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Development and Application of a Physics-Based Simulation Model to Investigate Residential PM2.5 Composition and Size Distribution Across the US

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SUMMARY

INTRODUCTION: Reducing $PM_{2.5}$ exposure in homes could substantially improve health.

METHODS: We have modified the Lawrence Berkeley National Lab Population Impact Assessment Modeling Framework to determine indoor $PM_{2.5}$ concentrations and exposures in a set of 50,000 homes representing the US housing stock. A mass-balance model calculated time-dependent pollutant concentrations within each home. The model included size- and species-dependent removal mechanisms and age-based occupancy patterns. We conducted an initial analysis of the impact of increasing central HVAC MERV rating on homes with central ducting on indoor concentrations of outdoor PM2.5.

RESULTS: On average, compared to homes with no filter, MERV6 reduced indoor concentrations by 6%, MERV11 by 19% and MERV14 by 39%. The impact varied by climate zone based on system run time and outdoor conditions that drive infiltration (temperature and wind) and outdoor aerosol composition.

CONCLUSIONS: The modeling framework will allow for the identifications of cost effective methods to control $PM_{2.5}$ indoors.

IMPLICATIONS: $PM_{2.5}$ exposures have a substantial impact on the health of occupants of the US housing stock. The impact of filtration on home energy use could have a sizeable net impact on the energy use of the housing stock. It is critical to provide guidance for energy efficient filtration to maximize the benefits and minimize the energy impacts. The correct filtration strategy for a given home will be a function of home location, characteristics, and occupant behavior. Costs and benefits of a given strategy may vary widely within a given location. LBNL has developed a tool to model the expected variations in costs and benefits associated with filtration across the US housing stock. This tool will aid us in providing guidance for filtration in US homes.

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INTRODUCTION

Atmospheric $PM_{2.5}$ varies in particle size distribution and composition both spatially and temporally as sources, atmospheric formation and ageing, and removal processes vary. Spatial variations occur over large regions, and from the sources that vary from urban to rural areas within regions. Temporal variations occur over diurnal, weekly, and seasonal time scales.

Elevated concentrations of $PM_{2.5}$ in the atmosphere have been associated with increased morbidity and mortality in the population.

Although the majority of health studies have correlated outdoor concentrations with health problems, most exposure to $PM_{2.5}$ occurs indoors (VanRyswyk et al. 2013). People spend more that 90% of their time indoors and more than 70% in their homes (Klepeis et al. 2001). Reducing concentrations in homes could provide an annual health benefit of $50-150 billion in the US (Logue et al. 2012).

A significant fraction of the $PM_{2.5}$ inside homes originated outdoors and is transported into the building by ventilation. In addition, there can be significant indoor sources of $PM_{2.5}$ with cooking and smoking the two most important (Wallace et al. 2004). A number of factors influence the concentration of $PM_{2.5}$ indoors. Loss mechanisms include deposition as outdoor air infiltrates through the building envelope, deposition to indoor surfaces, and particle removal by filtration. Some particles can undergo chemical reactions indoors, which can lead to a net gain or loss (Lunden et al. 2003a; Lunden et al. 2008). Lastly, particles can be emitted from a variety of indoor sources including combustion and chemical reactions.

The varied approaches to reducing indoor concentrations impact both occupant exposures and energy use. Providing guidance to effectively reduce indoor $PM_{2.5}$ concentrations at low energy cost requires an understanding of the variations in $PM_{2.5}$ sources, composition, and other parameters relevant to the US housing stock.

In order to compare the costs and benefits of various $PM_{2.5}$ control technologies, we modified the Population Impact Assessment Modeling (PIAM) framework to model $PM_{2.5}$concentrations and exposures across the US housing stock. The model currently includes infiltration of $PM_{2.5}$ from the outdoors as well as cooking. This initial analysis analyzed the impact of adding MERV rated filters to homes that have central duct systems.

