other process (e.g. coagulation, condensation, evaporation, chemical reaction, etc.).

In general, the mass-balance equation can be solved numerically, but it holds an analytical solution whenever O, P, λ, and λ_d are all constant in time. A well-mixed indoor air is a key assumption for

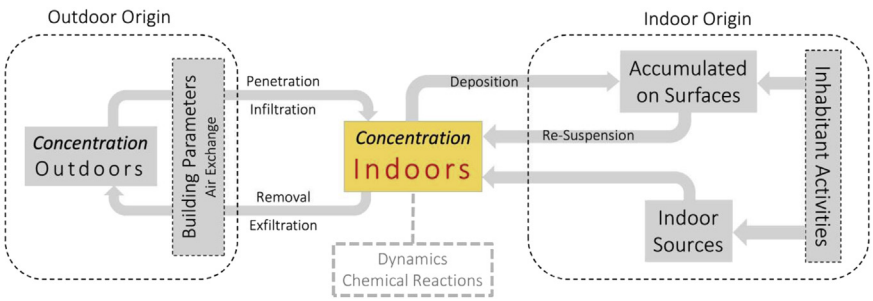

Fig. 2. A schematic diagram illustrating the main parts of an indoor aerosol model (IAM).

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the mass-balance equation to be valid (e.g. Hussein and Kulmala, 2008; Thatcher et al., 2002). Otherwise, spatial variation of indoor aerosol particle concentrations must be taken into account by, for example, utilizing Computational Fluid Dynamic (CFD) models (Hussein et al., 2005b; Gadgil et al., 2003; Feustel, 1999). In practice, the mass-balance equation is easier to adopt in exposure analysis.

The simplest form of IAM describes the dynamic behavior of a single component (e.g. total number concentration, number or mass concentration) inside a single compartment (e.g. Jamriska et al., 2003; Riley et al., 2002). In general, particles with different sizes behave differently depending on their physical and chemical properties; and thus, aerosol particles are treated by considering individual size-fraction where their properties and dynamic behavior is similar. Each particle size fraction requires a separate mass-balance equation. An additional term can be implemented in each mass-balance equation to describe the change rate due to coagulation, chemical reactions, or interaction with the surrounding vapors (condensation or evaporation).

Usually dwellings consist of more than one room and several floors; i.e. they are multi-compartment. Therefore, each compartment is assumed to have a well-mixed indoor domain; and thus, can be represented with a single mass-balance equation that incorporates internal air exchange rates between indoor compartments (e.g. Mølgaard et al., 2013; Hussein et al., 2006; Miller and Nazaroff, 2001; Thornburg et al., 2001; Mosley et al., 2001). In any case, each zone has its own parameters such as P, λ, λ_d, S, Re, and etc.

4. Model simulation scenarios

4.1. Indoor aerosol model (IAM) simulations

Indoor aerosol models (IAM) can be used to estimate the particle concentrations in an indoor environment. Initially, consider the outdoor concentration of a certain air pollutant is constant (O = constant) all the time and its concentration indoors is initially zero ($I = 0$ at $t_0 = 0$). Furthermore, assume P, λ_d, and λ are all constant. By omitting indoor sources, re-suspension, and chemical reaction/dynamics, the analytical solution of the indoor-to-outdoor concentration ratio is:

$$\frac{I(t)}{O} = \frac{P\lambda}{\lambda + \lambda_d}\left[1 - e^{-(\lambda+\lambda_d)t}\right]. \quad (3)$$

So the indoor concentration starts to increase and after a certain time, which depends on λ, it reaches a steady-state value (Fig. 3a). The smaller value of λ is the longer the time to reach the steady-state value.

