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Modeling indoor exposures to VOCs and SVOCs as ventilation rates vary

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SUMMARY
An important role of building ventilation is to limit the indoor concentrations of pollutants emitted from indoor sources. Changes in ventilation rate will impact the concentrations of VOCs and SVOCs in buildings depending on factors such as source location and phase partitioning. We used a fugacity-based mass balance model to simulate the impact of ventilation on indoor concentrations of VOCs and SVOCs. We found that increased ventilation is effective at controlling indoor exposures to VOCs emitted from indoor sources that have low octanol-air partitioning coefficients ($\log(K_{oa}) < 9$). For typical ventilation and filtration systems, increased ventilation is ineffective in controlling indoor concentrations of SVOCs with high octanol-air partitioning coefficients ($\log(K_{oa}) > 12$). This is because SVOCs are attached to particles, for which removal by filtration and deposition usually dominates. Results from this analysis are useful for identifying pollutants of concern while setting standards of minimum ventilation rates in commercial buildings.

KEYWORDS
Commercial buildings, fugacity model, phase partition, air filtration, intake fraction

1 INTRODUCTION

Building ventilation (outdoor air supply) is employed to limit the indoor air concentrations of pollutants emitted from indoor sources. The rates of ventilation are one of several factors that affect the indoor pollutant concentrations. Other key factors are the strengths of the indoor pollutant sources, the rates of pollutant removal by air filtration systems, deposition on surfaces, chemical interaction with surfaces, and the outdoor air pollutant concentration.

The American Society of Heating, Refrigerating and Air Conditioning Engineers provides a minimum ventilation standard for commercial buildings (ASHRAE 2010). In addition, ASHRAE (2010) also provides an optional performance-based indoor air quality procedure, which seeks to maintain indoor pollutant levels for contaminants of concern below levels specified by a cognizant authority. However, there is little data from the current literature that identifies indoor air pollutants whose concentrations are *actually sensitive* to variations in ventilation rates, and are expected to lower with increased ventilation.

This paper focuses on volatile organic compounds (VOCs) and semi-volatile organic compounds (SVOCs) for which there are indoor sources. It is part of a larger modeling effort that considers the effects of ventilation rates on exposure to organic and inorganic compounds from both outdoor and indoor sources in commercial buildings. A fugacity-based mass balance model is used to assess the dependence of pollutant removal and occupant exposures as a function of the fraction of outdoor air supply to the building. We analyze the impact of ventilation on indoor air concentrations of various compounds and summarize its importance for determining minimum ventilation rate requirements in commercial buildings.

2 MATERIALS/METHODS

We used a fugacity-based, mass-balance model (Bennett and Furtaw, 2004) to evaluate the impact of ventilation on VOCs and SVOCs. The model accounts for indoor sources, and the partitioning of chemicals among the major indoor compartments: air, particles, and surfaces (floors, walls, and ceilings). In this dynamic system, a difference in fugacity drives the diffusive flow between compartments from higher to lower fugacity. Fugacity, f (Pa), is defined as the ratio of the mass of compound, M (mol), to the fugacity capacity, Z (mol/m^{3}Pa), in a compartment of volume V (m^3).

$$f = \frac{M}{ZV} \tag{1}$$

Bennett and Furtaw (2004) detailed how fugacity capacities are computed in each of the compartments. For example, the room air compartment is composed of air and particles. The fugacity capacity of room air, Z_{air}, is therefore the sum of the air and particle phase that is modeled as having i size fraction.

$$Z_{air} = \frac{1}{RT} + \sum_i \frac{K_{p,i}\rho_{p,i}}{RT} \tag{2}$$

where R = 8.314 (Pa m^3/mol K) is the ideal gas constant, T (K) is ambient temperature, $K_{p,i}$ is the mass ratio of a pollutant associated with 1 μg of particles to 1 m^3 of air, and $\rho_{p,i}$ is the particle mass concentration (μg/m^3) in the room air for a given size fraction i.

