User Influence on Indoor Aerosol Model Calibration

Tareq Hussein[1]*, Bjarke Mølgaard[2], Kaarle Hämeri[2,3]

[1] *The University of Jordan, Department of Physics, Amman 11942, Jordan*
[2] *University of Helsinki, Department of Physics, P. O. Box 48, FI-00014 UHEL, Helsinki, Finland*
[3] *Finnish Institute of Occupational Health, Topeliuksenkatu 41 a A, FI-00250, Helsinki, Finland*

ABSTRACT

Calibration, or in other words "validation", of complex indoor aerosol models that simulate the dynamic behavior of particle number size distributions are often assumed to solely depend on the characteristics of the model and its setup. The user influence is rarely mentioned in that regard. This paper shows, with a simple exercise, the user influence on the calibration of an indoor aerosol model. It is also shown that a reasonable model simulation was achieved with a different understanding of the system modeled and several input parameter values. We utilized a single compartment and size-resolved indoor aerosol model approach to be calibrated against a model room. This kind of simple indoor aerosol models is very common in the literature and widely used in the analysis of indoor-to-outdoor relationship of aerosol particles. The input parameters for such indoor aerosol models are: outdoor particle number size distributions, indoor domain geometries, ventilation rate, penetration factor, and friction velocity (or deposition rate onto indoor surfaces). For simplicity, we considered the penetration factor and friction velocity are the only unknown input parameters to be chosen freely by the user so that the model is calibrated. We made it clear by this study that a user can influence the input parameter values significantly. Even though this suggests different sets of input parameter values can be valid for a model calibration, the model simulation differences between different calibration results remained within 1%. This implies that it is more challenging to calibrate a complex indoor aerosol model that requires many input parameters.

Keywords: Indoor-to-outdoor relationship; Size distribution; Iteration; Least-squares.

INTRODUCTION

Indoor aerosol models have been very useful tools to understand the importance of different mechanisms and to predict their effects on indoor air pollutants concentration under given circumstances (e.g. Nazaroff, 2004; Hussein and Kulmala, 2008). The degree of complexity of an indoor aerosol model relies on the implementation of processes (such as air flows, filtration, sources, sinks, aerosol dynamics, etc.), description on the particle size dependence, chemical reactions and interaction between different phases, etc. (e.g. Nazaroff and Cass, 1986; Nazaroff and Cass, 1989; Feustel, 1999; Ren and Stewart, 2003, Asmi *et al.*, 2004; Nazaroff, 2004; Hussein and Kulmala, 2008). In that sense, each model and approach has its own validity and ability to successfully explain the observations.

Utilization of indoor aerosol models brings up the issue of calibrating them against a certain measurement. The calibration results are mainly discussed based on the model characteristics (or processes), experimental setup, time series of aerosol data, statistical methods used in comparison between the model simulation and measurements, etc. However, the model-user is seldom mentioned as a factor influencing the model calibration; even though the user is the one who makes decisions on how to assign the input parameters and statistical methods used to make the comparison between the model simulation and the measurements. This is not an easy task for a non-expert user or even straight forward for an expert user to know in which aspects a model can be calibrated. Furthermore, the user might end up with several sets of input parameters values that provide similar model simulations, and thus, the user might be unable to approve the suitable set for that specific case.

In this study we aim at illustrating that (1) a user of an indoor aerosol model might influence the results of the model calibration and (2) there can be several sets of input parameters values lead to acceptable simulation results. To justify these objectives we employed two users to calibrate an indoor aerosol model against the same indoor-outdoor aerosol data set.

---
* Corresponding author. Tel.: 358-9-19150709;
 Fax: 962-6-5300253
 E-mail address: tareq.hussein@helsinki.fi

MATERIALS AND METHODS

Model Room

The model room that we considered in this study was an office room inside a building (Hussein *et al.*, 2004). This room was well sealed and there were no sources of indoor aerosol particles indoors. The total volume of the office V = 30 m^3 with total surface area to volume ratio S/V = 3.6 1/m. The office was equipped with a mechanical ventilation system: ventilation rate λ = 3 1/h and G3-class filter installed on the main central unit of the office. The ventilation rate was calculated from the incoming airflow and the total volume of the office room as $\lambda = Q/V$; the incoming airflow was obtained from the operation condition of the mechanical ventilation system. Since the office room was a part of a large building that shared the same mechanical ventilation system this required long duct lines to lead the fresh air into the office; and thus, the penetration factor is expected to be lower than the standards of G3-class filter.