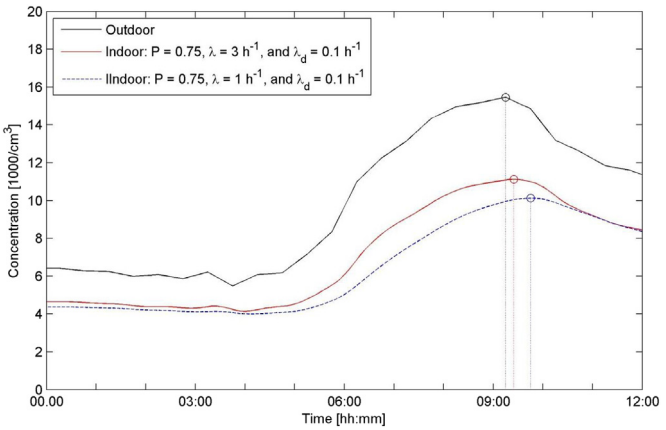

Fig. 4. Simple indoor aerosol model (IAM) simulations with realistic outdoor particle number concentration. The model simulation was performed with constant penetration factor (P) and deposition rate (λ_d) but the ventilation rate (λ) was either 3 h^{-1} or 1 h^{-1}, which illustrates the time-lag effect between the indoor and outdoor particle number concentrations. The indoor aerosol model simulation described in equation (2) was performed numerically for such real-life situations assuming no indoor sources, no re-suspension, and no chemical reaction/dynamics.

The steady-state value itself is proportional to P and inversely proportional to λ_d.

$$\left.\frac{I}{O}\right|_{\text{steady-state}} = \frac{P\lambda}{\lambda + \lambda_d} \rightarrow F_{INF}. \quad (4)$$

The I/O ration at steady-state conditions is often called the infiltration (F_{INF}) factor (e.g. Long et al., 2001). In other words, the F_{INF} is the equilibrium fraction of outdoor pollutants that penetrate indoors and remain suspended regardless to the air exchange path. While indoor sources take part in the instantaneous I/O ratio, they are not taken into account when calculating the F_{INF}. On the other hand, the penetration factor (P) is the fraction of outdoor pollutants that pass across the building shell or via the ventilation system into the indoor air. It is interesting here to show that F_{INF} is equivalent to P when λ_d is negligible (Fig. 3b). In general, the three parameters P, λ, and λ_d define the so called indoor-to-outdoor relationship of aerosols; or simply the F_{INF}. Although two of them (P and λ_d) are particle specific, but all of them are building specific.

In real-life situations, the outdoor concentration varies with time. This is illustrated in Fig. 4 with model simulations by using similar P and λ_d but different λ. It can be seen that the indoor particle number concentration responses rapidly with the varying outdoor particle number concentration when λ is higher. However,

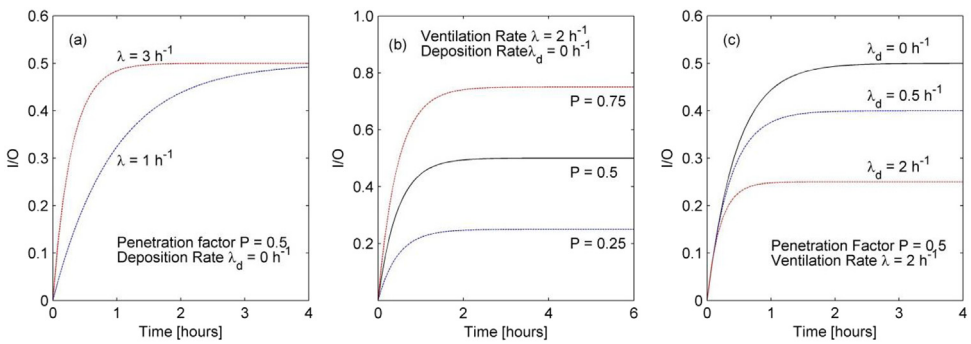

Fig. 3. Simple indoor aerosol model (IAM) simulations for the indoor-to-outdoor concentration ratio (I/O) with constant penetration factor (P), deposition rate (λ_d), ventilation rate (λ), and outdoor concentration. These calculations are based on the analytical solution of the mass–balance equation assuming no indoor sources, no re-suspension, and no chemical reaction/dynamics.

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there is time-lag between the indoor and the outdoor particle number concentration. As discussed before for the model simulation illustrated in Fig. 3a, this time-lag is longer when λ is smaller.

The situation becomes more interesting when we implement indoor sources (Fig. 5). In the given example all indoor sources elevated the indoor particle number concentrations to a similar value, but they were different in occurrence and amount of particles emitted.