METHODOLOGIES

The PIAM applies physics-based simulation model(s) to calculate one or more environmental or energy performance parameters for each home in a sample cohort developed to represent a population. Results from the individual homes are compiled to provide the statistics for population impacts. The approach can be applied at varying temporal or spatial scales; two recent applications examined the impact of air sealing and ventilation on annual energy use for homes across the U.S. (Logue et al. 2013)and the gaseous pollutant exposure impacts of cooking burners on the occupants of the Southern California housing stock (Logue et al. 2014).

We have expanded the PIAM Framework to determine indoor $PM_{2.5}$ concentrations. A single-zone mass balance model is applied to each home. The model includes factors that affect

particle transport and fate in the home including penetration, emissions, dilution, deposition, removal by filtration, chemical loss rates, and removal by air exchange. The model simulates particle dynamics by size and composition. The indoor air model uses the following governing mass-balance equation:

$$\overbrace{Change\ in\ mass}^{1} = \overbrace{Mass\ in}^{2} - \overbrace{Mass\ out}^{3} \quad (1)$$

$$\overbrace{\frac{dC_{in,i,j}}{dt}}^{1} = \overbrace{\frac{E_{i,j}}{V} + \left(A_{win}P_{i,win} + A_{infiltr}P_{i,infiltr} + \sum A_{mech}P_{i,mech}\right)C_{out,i,j}}^{2} - \overbrace{\left(k_{loss,i} + k_{evap,i,j} + A_{win} + A_{infiltr} + \sum A_{mech} + CE_{HVAC,i}A_{HVAC} + \sum CE_{recirc,i}A_{recirc}\right)C_{in,i,j}}^{3} \quad (2)$$

In Equation 2, the mass balance equation normalized by house volume, *i* refers to the particle size bin and *j* refers to a specific chemical constituent of $PM_{2.5}$. k_{loss} is the is a first order loss rate for physical loss processes like deposition to indoor surfaces. k_{evap} is the species dependent evaporative loss rate. C_{in} is the indoor concentration. C_{out} is the outdoor concentration. *P* is the particle penetration loss for the different ventilation processes that bring outdoor air indoors. *A* terms represent the airflow (ACH) through the window (A_{win}), infiltration ($A_{infiltr}$), any mechanically supplied air (A_{mech}), the central HVAC system (A_{HVAC}), and recirculation system A_{recirc}). CE_{recirc} is the fractional removal of particles from air flow through any recirculating or in room \air cleaning device. CE_{HVAC} is the size dependent removal efficiency of the central HVAC system.

In order to simplify the presentation of the equations, we introduce the two parameters which represent the household gain rate of $PM_{2.5}$ per unit outdoor concentration, G_i, and the loss rate of $PM_{2.5}$ per unit concentration indoors, Li,j. Using these parameters, Equation 2 becomes:

$$\overbrace{\frac{dC_{in,i,j}}{dt}}^{1} = \overbrace{\frac{E_{i,j}}{V} + GC_{out,i,j}}^{2} - \overbrace{LC_{in,i,j}}^{3} \quad (3)$$

where $C_{in\_I,ij}$ and $C_{in\_O,ij,}$ can be solved recursively from equation 3 as shown in Equations 4 and 5.

$$C_{in\_I,i,j}(t) = C_{in\_I,i,j}(t-1)\exp^{-(L_{i,ji}(t))\Delta t} + \frac{E_{i,j}(t)(1-\exp^{-(L_{i,ji}(t))\Delta t})}{(L_{i,j}(t))V} \quad (4)$$

$$C_{in\_O,i,j}(t) = C_{in\_O,i,j}(t-1)\exp^{-(L_i(t))\Delta t} + C_{out,i,j}(t)\frac{G_i(t)(1-\exp^{-(L_i(t))\Delta t})}{(L_i(t))} \quad (5)$$

The chemical components, denoted by *j*, are ammonium sulfate, ammonium nitrate, organic mass, elemental carbon, and "other". The size bins, denoted by subscript *i*, are those measured by the MOUDI instrument and are listed in Table 1. The total $PM_{2.5}$ concentration of indoor pollutants can be calculated by summing the contributions from indoors sources, $C_{in\_I,ij,}$ and outdoors, $C_{in\_O,ij}$:

$$C_{in} = \sum_{i,j}[C_{in\_I,i,j}(t) + C_{in_O,i,j}(t)] \quad (6)$$

Outdoor Pollutant Concentrations ($C_{out,i,j}$)

There are several sources of outdoor $PM_{2.5}$ data that vary in the detail with which the particles are characterized. We aggregated available daily, hourly, and speciation data for 2009-2012 from the EPA AirData site as well as available speciation data from the NASA NARSTO site.