The indoor-outdoor particle number size distributions (dry diameter 7–600 nm) were measured with a Differential Mobility Particle Sizer (DMPS) connected to an alternating valve that changed between indoor and outdoor air sampling each 5-minutes. The aerosol data-set consisted of 45 days that makes it long enough to provide sound statistical analysis. We performed a quality check to the aerosol data before pre-processing to eliminate time periods with possible malfunctions of instrument operation. The aerosol data was also corrected for particle losses in the sampling tubes.

Here, we use this aerosol data-set to only illustrate the user influence on model calibration and we do not aim to undergo constructive conclusion. This aerosol data-set was previously analyzed and published for constructive understanding about the indoor-to-outdoor relationship of aerosol particles (Hussein *et al.*, 2004, 2005).

Indoor Aerosol Model

We utilized a simplified version of the MC-SIAM that describes the dynamic behavior of particle number size distributions inside a single compartment; an approach that can be also found in the literature (e.g. Thatcher and Layton, 1995; Jamriska *et al.*, 1999; Kulmala *et al.*, 1999; Abt *et al.*, 2000a, b; Mosley *et al.*, 2001; Thornburg *et al.*, 2001; Riley *et al.*, 2002; Thatcher *et al.*, 2002; Jamriska *et al.*, 2003; Asmi *et al.*, 2004; Schneider *et al.*, 2004). For simplicity we omitted coagulation, thermal equilibrium, and re-suspension because these processes were not found relevant according to our investigations to the indoor-outdoor aerosol data sets used in this study. The mass-balance equation that describes the dynamic behavior of the number concentration N_i [1/cm^3] of particles in size-section "i" is

$$\frac{d}{dt} N_i = P_i \lambda O_i - \lambda N_i - \lambda_{d,i} N_i \qquad (1)$$

where N_i and O_i [1/cm^3] are the particle number concentration indoors and outdoors respectively, P_i is the penetration factor, $\lambda_{d,i}$ [1/s] is the deposition rate onto available indoor surfaces, and λ [1/s] is the ventilation rate.

For this model to be valid the indoor air is assumed to be turbulently well mixed, the physical properties of aerosol particles in a size-section are invariant, and the internal surfaces of the office are smooth, and thus, the three-layer deposition model by Lai and Nazaroff (2000) is valid here. This deposition model requires the friction velocity (u^* [m/s]) and the particle diameter (D$_p$ [m]) as input parameters to estimate the deposition velocities of aerosol particles. The model provides deposition velocities separately for upward facing, downward facing, and vertical surfaces. The total deposition rate on available indoor surfaces is

$$\lambda_{d,i} = \frac{1}{V} \sum_j A_j v_{ji} \qquad (2)$$

where V [m^3] is the volume of the indoor domain, A_j [m^2] is the surface area of an indoor surface, and v_{ji} [m/s] is the deposition velocity of an aerosol particle in size-section "i" towards an indoor surface "j".

The penetration factor also depends on the particle size and its value varies between 0 and 1 for each size-section. In general, aerosol particles are collected on the filter as well as deposited in the ventilation ducts. Therefore the penetration factor is expected to be slightly smaller than the ideal penetration factor of the standard filter, according to the manufacture guides, installed in the fresh air duct (e.g. Hussein *et al.*, 2005; Wu and Zhao, 2007).

After all, the input parameters required for the model simulation according to Eq. (1) are listed in Table 1. Some of these input parameters can be directly measured or estimated semi-empirically if needed (e.g. Hussein and Kulmala 2008).

User Selection, Post Processing of Aerosol Data, and Model Simulation

We selected two users for this study to calibrate an indoor aerosol model against the same indoor-outdoor aerosol data set. The first user (User-I) is an inexperienced user who received training on indoor aerosol model simulations. The second user (User-II) is the developer of the indoor aerosol model algorithm. User-II is considered experienced in indoor aerosol mode simulations.

