An Indoor Air Quality Model for Particulate Matter

Leslie E. Sparks, U. S. Environmental Protection Agency, Office of Research and Development, National Risk Management Research Laboratory, Air Pollution Prevention and Control Division, Research Triangle Park, NC 27711

ABSTRACT

The standard for particulate matter (PM) less than 2.5 µm in aerodynamic diameter ($PM_{2.5}$) proposed by the U.S. EPA has produced considerable interest in indoor exposures to PM. Indoor air quality (IAQ) models provide a useful tool for analyzing both the indoor exposure to PM and the impact of risk management options on exposure. Because analysis of the impact of PM exposures requires analysis over a particle size distribution, most existing IAQ models, which are designed to allow analysis of the impact of a single pollutant component, are not well suited for analysis of PM exposure. To overcome this limitation, a multicompartment IAQ model was developed for PM exposures for a full particle size distribution. The model allows analysis of the effect of: the building shell on the penetration of outdoor particles into the indoors, the deposition of particles to indoor surfaces, particle removal by air cleaners, and indoor particle sources. The use of the model is demonstrated by an analysis of both the time-varying impact of outdoor PM on indoor PM levels and the effect of a central furnace filter on indoor PM concentrations.

INTRODUCTION

As a result of EPA's proposed standard for particulate matter (PM) less than 2.5 µm in aerodynamic diameter ($PM_{2.5}$), a need for an indoor air quality (IAQ) model for PM has developed. IAQ models have been developed for PM. However, they are usually single-compartment models and treat only the steady state situation (see Thornburg et al.[1] for a discussion of some of these models). Existing multicompartment time-varying IAQ models generally allow modeling of one pollutant[2,3,4] and are thus unsuitable for modeling PM where many of the effects are due to particle size distribution. These single-pollutant models can be used to analyze PM by combining several model runs. However, this is inefficient and error prone. The IAQ model described in this paper allows analysis of the time-dependent behavior of up to eight different particle diameters and includes the effects of particle air cleaners, outdoor PM concentrations, air exchange rates, and PM sources.

THE MODEL

General equations

The new IAQ model is based on the multiroom IAQ model RISK[4]. The major changes made to RISK to allow modeling of PM were:

- Particle size distribution was added,
- Particle deposition was added,
- Particle penetration through the building fabric was added,
- Particle sources were added,
- Time-varying outdoor concentration was added, and
- Air cleaner efficiency as a function of particle diameter was added.

The new model is based on mass balance. The general mass balance equation for a single pollutant or particle size for room i of N rooms is:

Equation 1. Mass balance equation for room i of N rooms.

$$V_i \frac{dC_i}{dt} = C_a Pt\, Q_{a,i} + C_h Q_{h,i} + \sum_{j=1, j\neq i}^{j=N} C_j Q_{j,i} - C_i (Q_{i,a} + Q_{i,h}) - \sum_{j=1, j\neq i}^{j=N} C_i Q_{i,j} + S_i - R_i$$

where V_i is the volume of room i; C_i is the concentration in room i; C_a is the concentration outdoors; Pt is the penetration factor for pollutants into the indoors; $Q_{a,i}$ is the air flow from the outdoors into room i; C_h is the concentration leaving the heating, ventilating, and air conditioning (HVAC) system; $Q_{h,i}$ is the air flow from the HVAC system into room i; C_j is the concentration in room j; $Q_{j,i}$ is the air flow from room j into room i; $Q_{i,a}$ is the air flow from room i to the outdoors; $Q_{i,h}$ is the flow from room i into the HVAC system; $Q_{i,j}$ is the air flow from room i into room j; S_i is the source term for pollutants produced in room i; and R_i is the removal term for pollutants removed in room i, including those removed by sinks and in-room air cleaners. Note that most of the terms in Equation (1) may vary with time. In the model implemented here, C_a, the flow terms $Q_{a,i}$, $Q_{h,i}$, and $Q_{i,j}$ and the flows needed to balance them, and S_i are allowed to vary with time. The penetration term, Pt, the source term, S_i, and the removal term, R_i, are generally functions of particle diameter.

The term for the HVAC system is determined by the design of the HVAC system and the location of filters in the system. In a commercial system where mechanical ventilation is provided by the HVAC system, air is returned to the HVAC system from most rooms, and air cleaners are located after the outdoor air and room air are mixed (see Figure 1). The equation for the HVAC system is:

Equation 2. Equation for HVAC system.

$$C_h \sum_{i=1}^{i=N} Q_{h,i} + V_h \frac{dC}{dt} = (1-\eta) C_a Q_{a,h} + (1-\eta) \sum_{i=1}^{i=N} C_i Q_{i,h}$$

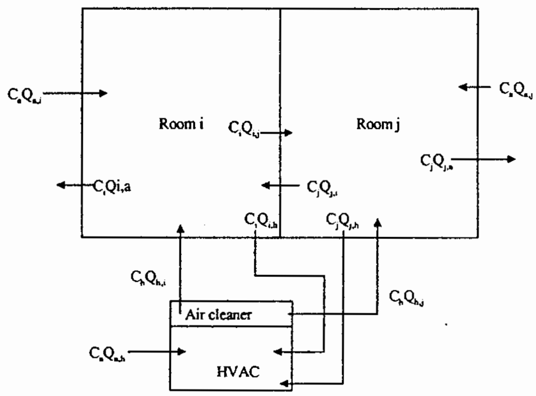
where V_h is the volume of the HVAC system, η is the efficiency of the air cleaner in the HVAC system, and $Q_{a,h}$ is the air flow from the outdoors into the HVAC system.