4.2. Indoor-to-outdoor relationship of aerosol particles

In the absence of indoor sources of aerosol particles, their behavior is closely related to those outdoors. This indoor-to-outdoor relationship is summarized by P, λ, and λ_d (e.g. Chen and Zhao, 2011; Hussein and Kulmala, 2008). Although it is very well known for indoor environments equipped with mechanical ventilation system, the indoor-to-outdoor relationship is complicated when natural ventilation is involved in the indoor–outdoor air exchange. In such cases, an IAM serves as a tool to quantify P, λ, and λ_d.

4.2.1. Penetration factor, P

The penetration factor (P) is the fraction of incoming outdoor aerosol particles into the indoor air across the building shell or through the ventilation system (e.g. Riley et al., 2002). P is a key parameter for estimating human exposure indoors to an outdoor pollutant source. P can be examined by investigating the indoor-to-outdoor concentrations (I/O) ratio (e.g. Hussein et al., 2006, 2005a and 2005b). Aiming at steady-state I/O ratio and in the absence of indoor sources, P can be quantified as:

$$P = \frac{\lambda + \lambda_d}{\lambda} \frac{I}{O}\bigg|_{\text{steady-state}} \tag{5}$$

which indicates that P is larger than the steady-state I/O ratio by a factor $(\lambda + \lambda_d)/\lambda$. Although, a steady-state I/O ratio might not be achieved, but this method is a starting point for quantifying P.

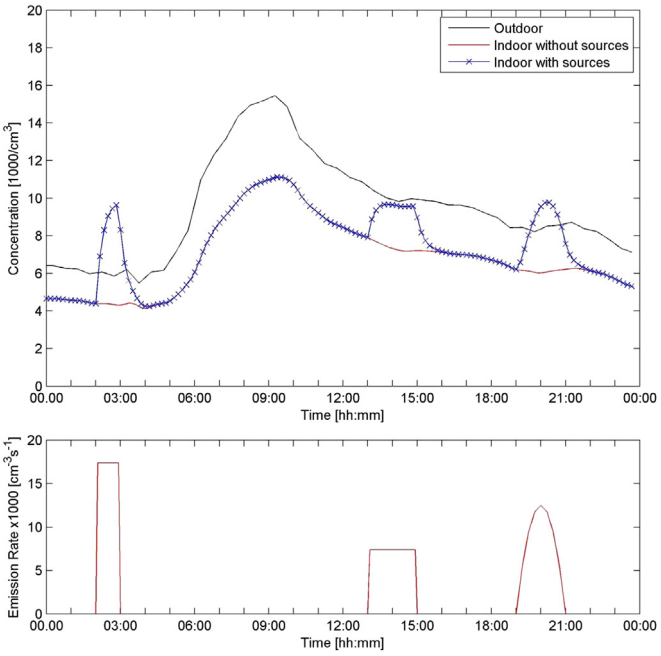

Fig. 5. Simple indoor aerosol model (IAM) simulations with a typical outdoor particle number concentration (upper plot) and three different scenarios of indoor sources (lower subplot). The model simulation was performed with $P = 0.75$, $\lambda_d = 0.1$ h^{-1}, and $\lambda = 3$ h^{-1}. The indoor aerosol model simulation described in equation (2) was performed numerically for such real-life situations.

Mechanical ventilation systems are equipped with filters of well-known filtration efficiency (Goodfellow and Tähti, 2001; Hanley et al., 1994). On contrary, P is complicated during natural ventilation because the airflow and the air path geometry are not controlled (Stephens and Siegel, 2012). Although modeling the P across the building shell has been presented in several previous studies, but more research is still needed to better understand the penetration across the building shell (e.g. Jeng et al., 2013; Chen et al., 2012). Similar to standard filters, the P across the building shell during natural ventilation has the maximum value in the diameter range 0.1–1.0 μm, but each dwelling has its own penetration curve. A unit value for P is easily achieved by wide opening of a window (e.g. Rim et al., 2013; Hussein et al., 2005b).