The first user, as will be described in this study, made the model calibration based on pure mathematical approach with the least-squares to determine the quality of the model simulations. The calibration made by the second user was mainly constrained on the educational guessing made for the input parameters based on the understanding of the measurements and the model development itself. Both calibrations were compared to a reference case where we assigned the actual (measured) values for the input parameters. Both approaches by the users assumed P and u^* to be unknown parameters and the model calibrations were based on the high time-resolution particle number

Table 1. Input model parameters used to simulate the indoor particle number concentrations, N_i.

Parameter	Symbol	Value	Notes
Outdoor particle number size distribution	O_i	Variable	Measured
Room volume	V	30 m^3	Measured
Indoor surface area:			
● Horizontal upward facing	$A_{i,\ up}$	20 m^2	
● Horizontal downward facing	$A_{i,\ down}$	19 m^2	Measured
● Vertical	$A_{i,\ vertical}$	70 m^2	
Ventilation rate		3 1/h	Measured
Penetration factor [a]	P_i	Iteration [b]	User defined
Friction velocity [a]	$u*$	Iteration [c]	User defined

[a] Penetration factor and friction velocity were assumed unknown and the user iterated them to obtain acceptable model simulation. [b] Kindly see Figs. 3 and 4. [c] User-I iterated $u*$ between 1 and 25 cm/s.

size distribution, although we present the comparison here for the indoor-to-outdoor concentration (I/O) ratios.

User-I post processed the measured particle number size distributions by running a routine quality check for each size-section. He omitted size-sections of aerosol particles with diameters below 10 nm and above 400 nm. After that he omitted the lower and upper 5% of measured data of each size-section. He calibrated the model by iterating $u*$ within the range 1–25 cm/s and then allowing the model to find the best-fit P_i that minimizes the LSQ value for each $u*$. In other words, each $u*$ had a corresponding best-fit penetration curve denoted by P^{u*}. The model simulations were performed by this user with 24 size-sections within the particle diameter 10–400 nm.

We recall here the model calibration made by Hussein *et al.* (2005) as **User-II**. According to this user the aerosol data was post processed for quality check by omitting time periods due to suspicion in the quality of the measured number size distribution. This user iterated $u*$ and P_i simultaneously with certain constrains based on the understanding of the measurements and the model behavior. The model simulations were performed with 29 size-sections within the particle diameter 7–600 nm.

The model simulation quality for a certain particle size-section "i" was determined by the normalized least square value

$$LSQ_i = \sum_t \frac{\left[N_{sim,i}(t) - N_{meas,i}(t) \right]^2}{N_{sim,i}(t) N_{meas,i}(t)} \qquad (3)$$

where N_{meas} and N_{sim} [1/m^3] are respectively the measured and simulated particle number concentration, and t is the time (simulation time step $dt = 300$ s).

The overall model simulation quality is then determined from the sum of Eq. (3) over all particle size-sections considered in the model simulation as follows

$$LSQ = \sum_i LSQ_i. \qquad (4)$$

Note that the model simulation quality was judged based

on the prediction of each time-step, i.e. 5 minute resolution, and the normalized LSQ is useful to make equal weighting for the high and low concentration in Eq. (3). For instance, the normalization by the measured and simulated concentrations gives a bigger weight for small concentrations, and thus, the model simulation quality is judged equally to all concentrations.

MODEL CALIBRATION RESULTS

From analytical point of view, the data processing approach used by User-I is more reliable. However, the approach used by User-II is more physically acceptable because he was more aware about the aerosol measurement itself. Fig. 1 shows the indoor-to-outdoor concentration ratio of aerosol particles as obtained by these two users after post processing the aerosol data. Table 1 lists the input parameters assigned by both users. They both used the measured values for O_i, λ, V, and A_j whereas $u*$ and P_i were user-defined (iterated) to allow for acceptable model simulation quality based on the judgment of the user.

As a **"reference case"** we made model simulations according to User-I but instead of allowing iterated input for P_i we used the penetration factor curve of G3-class filter (Hanley *et al.*, 1994, Goodfellow and Tähti, 2001) and $u*$ was iterated to minimize the LSQ. According to the LSQ value the best-value for the friction velocity $u*$ was 12.7 cm/s at a LSQ = 7.47 × 10^3 (Fig. 2).