The volume of the HVAC system is generally very small relative to the building volume, and the various air flow rates and the change of concentration with time in the HVAC system can be neglected. The equation for the concentration leaving the HVAC system is then:

Equation 3. Final equation for HVAC system.

$$C_h = \frac{(1-\eta)(C_a Q_{a,h} + \sum_{i=1}^{i=N} C_i Q_{i,h})}{\sum_{i=1}^{i=N} Q_{h,i}}$$

Figure 1. Diagram of two compartments with an HVAC system.



In Figure 1, $Q_{a,j}$ is the air flow from the outdoors into room j, $Q_{j,a}$ is the air flow from room j to the outdoors, $Q_{j,h}$ is the air flow from room j into the HVAC, and $Q_{h,j}$ is the air flow from the HVAC into room j.

For a typical residential system: heating and air conditioning (HAC) are provided, there is no outdoor air entering the HAC system, air is returned to the HAC system from one location, and the filter is typically located on the return side of the system (Figure 2). The equation for the HAC system is then:

Equation 4. Equation for residential HAC system.

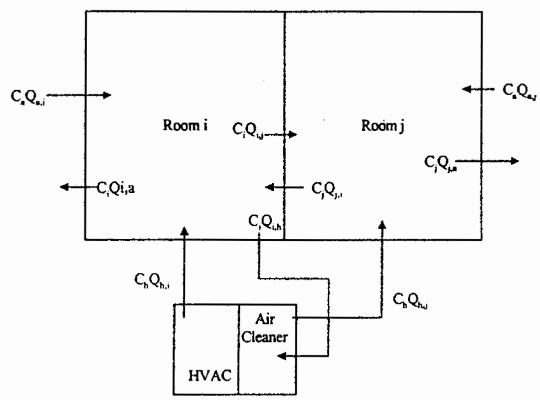
$$C_h = \frac{(1-\eta) C_r Q_{r,h}}{\sum_{i=1}^{i=N} Q_{h,i}}$$

where C_r is the concentration at the return location and $Q_{r,h}$ is the air air flow from the return location to the HVAC system. If outdoor air does enter a typical residential system due to leaks in the system, the air is not cleaned and the resulting concentration is given by:

Equation 5. Equation for HAC system with outdoor air leakage into the system.

$$C_h = \frac{C_a Q_{a,h} + (1-\eta) C_r Q_{r,h}}{\sum_{i=1}^{i=N} Q_{h,i}}$$

Figure 2. Two rooms with an HAC system.



The air entering a room from all locations must equal the air leaving the room to all locations, the total amount of outdoor air entering the building must equal the total amount of outdoor air leaving the building, and the total air entering the HVAC system from all locations must equal the total air leaving the HVAC system to all locations. Additional equations are necessary to describe the source and removal terms. The entire system of equations is solved numerically using techniques described by Yamamoto et al.[5]

Particle size distribution calculations

The model allows calculation of concentration for a maximum of eight different particle diameters. The particle data are entered into the model using data entry tables. The user enters the particle diameter and appropriate data for that diameter. If the user uses the model defaults for penetration, particle deposition, or air cleaner efficiency, the user must use the physical particle diameter. Because the $PM_{2.5}$ standard is based on aerodynamic diameter, the model provides an option to convert from physical diameter to aerodynamic diameter using[6]:

Equation 6. Equation for converting between aerodynamic and physical diameter.