4.2.2. Deposition rate, λ_d

Dry deposition onto indoor surfaces can be as significant as the ventilation in removing aerosol particles from the indoor air. It depends on the fluid and airflow properties, surface roughness and physical state, and the particle properties. Dry deposition indoors occurs in two stages: convection of aerosols from the core of the room towards a surface and then transport across the boundary layer before ending up in contact with the surface (Guha, 1997). The most important mechanisms to be considered for particle transport across the boundary layer are Fickian diffusion, gravitational settling, thermophoresis, electrophoresis, and turbophoresis (e.g. McMurry and Rader, 1985; Zhao and Wu, 2006).

The value of λ_d is usually calculated after knowing the geometries of the indoor environment:

$$\lambda_d = \sum_i \frac{A_i}{V} V_{d,i} \tag{6}$$

where $V_{d,i}$ [m/h] is the dry deposition velocity towards an indoor surface with area A_i [m^2] inside an indoor environment with volume V [m^3]. The summation index runs over all available surfaces indoors. The dry deposition velocity can be calculated by using three-layer deposition models (e.g. Hussein et al., 2012b; Lai and Nazaroff, 2000), which require accurate information on the indoor air turbulent intensity and the physical properties of aerosol particles.

Alternative methods can be used to estimate an average value for λ_d. The first method is to undergo routine measurements with indoor sources performed during certain time periods. Following the decay rate of the aerosol particle concentrations would allow for a direct estimate of λ_d.

$$\lambda_d = \frac{1}{t_2 - t_1} \ln\left(\frac{I(t_1)}{I(t_2)}\right) - \lambda \tag{7}$$

where $t_2 - t_1$ is the time period chosen to calculate the slope of the decaying particle concentration right after the source. As an example, Fig. 6 illustrates a case with $P = 0.5$, $\lambda = 2$ h^{-1}, and $\lambda_d = 0.1$ h^{-1}. We could chose the time period between $t_1 = 15{:}00$ and $t_2 = 18{:}00$ to calculate the decaying slope of the particle number concentration from about $I(t_1) = 5.125 \times 10^6$ cm^{-3} to about $I(t_2) = 9.572 \times 10^3$ cm^{-3}. This yields $\lambda_d = 0.09$ h^{-1}, which is within 10% of the real value used to simulate this indoor case.

Another method to estimate λ_d is by using the steady-state I/O ratio.

$$\lambda_d = \frac{P\lambda}{I/O|_{\text{steady-state}}} - \lambda \tag{8}$$

Applying this to the same previous case yields $\lambda_d = 0.11$ h^{-1}. Here we used O ~10,000 cm^{-3} and I ~4750 cm^{-3} during the time

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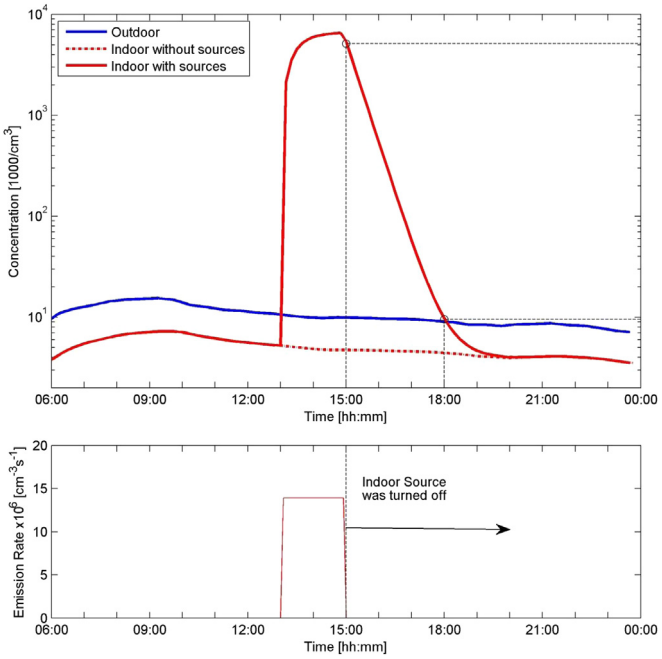

Fig. 6. Illustration of the method suggested for calculating the deposition rate (λ_d) for a case modeled with an indoor source scenario (lower plot). The model simulation was performed with $P = 0.5$, $\lambda_d = 0.1$ h^{-1}, and $\lambda = 2$ h^{-1}. The slope of the straight line between the two circles (upper plot) yields a value for $\lambda_d = 0.09$ h^{-1}.

period 13:00–18:00; i.e. they justify the condition of steady-state. Again this method gave an estimate within 10% of the real value used in the model simulation.