According to **User-I**, the model was calibrated with $u*$ = 6.6 cm/s and its corresponding penetration factor $P^{6.6}$ at LSQ = 6.32 × 10^3 (Figs. 2–3). The deviation in the LSQ was less than 1% when the friction velocity was changed from 2 cm/s to 12 cm/s with their respective penetration factors $P^2 – P^{12}$. This is very challenging for an inexperienced user to chose the physically correct combination of u* and P^{u*}.

It is obvious that User-I provided better match to the measurements when compared to the **reference case** with improvement of about 16% according to the LSQ value. However, the duct lines must be taken into account here because they act as an additional filter to collect aerosol particles while transported from the outdoor air to the office. Therefore the penetration factor curve P^{12} is not physically

realistic for one important reason: the penetration factor of the smallest particles is very close to that of a G3-class filter and this means that the effect of duct-lines was not taken into consideration.

According to **User-II** the model was calibrated with $u*$ = 19 cm/s and best-fit penetration factor as shown in Fig. 4; the LSQ was 1.00×10^4. Note that the best-fit penetration factors as assumed by the users are very close to each others

for particle diameters > 100 nm. The main difference was for ultrafine particles (UFP, diameter < 100 nm). This is explained by the fact that $u*$ assumed by User-II ($u*$ = 19 cm/s) was higher than that assumed by User-I ($u*$ = 6.6 cm/s). To compensate for this difference, the model calibration required to have higher penetration factor for UFP according to User-II. This clearly illustrates how $u*$ and P are collinear parameters instead of being orthogonal.
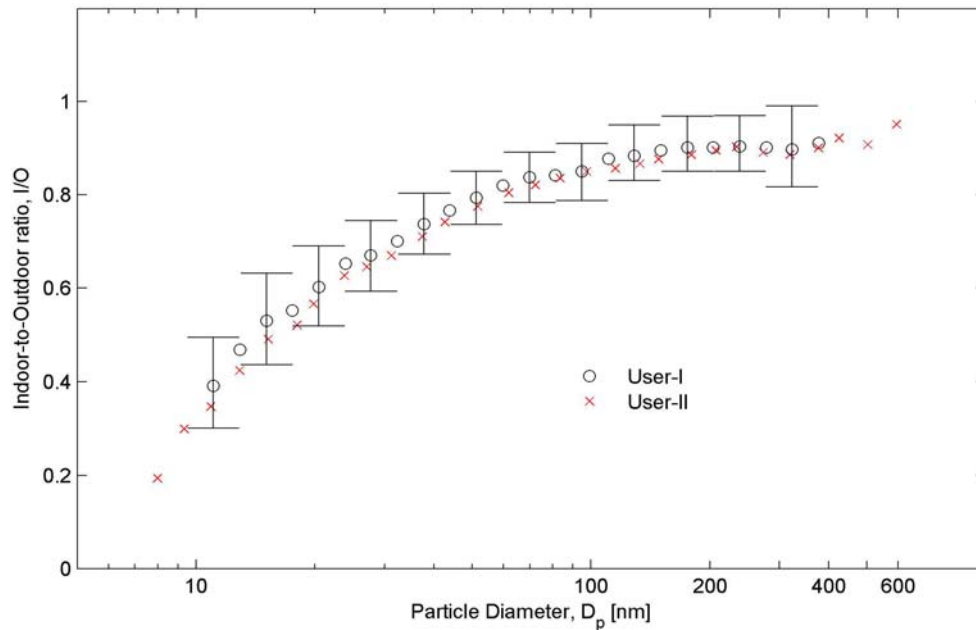