$$d_A = d\sqrt{C' \rho}$$

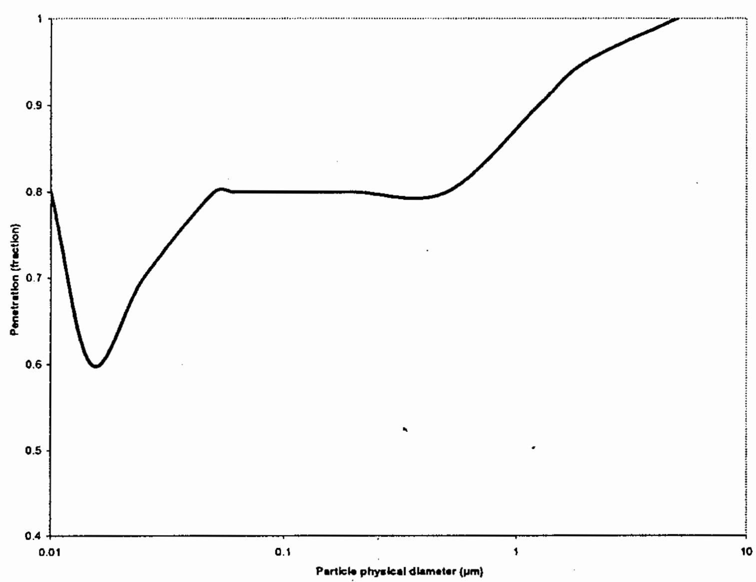
where d_A is the particle aerodynamic diameter, d is the particle physical diameter, C' is the Cunningham correction factor, and ρ is the particle density. Particle concentration may be entered as number concentration, volume concentration, or mass concentration as long as the same concentration units are used to describe all particle concentrations and source emission rates.

Particle penetration

For particles, the penetration factor, Pt, is a function of particle diameter and is not well known. Several studies of penetration have been reported in the literature, but there is no consensus about the proper values to use. McMurry *et al.*[7] reported that the penetration varied from 0.2 to 0.4 for particles with diameters between 0.01 and 0.1 µm. Thatcher and Layton[8] reported that the penetration was unity for particles with diameters less than 10 µm. Tung *et al.*[9] reported an average penetration factor of 0.78 for particles with aerodynamic diameters less than 10 µm (PM_{10}) in an enclosed office. Thornburg et al.[1] reported data and modeling showing that the penetration for a residence without an HVAC system varied from 0.5 to 0.8 for particle diameters over the range of 0.02 to 8 µm. It is difficult to compare these studies, because many authors do not define whether their results are for particle aerodynamic or physical diameter.

The new model allows the user to enter values of penetration for various particle diameters or the user may use default values provided by the model. The model defaults are based on experiments conducted in EPA's IAQ research house at Research Triangle Park, NC, literature values, and modeling. The default values, based on physical diameter, are shown in Figure 3.

Figure 3. Default penetration as a function of particle physical diameter.



Particle deposition

The deposition of particles onto indoor surfaces is a major loss mechanism for particles. The loss of particles due to deposition can be described in terms of deposition loss rate with units of inverse hours or in terms of deposition velocity with units of meters per hour. The model uses deposition velocity with the loss of particles due to deposition given by:

Equation 7. Equation for deposition losses of particles indoors.

$$R_d = C v_d A$$

where R_d is the loss due to deposition, C is the particle concentration, v_d is the deposition velocity, and A is the area of the surface.

The deposition velocity has been studied both experimentally and theoretically by several investigators. Nazaroff and Cass[10] present a set of equations to predict the deposition velocity for the ceilings, walls, and floors of indoor spaces. Lai and Nazaroff [11] provide a model for deposition velocity that accounts for near-surface turbulence. Fogh et al. [12] present data on deposition rate as a function of particle size. Goddard et al.[13] and Byrne et al.[14] present data on particle deposition rate in occupied rooms. Sparks et al.[15] present data on particle deposition rate obtained from chamber and research house experiments. The theoretical and experimental values of particle deposition are strong functions of the air turbulence. Lai and Nazaroff's model predicts that deposition rate can vary by about an order of magnitude for typical turbulence conditions found indoors.

The deposition rate can be calculated if the deposition velocity and the surface to volume ratio are known. For a space with N surfaces, the deposition rate, λ_d, is given by:

Equation 8. Equation for converting deposition velocity to deposition rate.

$$\lambda_d = \frac{1}{V} \sum_{i=1}^{i=N} v_{di} A_i$$

where v_{di} is the deposition velocity to surface i and A_i is the area of the surface i. An overall deposition velocity can be estimated from the deposition rate by assuming that particles deposit to all surfaces equally and is given by:

Equation 9. Equation for converting deposition rate to overall deposition velocity.