4.2.3. Ventilation rate, λ

The ventilation rate (λ) refers to the amount of fresh air entering an indoor space; i.e. $\lambda = Q_0/V$, where Q_0 is the fresh airflow rate into the indoor domain and V is the volume of that indoor domain. A typical value of λ ranges between 0.5 and 3 h^{-1} for apartments and offices and it can be lower than 0.5 h^{-1} for very tight dwellings. The importance of the air exchange rates (AER) in the indoor-to-outdoor relationship comes from the fact that it determines the entry and removal of air pollutants in the indoor air. Therefore, a balance-point should be approached in order to optimize the entry rate of outdoor air pollutant and the removal rate of an indoor generated pollutant (e.g. Chen and Zhao, 2011; Li and Chen, 2003). Therefore, AER is one of the most important parameters to understand the indoor-to-outdoor relationship of aerosol particles, and thus human exposure assessment (e.g. Breen et al., 2013; Pandian et al., 1993).

Aerosol particles are exchanged between the outdoor air and the indoor air via two main types of ventilation: natural and mechanical. Usually, natural ventilation occurs via uncontrolled paths such as windows, doors, cracks, and leaking paths across the building shell; the latter two are also commonly known as infiltration/exfiltration (e.g. Chen and Zhao, 2011; Li and Delsante, 2001; Linden, 1999). The mechanical ventilation controls the rate of air exchange between the indoor air and the outdoor air via well-defined duct lines, which consists mainly of fresh air ducts and exhaust air ducts (e.g. Jamriska et al., 2003).

As could be seen in the previous examples, λ is an important for estimating P and λ_d. Usually, λ is measured in the field by injecting trace gases indoors and following their fate. Alternatively, equation (7) can be used with an assumption that $\lambda >> \lambda_d$. This condition is often possible to be satisfied for aerosol particles in the diameter range 0.1–1.0 μm, where neither diffusion nor inertial processes are efficient. We can then estimate λ as:

$$\lambda \leq \frac{1}{t_2 - t_1} \ln\left(\frac{I(t_1)}{I(t_2)}\right) \quad 0.1\ \mu\text{m} < D_p < 1\ \mu\text{m} \tag{9}$$

4.3. Quantification of indoor sources

Indoor aerosols are produced indoors as a result of inhabitants' activities via combustion or mechanical and their concentrations might become considerably high inside air-tight indoor environments (Jones, 1999). The most powerful method to estimate source strengths of indoor aerosols is semi-empirical modeling, which is based on the indoor–outdoor measurements and IAM simulation (e.g. Hussein et al., 2005b). It is based on two mass-balance equations:

$$\begin{cases} \frac{d}{dt} I_{sim} = P\lambda O_{meas} - (\lambda + \lambda_d) I_{sim} \\ \frac{d}{dt} I_{meas} = P\lambda O_{meas} - (\lambda + \lambda_d) I_{meas} + S \end{cases} \tag{10}$$

where the first one is written for simulating the indoor particle concentrations (I_{sim}) in the absence of the indoor source and the second one represents the change rate as if indoor sources are included. The difference between these two equations gives an estimate for the source term.

$$S = (\lambda + \lambda_d)(I_{meas} - I_{sim}) + \frac{d}{dt}(I_{meas} - I_{sim}) \tag{11}$$

As an example, we can reconsider the model simulations made in the previous section (Fig. 5) to illustrate the quantification of the source term in real-time basis (Fig. 7). While this method assumes that aerosol particles are primary, the process behind secondary particle formation must be taken into account separately.