Fig. 1. Measured indoor-to-outdoor concentration ratio (I/O) according to the two users after post processing the aerosol data. *The bars indicate the quartile values.*
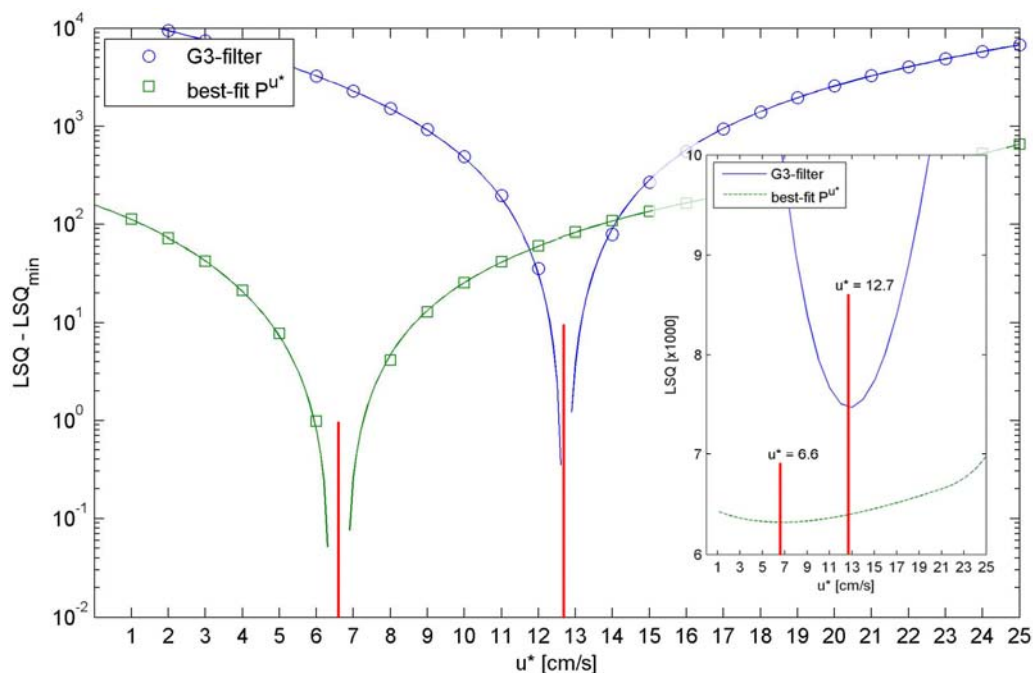

Fig. 2. Model simulation quality by using combinations of friction velocities ($u*$) and best-fit penetration (P^{u*}) at that $u*$ according to User-I. The figure also shows the simulation quality when assuming the penetration factor as G3-class filter.
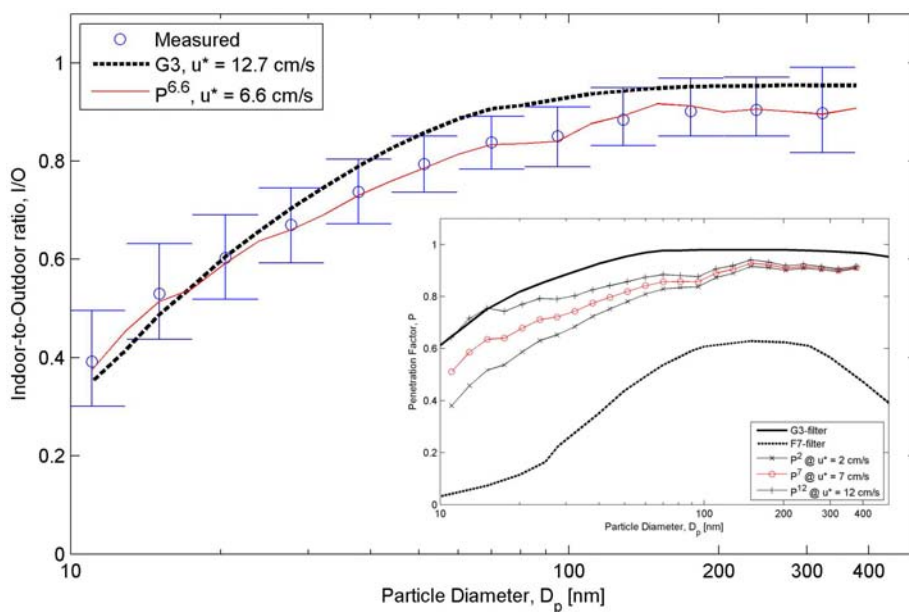
Fig. 3. Simulated indoor-to-outdoor concentration ratios (I/O) according to User-I at the best-fit combinations of $u*$ and P^{u*}. This model simulation is also compared to the measured I/O and another simulation with G3-class filter and $u* = 12.7$ cm/s.
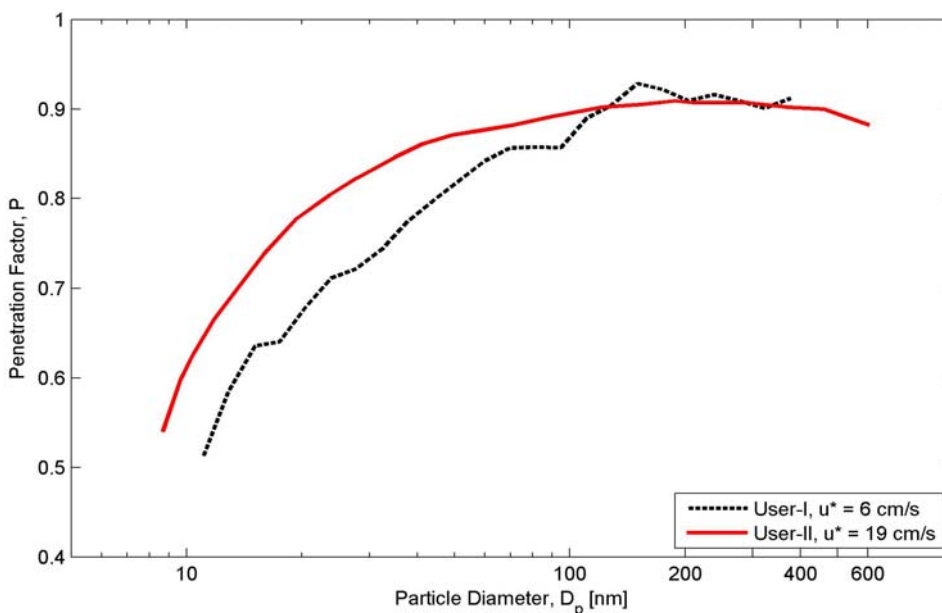