$$v_d = \frac{\lambda_d V}{A}$$

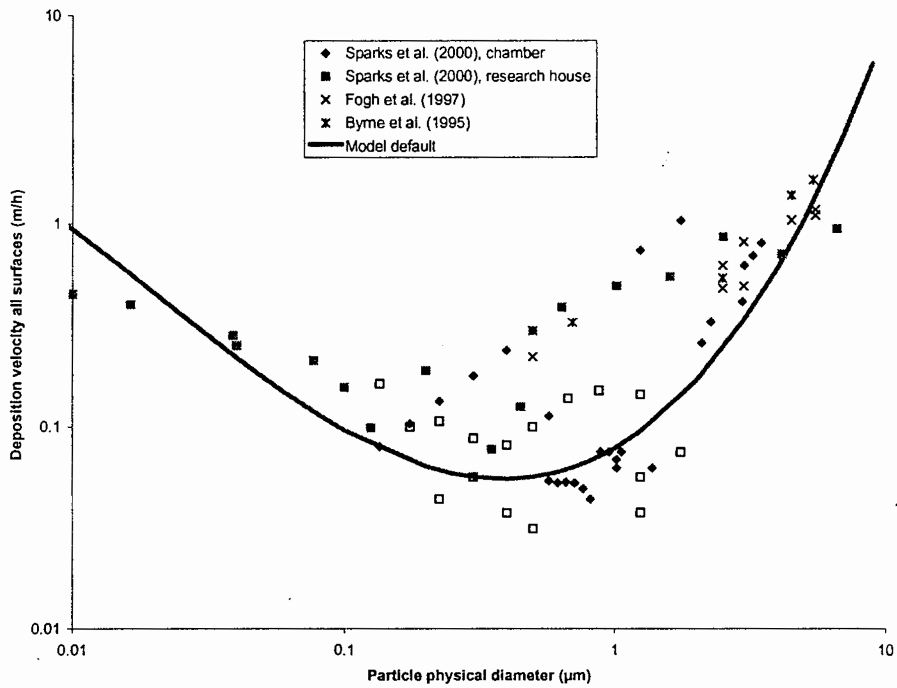
where A is the total area available for deposition.

The model allows the user to enter the deposition rate directly or the user can use model defaults. The model defaults for particle deposition velocity and results from the literature are shown in Figure 4. The default deposition velocities were estimated from deposition rate data by assuming that all particles deposit to all surfaces equally. If data or calculations for deposition velocity to different surfaces are available, they can be used in the model.

Particle sources

Because of the lack of data on indoor PM emissions as a function of particle diameter, the current version of the model does not provide default PM sources. The model does allow the user to specify the emission rate for each particle diameter that is modeled. It is critical that the units used to describe source emission rates be consistent with those used to describe outdoor concentrations. For example, if outdoor concentrations are entered as particles per cubic centimeter, then the source emission rate must be entered as particles per hour per unit source. Results of ongoing research on indoor PM sources will be incorporated into the model as soon as they become available.

Figure 4. Model default particle deposition velocity as a function of particle physical diameter.



Particle air cleaners

Air cleaners can have a significant impact on the indoor particle concentration. Because of the large amount of air recirculated in many buildings, even relatively low efficiency air cleaners can significantly reduce indoor particle concentrations. Any analysis of field data should account for the effect of air cleaners.

Hanley et al.[16] provide data on the efficiency of a wide range of particulate air cleaners. These data have been extended with results from EPA's environmental technology verification (ETV) program. Air cleaner efficiencies for several devices based on Hanley et al. and the ETV data are shown in Figure 5 along with the typical particle physical diameter range of some typical indoor air pollutants.

The model allows the user to enter air cleaner efficiency for the diameters used in the model or the user can select model defaults for a range of air cleaners. The default air cleaners and their efficiencies are shown in Figure 6.

Figure 5. Air cleaner efficiencies as a function of particle physical diameter and physical diameter range of typical indoor pollutants.

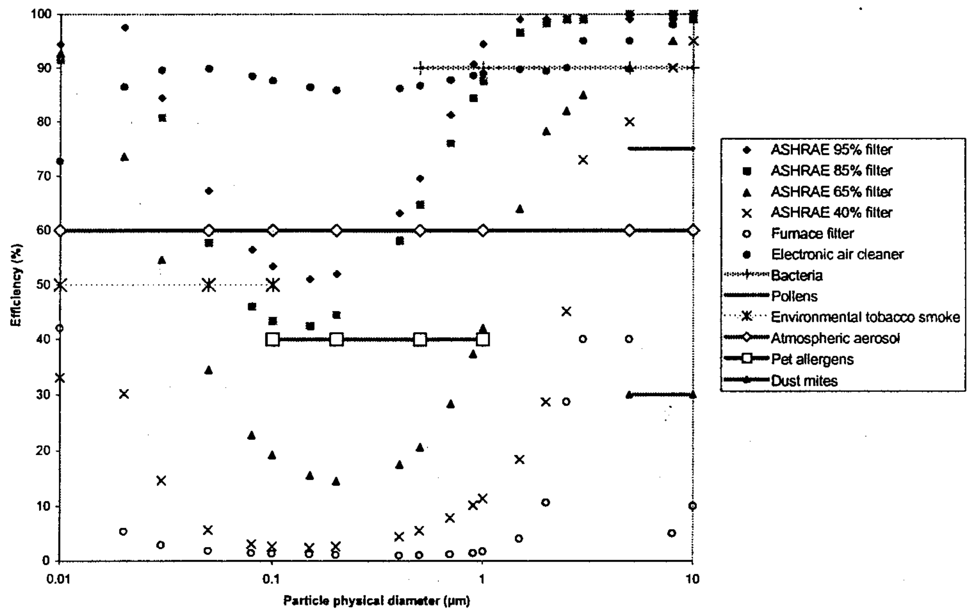
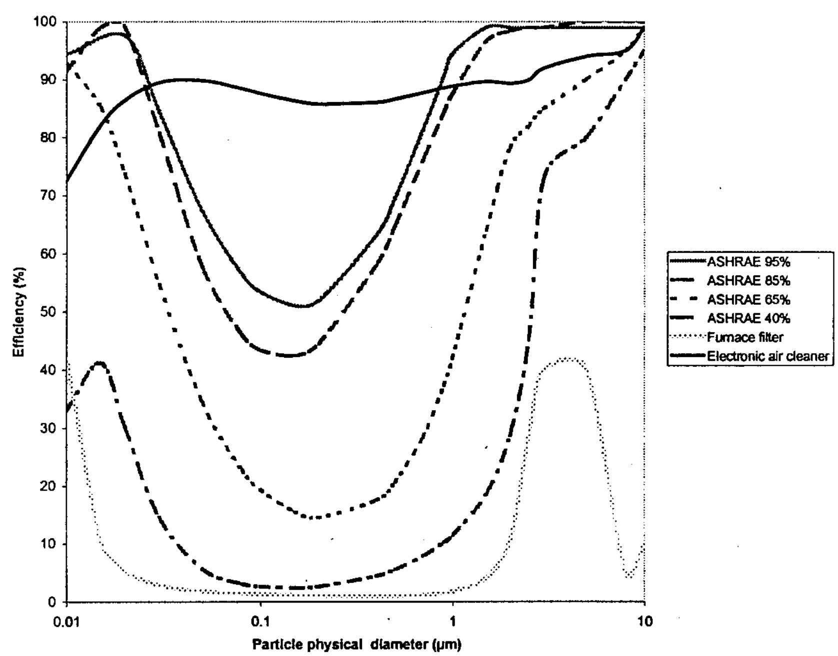