There is a pressing need for publically available databases with indoor sources' emission factors because each source has its own characteristics and occurrence. Only a small number of studies focused on the particle number size distributions and even few

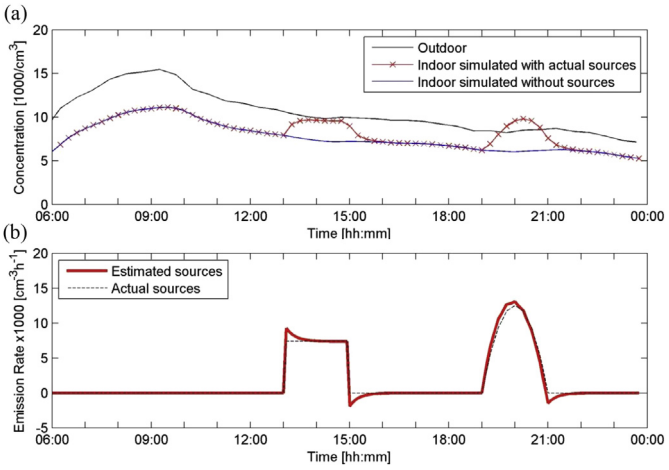

Fig. 7. Illustration for the semi-empirical estimation of indoor sources: (a) is the particle concentrations outdoors and indoors. The indoor model simulations were made twice: with sources and without sources, and (b) is the presumed emission rate (actual) and the quantified one (estimated) based on the semi-empirical method described in the text. The indoor aerosol model simulation described in equation (2) was performed numerically for such real-life situations.

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presented detailed quantification of aerosol particle emissions (e.g. Torkmahalleh et al., 2012; Buonanno et al., 2009; Pagels et al., 2009, Afshari et al., 2005; He et al., 2004; Fan and Zhang, 2001).

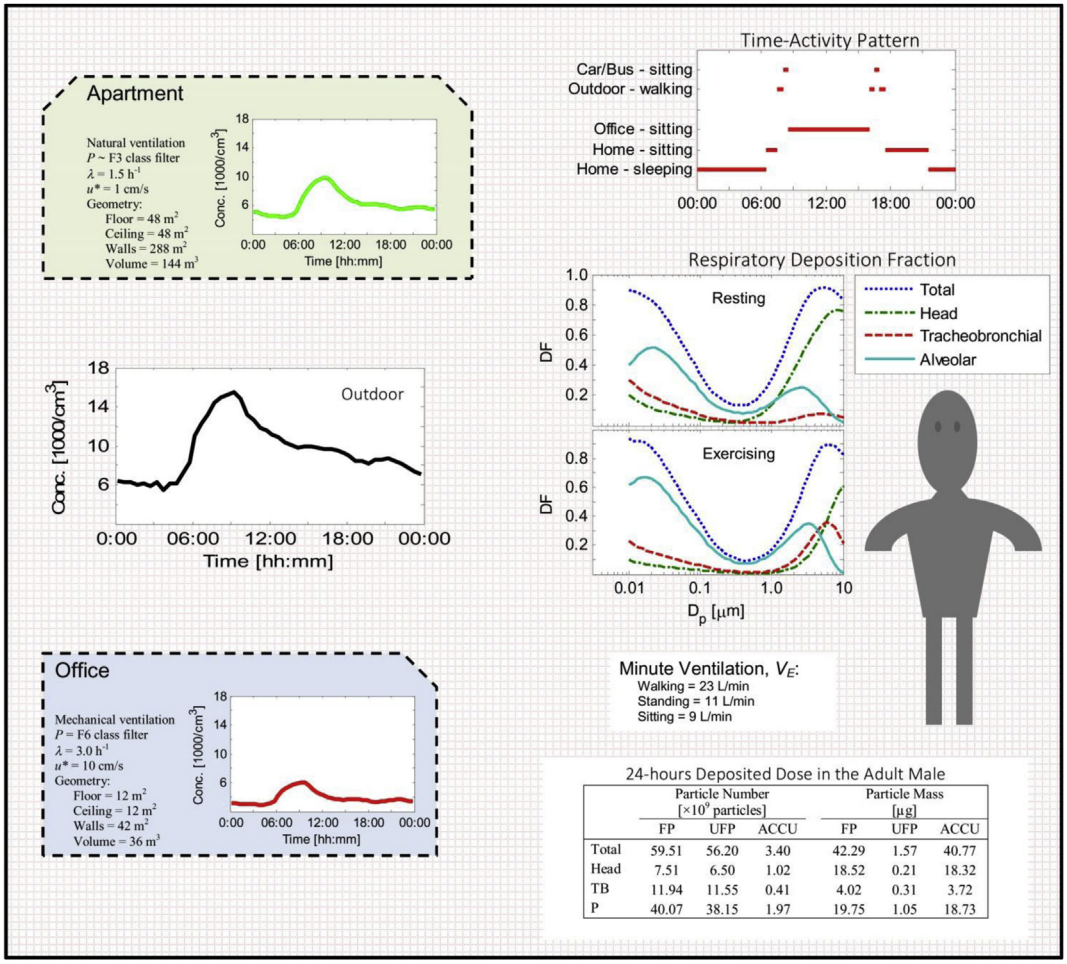
4.4. Scenarios of exposure and deposited dose