Fig. 4. Comparison between the best-fit penetration factors according to the model calibrations by the two users.

SUMMARY

The simple investigation presented in this study showed that the model user might influence the calibration of an indoor aerosol model. We presented two model calibration results made independently by two users for the same aerosol data-set. Each user followed a certain post processing procedure for the aerosol data that did not affect overall median indoor-to-outdoor concentration ratios of aerosol particles. The users applied a single compartment and size-resolved indoor aerosol model approach to a model room. This kind of indoor aerosol models is very common in the literature and widely used in the analysis of indoor-to-outdoor relationship of aerosol particles. The input parameters for such indoor aerosol models are: outdoor particle number size distributions, indoor domain geometries, ventilation rate, penetration factor, and friction velocity (or deposition rate onto indoor surfaces). For simplicity, the users considered the penetration factor and friction velocity are the only unknown input parameters.

It was also shown in this study that an acceptable match between the measured data and simulated data was achieved by using several sets of input parameters values.

Therefore, it is very clear by this study that a user can also influence the decision on the input parameters values significantly without changing the model simulation results. Even though this suggests different sets of input parameters, the model simulation differences remained within 1% between both users. This implies that complex indoor aerosol models cannot be validated, in general, but they should be calibrated based on a standard procedure to allow for comparable results between different methods.

REFERENCES

Abt, E., Suh, H.H. and Catalano, P. (2000b). Relative Contribution of Outdoor and Indoor Particle Sources to Indoor Concentrations. *Environ. Sci. Technol.* 34: 3579–3587.

Abt, E., Suh, H.H., Allen, G. and Koutrakis, P. (2000a). Characterization of Indoor Particle Sources: A Study Conducted in the Metropolitan Boston Area. *Environ. Health Perspect.* 108: 35–40.

Asmi, A.J., Pirjola, L.H. and Kulmala, M. (2004). A Sectional Aerosol Model for Submicron Particles in Indoor Air. *Scand. J. Work Environ. Health* 30 (Suppl 2): 63–72.

Feustel, H.E. (1999). COMIS–an International Multizone Air-flow and Contaminant Transport Model. *Energ. Buildings* 30: 3–18.

Goodfellow, H.D. and Tähti, E. (2001). *Industrial Ventilation Design Guidebook*, Academic Press, California, p. 685.

Hanley, J.T., Ensor, D.S., Smith, D.D. and Sparks, L.E. (1994). Fractional Aerosol Filtration Efficiency of In-Duct Ventilation Air Cleaners. *Indoor Air* 4: 169–178.