Figure 6. Default air cleaner efficiencies as a function of particle physical diameter provided by model.



COMPARISON OF MODEL AND MEASUREMENTS

Modeling impact of outdoor PM on indoor PM

One of the uses of the IAQ model is in analyzing the effects of outdoor PM on indoor PM. The major parameters necessary for this analysis are the penetration of outdoor particles into the indoors, the deposition of indoor particles, and the efficiency of any indoor air cleaners. Several investigators, for example Thatcher and Layton[8] and Thornburg et al.[1], have used a single-compartment steady-state model to analyze the impact of outdoor PM on indoor PM. In many cases, the outdoor PM concentration varies significantly with time and an analysis with a dynamic model is needed.

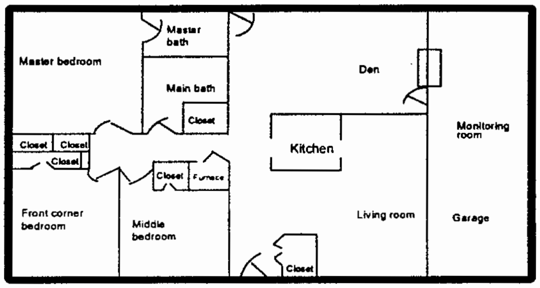
The analysis that follows is based on data collected in EPA's IAQ research house. The research house is a typical three-bedroom ranch style house with a volume of 300 m^3. The house is unoccupied and unfurnished. The floor plan for the test house is shown in Figure 7. The house has central air conditioning and a natural gas central heating system. Exhaust fans are provided in the hall bathroom and for the kitchen stove hood. The exhaust fans were not operated during these experiments. The monitoring room, isolated from the rest of the house, is not considered in any modeling. For these experiments the house was operated with the HAC system fan on continuously and with the thermostat set to maintain an indoor temperature of 22° C. The furnace filter was removed. Air flows from the HAC into each room were measured as was the air flow from the hall to the HAC return. The total HAC air flow was about 1,800 m^3/h or 6 house volumes/h. All interior doors were open for these experiments. Indoor PM was measured in the master bedroom.

Indoor and outdoor particle size distributions were collected over the particle physical diameter range of 0.015 to 7.5 µm using a scanning mobility particle sizer (SMPS) for the range of 0.015 to 0.6 µm and a single-particle laser counter (Lasx) for the range of 0.1 to 7.5 µm. Indoor and outdoor data were collected using the same instrument. In general the SMPS and the Lasx were in good agreement where their measurements overlapped. The instruments sampled the outdoors for 30 minutes and then sampled the indoors for 30 minutes. An automatic valve was used to switch the sample from outdoors to indoors. Even with 30-minute sampling, the number of particles with diameters larger than 3 µm was too low to provide valid count statistics.

The air exchange rate with the outdoors was determined using sulfur hexafluoride (SF_6). SF_6 was injected periodically and the decay method was used to determine the air exchange rate. A meteorology station at the research house provided data on wind speed, wind direction, relative humidity, and outdoor temperature. Indoor temperature and relative humidity were also measured.

The model calculated for particle physical diameters of 0.015, 0.05, 0.077, 0.1, 0.2, 0.35, 0.5, and 1.25 µm. The model default settings for penetration and deposition were used. The measured air exchange rates were used in the modeling. The results are shown in Figure 8.