To illustrate the application of the combined modeling approach presented in this study, we will consider a healthy adult male who lives in a studio and works at an office; which are located in a suburban area. The first scenario is to calculate the respiratory tract deposited dose by ignoring indoor sources, whereas the second one is by including indoor sources. So far, exposure to indoor-generated particles has not been assessed in epidemiological studies (e.g. Morawska et al., 2013).

All components needed for the deposited dose calculation are elaborated in Fig. 8. The time activity pattern of such a subject (adult-male) can be as follows: gets up around 06:30 and stays at home for a while before going to work, returns back home around 17:00, goes to bed around 21:30, and commutes to and from work by local transportation and few minutes walking. Such a subject has a respiratory tract deposition fraction (*DF*) as indicated in Fig. 8, which were generated based on the ICRP and MPPD calculations. The minute ventilation (V_E) can be 23, 11, and 9 L/min for walking, standing, and sitting; respectively (Holmes, 1994). The outdoor particle number size distribution can be obtained from a routine measurement; here we generated a case for a typical workday in the urban atmosphere. The corresponding indoor size distributions were simulated with an IAM for an apartment and an office according to the model parameters indicated in Fig. 8.

As shown in the table of Fig. 8, the 24-h total deposited dose of fine particles (FP, diameter < 1 μm) would be about 60 × 10^9 particles (42 μg). Most of this deposited dose was accumulated in the alveolar region of the lung. Based on the mass concentration (assuming unit density), which is mainly in the accumulation and coarse fraction, the 24-h total deposited dose of FP was equally accumulated in the head airways and alveolar region.

It is expected that the deposited dose would be higher if he lives and works in an urban area. The situations become even more serious for people living and working nearby major roads and road conjunction, where the concentrations are extremely high. As for the particle density, we assumed particles having unit density. This is not realistic for most ambient particle types. Particle density of mechanically generated particles and also particles in the accumulation size fraction tend to have density larger than 1 g/cm^3, while combustion particles which may be highly agglomerated typically have an effective density below 1 g/cm^3.



	Particle Number [×10^9 particles]			Particle Mass [μg]		
	FP	UFP	ACCU	FP	UFP	ACCU
Total	59.51	56.20	3.40	42.29	1.57	40.77
Head	7.51	6.50	1.02	18.52	0.21	18.32
TB	11.94	11.55	0.41	4.02	0.31	3.72
P	40.07	38.15	1.97	19.75	1.05	18.73

Fig. 8. A schematic diagram illustrates a scenario of 24-h deposited dose calculations for an adult male on a workday assuming no indoor sources. The figures on the left hand side are the total number concentrations (middle) outdoors, (upper) at home/apartment, and (lower) at office; concentrations in home/apartment and office were simulated with IAM assuming no indoor sources i.e. on the basis of outdoor concentrations only. The indoor parameters are indicated in the corresponding boxes as: penetration factor (*P*), ventilation rate (λ), friction velocity (*u**), and indoor environment surface areas and volume. The figure on the upper right corner is the time–activity pattern and bellow it is the respiratory parameters of an adult male. The table lists the calculated regional deposited dose for this person based on particle number and mass.