Using the aggregated data from these sites, the PIAM model creates a weeklong, outdoor, minutely profile of $PM_{2.5}$ mass divided into the 30 bins defined by chemical species and particle size. Values used are average for the modeled season.

For each home, a representative county is stochastically selected by sampling from the counties located in the specified climate zone, state combination for that home weighted by county population. For the selected county, the closest monitoring sites with $PM_{2.5}$ daily data, hourly data, speciation data, and size distribution data are selected based on the distance between the county center and the location of measurement sites. Briefly the four major steps used to develop outdoor concentration profiles from monitoring data are as follows; profiles are developed for a typical weekday (Monday through Friday) and a typical weekend day (Saturday, Sunday).during each season. 1) The hourly data is first used to develop diurnal profiles of the pattern of hourly concentrations relative to daily averages. 2) From the daily data we determine average outdoor concentration for weekends and weekdays. The weekend and weekday non-dimensional diurnal profiles are multiplied by the weekend and weekday daily average concentrations to develop quantitative diurnal concentration profiles. 3) The weekend/weekday diurnal profiles are then separated into five diurnal profiles, one for each chemical species based on the closest speciation site data. 4) The average weekend/weekday fraction of each chemical species mass in each particle size bin is determined from data from the closest monitoring site with size distribution data. Organic mass was determine by multiplying the organic carbon by 1.4, the mean organic mass to organic carbon ratio found by Russell (2003).

Representative Housing Stock Development

We developed a weighted, representative set of 50,877 US homes for use in modeling conditions across the US housing stock based on the Residential Energy Consumption Survey (RECS) (US EIA 2009). The model requires several housing parameters that are not available in the RECS; these parameters were estimated or assigned based on home characteristics that were specified in the RECS. The estimated or assigned parameters include normalized leakage of the building envelope, home size, hourly weather conditions, and thermostat temperatures for RECS entries that did not have specified values. Full details of this process are described in Logue et al (2013).

When applying this model to the existing database of homes, we used an existing, simple airflow model to determine the hourly air exchange rate due to natural ventilation based on home characteristics and window opening size. Walker and Wilson (1998) developed an algorithm to calculate infiltration through the building envelope as a function of a limited number of home characteristics, outdoor weather data, and home leakage area. The size of window opening in each home is determined as a function of outdoor temperature and whether or not the home had cooling based on the algorithm implemented by Baxter (2013).

In the US housing stock, 71% of homes reported having ducted heating systems and 76% reported having some level of ducted cooling in the home (US EIA 2009). One option for controlling $PM_{2.5}$ is to increase the MERV filter rating of the duct system and potentially increase the run time of the system. To access the impact of these types of systems on concentrations, we need to estimate the airflow and runtimes of central HVAC systems. In previous work, we conducted simulations for three homes representing new, average, and old construction, corresponding to homes built according to the 2008 California Title 24 standard, a typical 1980s home and a typical 1940s home. Logue et al (2013) determined the average fractional hourly run time of the HVAC system for each home for heating and cooling as a function of the indoor-set point and outdoor temperature difference for a set of IECC climate

zones. We are using this data to estimate the hourly run time of the heating and cooling system, when present, as a function indoor-set point temperatures and outdoor temperatures for each of the modeled homes.