Figure 7. Floor plan of EPA's IAQ research house.



Several useful metrics can be used to compare quantitatively model predictions and measurements. Some of the more useful are:

1. The average relative error between measurements and predictions given by:

Equation 10. Equation for the average absolute value of the relative difference between predicted and measured concentrations.

$$\frac{\sum_{i=1}^{n}\left|\frac{c_{pi}-c_{oi}}{c_{oi}}\right|}{n}$$

where c_{pi} is the value of the i^{th} predicted concentration, c_{oi} is the value of the i^{th} observed concentration, and n is the number of observations.

2. The normalized mean square error (NMSE) given by:

Equation 11. Equation for normalized mean square error.

$$NMSE = \overline{(c_p - c_o)^2} / (\overline{c_p} \bullet \overline{c_o})$$

where $\overline{(c_p - c_o)^2}$ is the average value of the square of the difference between predicted and observed concentration, $\overline{c_p}$ and $\overline{c_o}$ are the average of the predicted and observed concentrations, respectively.

3. The regression intercept (a), regression slope (b), and correlation coefficient (r) calculated for the least squares linear fit of the predicted concentrations to the measured concentrations.

4. The bias between model predictions and measurements can be measured by the fraction bias (FB) given by:

Equation 12. Equation for fraction bias.

$$FB = 2 \bullet \frac{(\bar{c}_p - \bar{c}_o)}{\bar{c}_p + \bar{c}_o}$$

American Society for Testing and Materials (ASTM)[17] recommendations for acceptable values of these parameters are given in Table 1.

Table 1. ASTM criteria for comparing model predictions with measurements

Criterion	Recommended value
Correlation coefficient (r)	>0.9
Normalized mean square error (NMSE)	<0.25
Regression intercept (a)	<25% of the average value of the measurements
Regression slope (b)	0.75 to 1.25
Fractional bias (FB)	Absolute value <0.25

Quantitative comparisons of the model predictions and experimental data are shown in Table 2.

Figure 8. Comparison between model predictions and research house data.