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Taking into account exposure to particles produced indoors. We assumed a printing job in the office that lasted about 5 min with a size distribution of emitted particles as shown in Fig. 9. The 24-h deposited dose increased from 42 μg to about 46 μg, which is very little change (Table 1). However, the difference is huge when looking at the deposited dose based on particle number, which increased from 60×10^9 particles to more than 325×10^9 particles for FP. Basically, the person would have other print jobs and other activities at work; so the exposure and deposited dose during the time spent at work would be even more than what is shown here. Besides that, while being at home, this person would prepare food and conduct other activities that are known to generate particles in high amounts. Therefore, the 24-h exposure and deposited dose is expected to be more than what is calculated here. Recent studies have shown that indoor sources contribute to about 60% of our exposure to UFP at home (e.g. Bekö et al., 2013; Bhangar et al., 2011).

These two scenarios evidently illustrate that exposure should be evaluated based on other metrics (particle number and surface area) besides particle mass concentration. For example, by including an indoor source for 5 min increased the deposited dose by about 10% based on particle number whereas the increment was more four folds based on particle number.

5. Conclusions

As described and demonstrated in this paper, indoor aerosol models (IAM's) have been utilized in a variety of applications. IAM's substantially improves personal exposure assessment and saves time, efforts, and money in replacing measurements with real-time model simulations, which provides useful data in larger population samples needed for epidemiological studies. In combination with respiratory tract modeling, the deposited dose can be quantified in various metrics including particle mass, number, and chemically active surface area. Evaluation of these alternative metrics against traditional particle mass exposures and doses will likely improve our understanding of the health effects currently associated with outdoor particle concentrations.

To support the proposed combined modeling approach, a detailed information about the indoor environment (geometry, conditioning, etc.) is a must. At the moment such information are not widely available for most of the cities. There is still a lack of information about the physical–chemical properties and emission rates of aerosol particle produced indoors. In reality, indoor sources are very complicated and even the same activity might produce different types of aerosols; even if the same type is reproducible, it can be so that the emission rate of the same process is different. Therefore, there is a need to increase the knowledge about indoor sources and their emission factors. Detailed time and size-resolved data-base of outdoor aerosols is also needed. This can be obtained by expanding existing monitoring networks to measure other particle metrics than mass concentration i.e. time and size resolved number concentration. Nowadays, it is possible to utilize urban model forecasts to obtain high resolution (both time and space) of aerosol data bases representing the past, current time, and the future. Time–activity patterns of urban population have been investigated in several cities; however, it still needs more efforts to expand for many other cities worldwide. Most importantly, the deposited fraction in human; this part is still not very well understood and needs more investigations and laboratory measurements to quantify the deposition curves of people with different health conditions, gender, and age.

While any approach has advantages and disadvantages, we foresee this combined modeling approach presented in this article is very promising. With respect to costs and efforts, it presents useful alternative to experimental investigations.

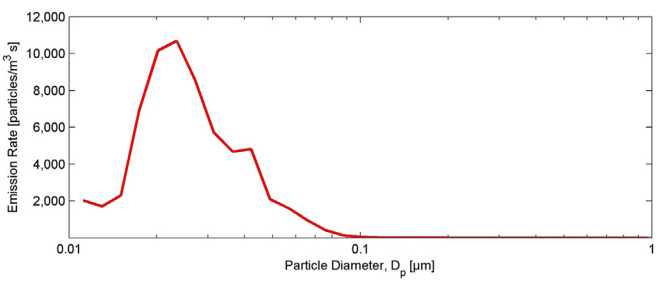

Fig. 9. A sample size distribution ($dS/d\log(D_p)$) of printer emissions.

Table 1
Calculations of 24-h regional inhaled dose for the same scenario illustrated in Fig. 8 but with inclusion of an indoor source – A print job (5 min at noon and emission rate size distribution shown in Fig. 9).

	Particle number [$\times 10^9$ particles]			Particle mass [μg]		
	FP	UFP	ACCU	FP	UFP	ACCU
Total	327.46	324.10	3.46	45.77	5.01	40.82
Head	41.44	40.43	1.03	18.98	0.65	18.33
Tracheobronchial	69.44	69.04	0.42	4.75	1.03	3.73
Alveolar	216.58	214.63	2.01	22.05	3.33	18.76

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