Hussein, T. and Kulmala, M. (2008). Indoor Aerosol Modeling: Basic Principles and Practical Applications. *Water Air Soil Pollut. Focus* 8: 23–34.

Hussein, T., Hämeri, K., Aalto, P., Asmi, A., Kakko, L. and Kulmala, M. (2004). Particle Size Characterization and the Indoor-to-outdoor Relationship of Atmospheric Aerosols in Helsinki. *Scand. J. Work Environ. Health* 30 (Suppl 2): 54–62.

Hussein, T., Korhonen, H., Herrmann, E., Hämeri, K., Lehtinen, K.E.J. and Kulmala, M. (2005). Emission Rates Due to Indoor Activities: Indoor Aerosol Model Development, Evaluation, and Applications. *Aerosol Sci. Technol.* 39: 1111–1127.

Jamriska, M., Morawska, L. and Ensor, D.S. (2003). Control Strategies for Sub-micrometer Particles Indoors: Model Study of Air Filtration and Ventilation. *Indoor Air* 13: 96–105.

Jamriska, M., Thomas, S., Morawska, L. and Clark, B.A. (1999). Relation between Indoor and Outdoor Exposure to Fine Particles near a Busy Arterial Road. *Indoor Air* 9: 75–84.

Kulmala, M., Asmi, A. and Pirjola, L. (1999). Indoor Air Aerosol Model: The Effect of Outdoor Air, Filtration and Ventilation on Indoor Concentrations. *Atmos. Environ.* 33: 2133–2144.

Lai, A.C.K. and Nazaroff, W.W. (2000). Modeling Indoor Particle Deposition from Turbulent Flow onto Smooth Surfaces. *J. Aerosol Sci.* 31: 463–476.

Mosley, R.B., Greenwell, D.J., Sparks, L.E., Guom, Z., Tucker, W.G., Fortmann, R. and Whitfeld, C. (2001). Penetration of Ambient Fine Particles into the Indoor Environment. *Aerosol Sci. Technol.* 34: 127–136.

Nazaroff, W.W. (2004). Indoor Particle Dynamics. *Indoor Air* 14 (Suppl 7): 175–183.

Nazaroff, W.W. and Cass, G.R. (1986). Mathematical Modeling of Chemically Reactive Pollutants in Indoor Air. *Environ. Sci. Technol.* 20: 924–934.

Nazaroff, W.W. and Cass, G.R. (1989). Mathematical Modeling of Indoor Aerosol Dynamics. *Environ. Sci. Technol.* 23: 157–166.

Ren, Z. and Stewart, J. (2003). Simulating Air Flow and Temperature Distribution Inside Buildings Using a Modeified Version of COMIS with Sub-zonal Divisions. *Energ. Buildings* 35: 257–271.

Riley, W.J., Mckone, T.E., Lai, A.C.K. and Nazaroff, W.W. (2002). Indoor Particulate Matter of Outdoor Origin: Importance of Size-dependent Removal Mechanisms. *Environ. Sci. Technol.* 36: 200–207.

Schneider, T., Jensen, K.A., Clausen, P.A., Afshari, A, Gunnarsen, L., Wåhlin, P., Glasius, M., Palmgren, F., Nielsen, O.J. and Fogh, C.L. (2004). Prediction of Indoor Concentration of 0.5–4 μm Particles of Outdoor Origin in an Uninhabited Apartment. *Atmos. Environ.* 38: 6349–6359.

Thatcher, T.L. and Layton, D.W. (1995). Deposition, Resuspension, and Penetration of Particles within a Residence. *Atmos. Environ.* 29: 1487–1497.

Thatcher, T.L., Lai, A.C.K., Moreno-Jackson, R., Sextro, R.G. and Nazaroff, W.W. (2002). Effects of Room Furnishings and Air Speed on Particle Deposition Rates Indoors. *Atmos. Environ.* 36: 1811–1819.

Thornburg, J., Ensor, D.S., Rodos, C.E., Lawless, P.A., Sparks, L.E. and Mosley, R.B. (2001). Penetration of Particles into Buildings and Associated Physical Factors. Part I: Model Development and Computer Simulations. *Aerosol Sci. Technol.* 34: 284–296.

Wu, J. and Zhao, B. (2007). Effect of Ventilation Duct as a Particle Filter. *Build. Environ.* 42: 252–2529.