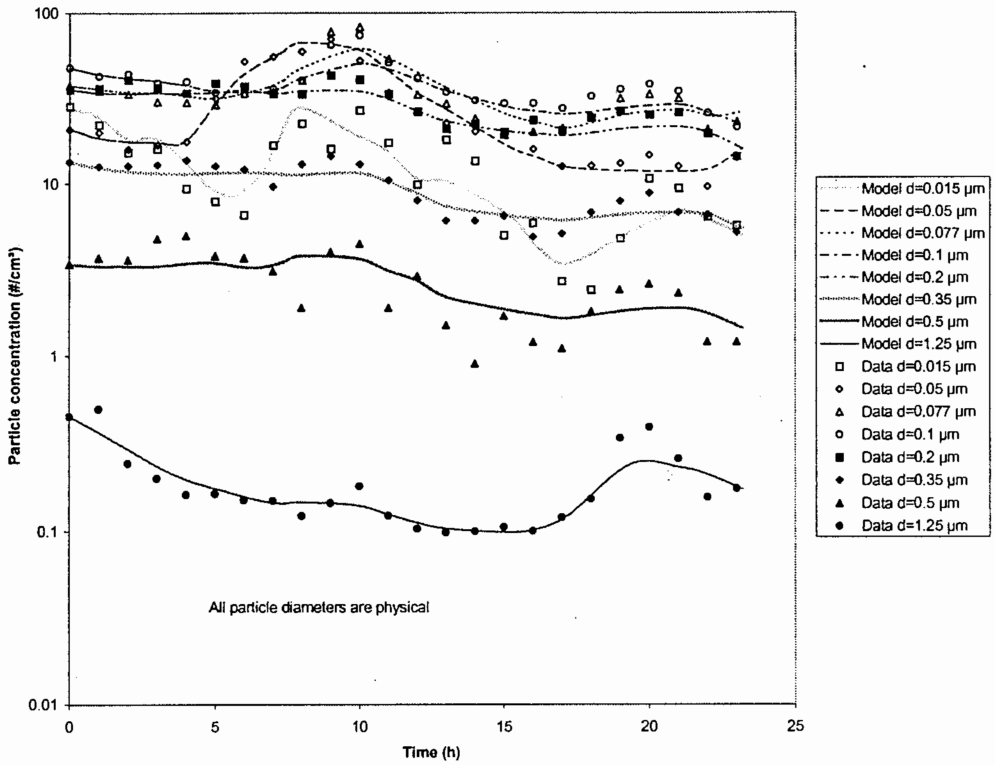


Table 2. Quantitative comparison of model predictions and experimental data

Diameter µm	0.015	0.05	0.077	0.1	0.2	0.35	0.5	1.25
NMSE	8.43E-05	1.91E-03	2.37E-04	6.57E-03	5.04E-03	1.02E-03	5.46E-05	1.13E-03
FB	-9.18E-03	4.36E-02	1.54E-02	-8.10E-02	-7.10E-02	-3.19E-02	-7.39E-03	-3.36E-02
r	0.90	0.97	0.91	0.90	0.95	0.95	0.79	0.90
a	0.85	0.44	13.00	11.00	3.50	2.00	1.10	0.05
b	0.92	1.03	0.63	0.62	0.80	0.75	0.55	0.70
25% of average value of concentration (ASTM recommended value of a)	3.01	6.76	8.51	8.63	6.72	2.25	0.65	0.05
Average absolute value of relative residual	0.25	0.12	0.16	0.12	0.11	0.12	0.23	0.14
Maximum absolute value of relative residual	0.75	0.45	0.55	0.48	0.28	0.41	0.53	0.53

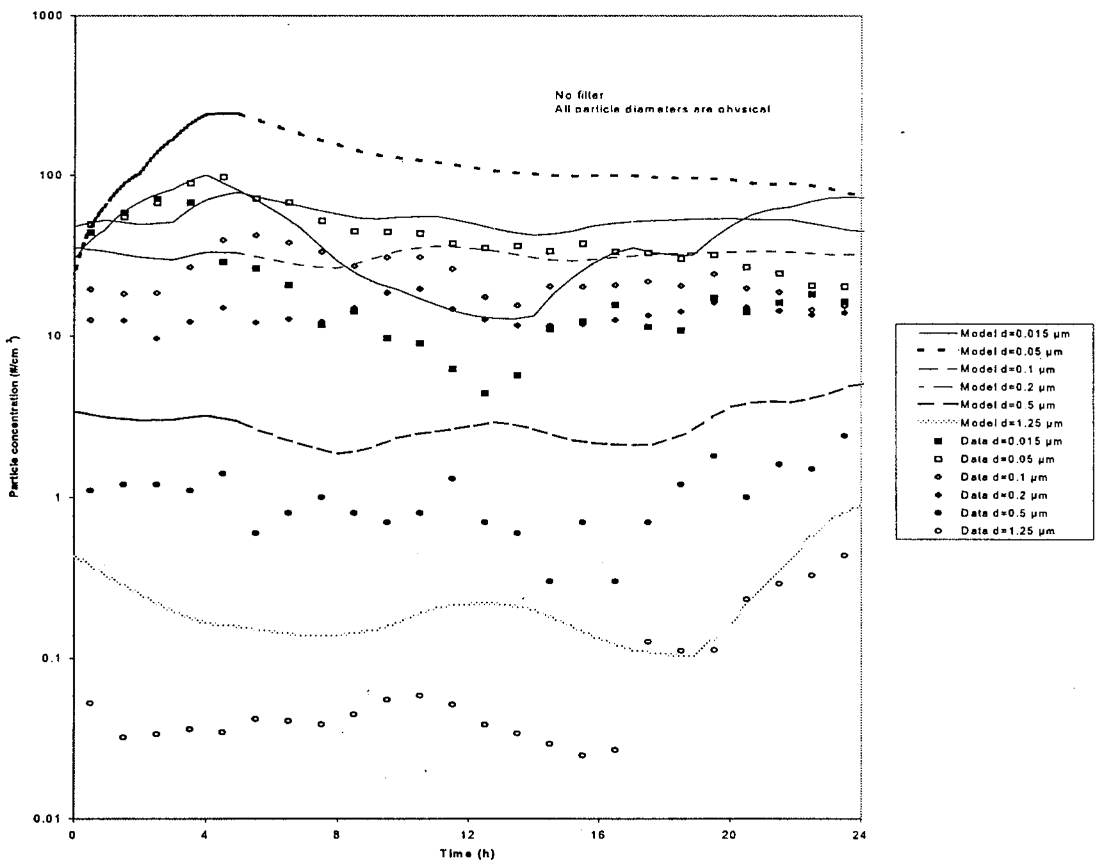
ASTM recommends that the suitability of an IAQ model be determined by an evaluation of all the quantitative factors. A model may meet one or more criteria and still be inadequate, or a model may fail one or more criteria and still be adequate for the task at hand. Except for the slope and intercept for diameters 0.077, 0.1, and 0.5 µm, the values are within ASTM guidelines. Much of the disagreement between the model predictions and the data is due to uncertainty in the values of deposition rate and penetration factor. Research is ongoing to provide better information on both of these factors.

Effect of furnace filter on indoor PM

An experiment with the furnace filter in place was conducted to determine if a common furnace filter had an impact on indoor PM concentrations. Although the single-pass efficiency of a furnace filter is low, the recirculation rate through the filter is about 6 house volumes per hour. Thus some effect could be expected. The comparison of measurements and data for no filter is shown in Figure 9. The agreement between model and data is poor.