Size and species dependent model parameters

Deposition rates are a function of physical particle size and home characteristics. Thatcher et al (2003) and Long et al. (2001b) measured size dependent deposition rates in homes in winter and summer. For each size bin, Long and Thatcher reported the median and standard deviation of the measured deposition rate. We determined the median and standard deviation of the expected deposition rate for each of our defined particle bins by combining the weighted values for the bins used in sited studies assuming a normal distribution. For the model implementation, for each home, we selected one of the sets of data, sampled from the distribution for the size bin with the lowest variability, and then assigned the same percentage change in deposition for all of the size bins.

Particle penetration factors depend on particle size, but it is not a very strong dependence (Long et al. 2001b; Chen and Zhao 2011) for the particle size bins that are significant contributors to $PM_{2.5}$ mass. We assigned penetration factor as a function of how air enters the home. For air that is supplied through the windows, we assume that the penetration factor is 1.0.. When air infiltrates through the building envelope, we used a similar approach as we did for the particle first order deposition loss rate using penetration data from Thatcher et al. (2003) and Long et al (2001a).

Previous work by Lunden et al. (2003b) showed that ammonium sulfate could be modeled effectively using penetration, deposition loss rate values, and the building air exchange rate. Lunden et al. (2003a) found that ammonium nitrate loss rates are higher than those expected just from deposition alone. We used the fit derived by Herring et al. (2007) of the Lunden et al. data to estimate the evaporative loss rate of ammonium nitrate as a function of home temperature and particle size. Lunden et al. (2008) showed that elemental carbon follows a similar behavior as ammonium sulfate indoors, but that organic carbon concentrations are impacted by chemical transformation indoors. We used the measured data reported by Thatcher et al. (2003) and Lunden et al. (2008) to estimate a first order chemical evaporative loss rate for organic mass as a function of particle size.

Table 1. Total capture efficiency for ducts and filter for base case (BC) and three analysis scenarios (S1,S2 and S3).

Size Range		BC	S1	S 2	S3	Size Range		BC	S1	S2	S 3
<.1 μm	Bin 1	5%	9%	35%	51%	.56-1.0 μm	Bin 5	10%	19%	33%	60%
.1-.18 μm	Bin 2	5%	6%	24%	42%	1-1.8 μm	Bin 6	13%	39%	53%	82%
.18-.32 μm	Bin 3	5%	6%	22%	40%	1.8-2.5 μm	Bin 7	13%	47%	64%	91%
.32-.56 μm	Bin 4	18%	20%	33%	54%	MERV number		NA	6	11	14

Analysis Scenarios

For this initial application, we explored the impact of in-duct systems on $PM_{2.5}$ concentrations in US homes that have central duct systems. The analysis looked at a 37,819 home subset of the representative housing stock, which represents the 76% of the US housing stock with some level of ducting. We assumed that all homes ran the central duct system to provide heating and cooling. We assumed a base case of a duct system solely to provide heating and cooling with no filter in place. We compared the base case to filters in the duct systems with MERV ratings of 1) MERV6,, 2) MERV11, and 3) MERV14. Our analysis did not consider

the impacts of increased MERV filters on filter bypass, duct leakage, or reductions in duct flow rate due to increased pressure drop. MERV filter particle capture efficiency values were taken from two sources (Hanley et al. 1994; EPA 2008). A MERV14 filter likely has too large of a pressure drop for most existing home HVAC systems, however the results can be thought of as providing an upper bound on the potential benefits from adding a higher MERV filter to existing duct systems. Duct only capture efficiencies were taken for home HVAC system efficiencies measured by Stephens and Siegel (2012; 2013). We combined the duct and filter capture efficiencies using the formula given by Stephens and Siegel (2012):

$$CE_{HVAC} = CE_{ducts+filter} = 1 - (1 - CE_{ducts})(1 - CE_{filter}) \quad (7)$$

The total calculated duct and filter particle removal efficiency for each particle size bin is shown in Table 1. There are no data for the 0.1-0.3 μm size range, which encompasses most of two of our seven modeled size bins (0.1-0.18 μm bin and 0.18-0.32 μm bin). For those bins we assumed the same duct capture efficiency as for the smallest modeled bin (<0.1 μm).