The comparison between model predictions and data when the default values of furnace filter efficiency are used is shown in Figure 10. The agreement between model and data is greatly improved. This indicates that the effect of the furnace filter must be taken into account when data are analyzed. In buildings with more efficient filtration, the effect of the filter would be much greater.

Figure 9. Comparison of model predictions with no furnace filter and research house data with a furnace filter.



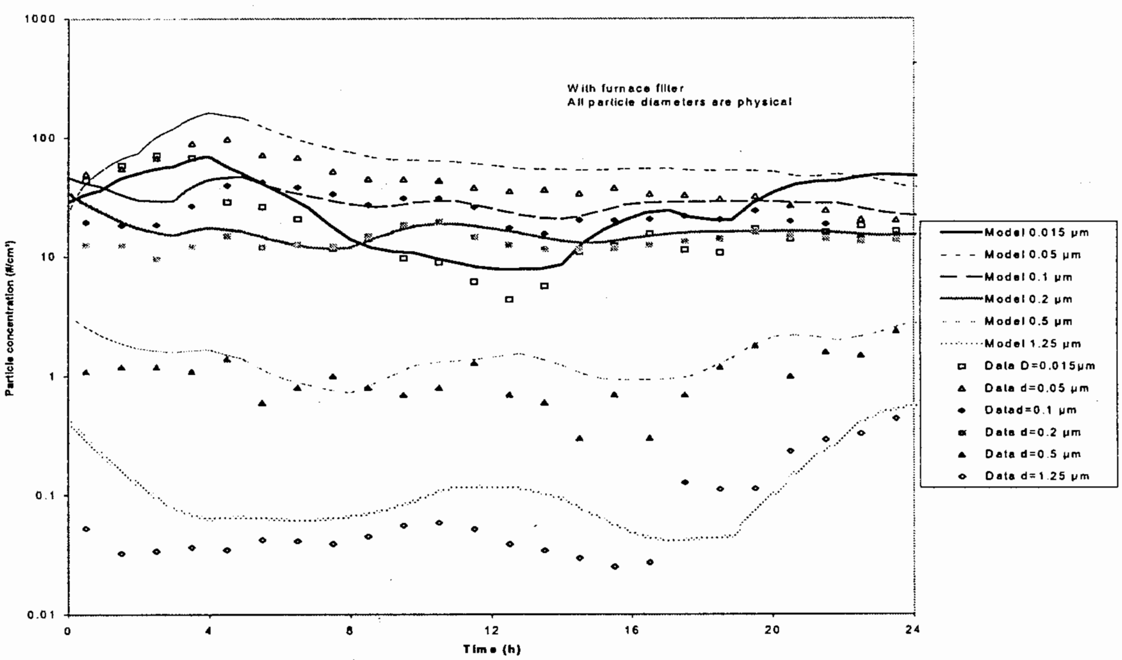
CONCLUSIONS

An IAQ model for PM has been developed. The model allows analysis of up to eight different particle diameters at a time. When the default values of penetration and particle deposition are used, the model predictions are in fair agreement with experimental data from an IAQ research house for situations with and without a furnace filter in the HAC system. The results of modeling measurement show that even a low efficiency filter has an effect on the relationship between indoor and outdoor PM.

MODEL AVAILABILITY

The model is available from EPA's web site at:
http://www.epa.gov/docs/crb/iemb/index.htm
or on CD-ROM by contacting L. E. Sparks, Indoor Environment Management Branch, Air Pollution Prevention and Control Division, National Risk Management Research Laboratory, U. S. Environmental Protection Agency, MD-54, Research Triangle Park, NC 27711. The model requires Windows 95 or 98 and at least 64 MB of RAM.

Figure 10. Comparison of model predictions with furnace filter and research house data with furnace filter.



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16. ABSTRACT The paper discusses an indoor air quality (IAQ) model for particulate matter (PM). The standard for PM < 2.5 micrometers in aerodynamic diameter (PM 2.5) proposed by the U.S. EPA has produced considerable interest in indoor exposures to PM. IAQ models provide a useful tool for analyzing both the indoor exposure to PM and the impact of risk management options on exposure. Because analysis of the impact of PM exposures requires analysis over a particle size distribution most existing IAQ models, which are designed to allow analysis of the impact of a single pollutant component, are not well suited for analysis of PM exposure. To overcome this limitation, a multicompartment IAQ model for PM exposures for a full particle size distribution was developed. The model allows analysis of the effect of: the building shell on the penetration of outdoor particles into the indoors, the deposition of particles to indoor surfaces, particle removal by air cleaners, and indoor particle sources. The use of the model is demonstrated by an analysis of both the time-varying impact of outdoor PM on indoor PM levels and the effect of a central furnace filter on indoor PM concentrations.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS		b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group	
Pollution	Air Filters	Pollution Control	13B	13K
Particles		Stationary Sources	14G	
Mathematical Models		Particulate	12A	
Exposure		Indoor Air Quality	6S	
Analyzing			14B	
Air Cleaners			13A, 13I	

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