RESULTS AND DISCUSSION

Table 2 presents summary results for each scenario in each US climate zone and the US average. Figures 1 and 2 present the distributional results for the concentrations indoors and outdoors of homes for each of the operating conditions. The box in each plot shows the 25-75th percentiles of the home/occupant data for each modeled condition. The line in the center of each box shows the median, and the whiskers extend to the 5th and 95th percentiles.

Table 2. Mean weekly average concentrations (conc.) in the US housing stock

Climate zone	*1*	*2a*	*2b*	*3a*	*3b*	*3c*	*4a*	*4b*
Num. of Homes (thousands)	1,338	10,783	1,938	13,629	7,072	1,661	18,583	724
Indoor Conc. (μg/m^3)								
no filter	3.8	3.3	1.8	3.5	2.7	2.2	3.8	1.7
MERV 6 filter	3.7	3.2	1.8	3.3	2.6	2.1	3.6	1.6
MERV 11 filter	3.7	2.8	1.5	2.9	2.2	1.9	3.0	1.4
MERV 14 filter	3.6	2.3	1.2	2.3	1.8	1.6	2.2	1.0
Outdoor Conc. (μg/m^3)	7.1	8.8	8.6	9.9	10.8	8.7	10.2	6.2

Climate zone	*4c*	*5a*	*5b*	*6a*	*6b*	*7*	*8*	*All US*
Num. of Homes (thousands)	1,856	18,510	3,244	5,597	856	790	34	86,614
Indoor Conc. (μg/m^3)								
no filter	2.9	4.2	2.5	3.8	2.8	2.7	8.7	3.5
MERV 6 filter	2.6	3.9	2.4	3.5	2.5	2.5	7.3	3.3
MERV 11 filter	2.2	3.3	2.0	2.9	2.2	2.1	6.0	2.8
MERV 14 filter	1.7	2.4	1.5	2.0	1.5	1.5	4.3	2.2
Outdoor Conc. (μg/m^3)	9.1	11.7	9.1	11.7	9.2	7.7	23.6	10.2

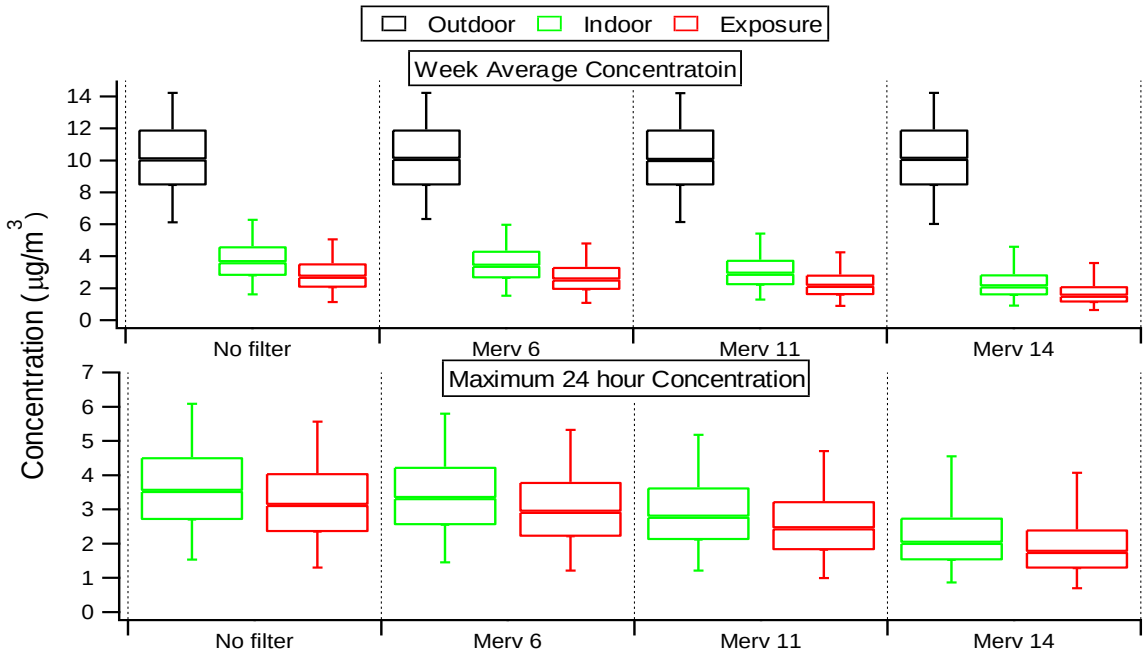

Figure 1. Week average and maximum 24-h concentrations for modeled week.

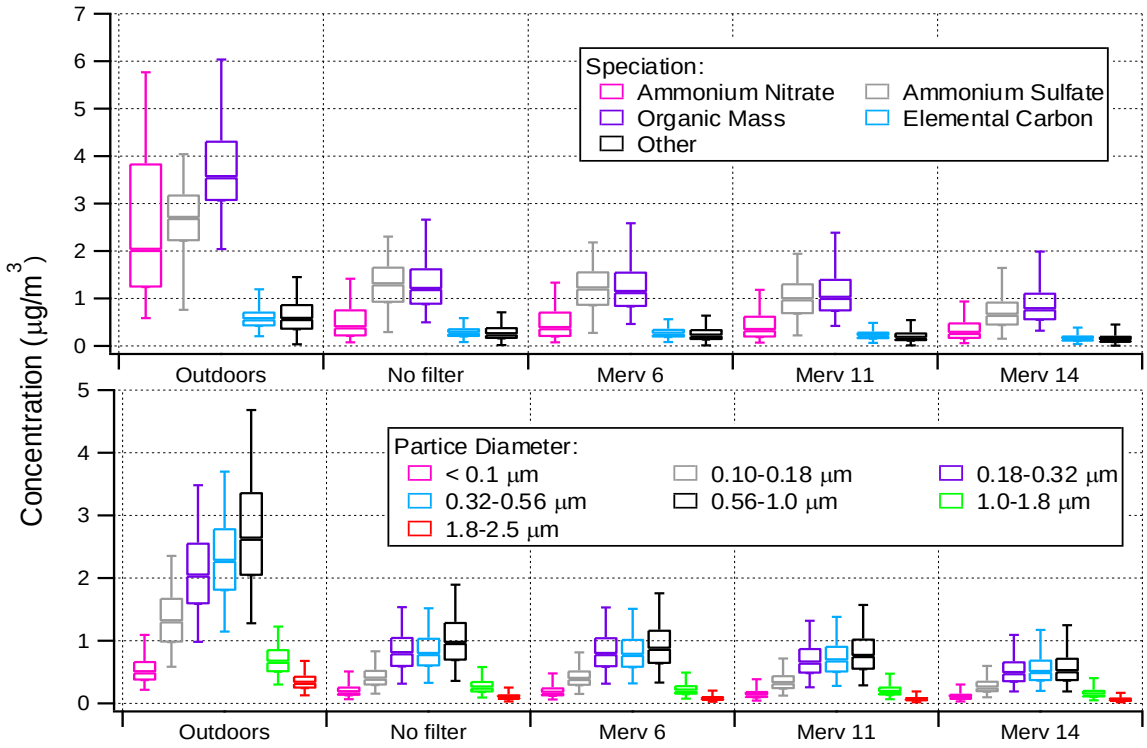

Figure 2. Week average speciation and size distribution for modeled week.

CONCLUSIONS

The results indicate that if no other changes are made, adding a higher MERV filter can reduce indoor concentrations by up to 39%, but that low MERV (MERV6), and moderately high (MERV11) filters had a much smaller impact, 8% and 20% respectively.

This work was intended to demonstrate the capabilities of the PIAM framework for assessing indoor $PM_{2.5}$ concentrations across the US housing stock. Going forward, this tool will allow

us to determine cost effective methods of controlling $PM_{2.5}$ in the residential housing stock based on home characteristics and for assessing indoor exposures across the population.

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