Model Setup

A schematic of the model used in this study is shown in Figure 1. The model includes features of a commercial building ventilation system, where the indoor air is recirculated and air filters are present. The model by Bennett and Furtaw (2004) has been validated in a residential setting where the partitioning of pesticide to air and carpet was measured in a test house following an indoor application. Because this is the only fugacity model available which deals with indoor environments, we assumed that the model and its parameters apply in commercial buildings.

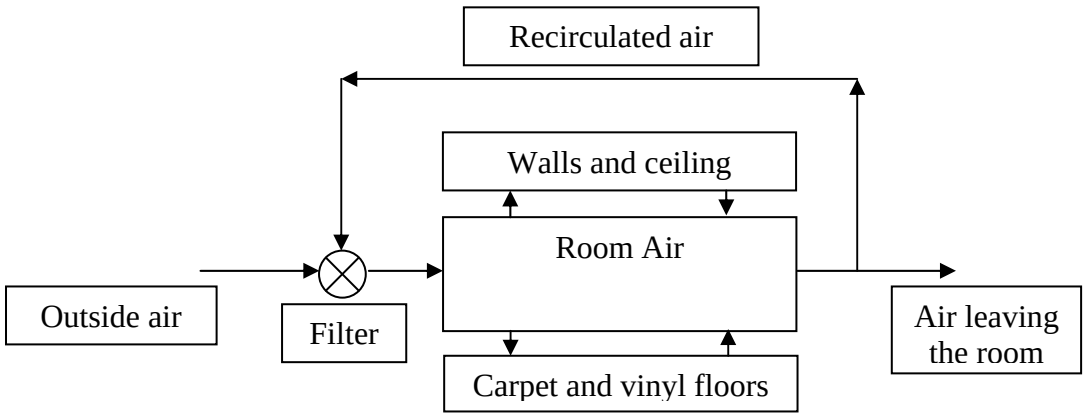


Figure 1. Fugacity-based mass-balance model, adapted from Bennett and Furtaw (2004), used to describe the mass flow and partitioning of pollutants in and out of a commercial building.

The contaminant mass flow and accumulation in the different compartments are solved by a set of differential equations. Initially, all compartments were free of contaminants. We considered VOCs and SVOCs with octanol-air partitioning coefficients, $\log(K_{oa})$, ranging from <9 to >12. Simulations were run for one year to reach quasi-equilibrium. For analyses presented in this paper, we assumed that all particles were generated outdoors, and there were only indoor sources of VOCs and SVOCs. This is representative of commercial buildings where there are generally many sources of VOCs and SVOCs such as building materials, furniture, etc., but few particle sources (Bennett et al., 2011). The indoor air is assumed well-mixed. This space has a 4 h^{-1} total air supply rate, which is made up by outdoor air and recirculated air. The fraction of outdoor air to total air supply considered ranges from 0.05 to 1. Commercial buildings typically provide fraction of outdoor air between 0.1 and 0.4 to meet the minimum ventilation requirement (Persily and Gorfain 2008). This corresponds to an outdoor air-exchange rate of 0.4 to 1.6 h^{-1}. Uncontrolled air leakage into the space through the building envelope is assumed negligible.

Particles

Particles are modeled in three size bins: 10 µm to 2.5 µm, 2.5 µm to 1 µm, and < 1µm. The removal efficiencies of the air filter are 90%, 65%, and 50%, respectively, for particles in these three size bins (Fisk et al. 2002). This roughly corresponds to a filter with MERV 13 rating. We assumed negligible filter bypass. Particle deposition and resuspension are modeled as a first-order processes. The deposition and resuspension rate constants, as well as the organic carbon fraction of the particles, are the same as used in Bennett and Furtaw (2004).

Indoor Surfaces

The indoor surfaces and their parameters are the same as modeled in Bennett and Furtaw (2004). The modeled space has 20% vinyl flooring and 80% carpet. Fugacity capacity of the vinyl floor is calculated as the sum of its components including the vinyl, the organic film on the floor surface, and the particles settled on the surface. Similarly, the fugacity capacity of the carpet is calculated as the sum of the carpet and the particles that have settled on it. Besides flooring, chemicals also partition to walls and ceiling. Fugacity capacity of the walls and ceiling is computed from the mass-transfer coefficient determined from experimental data.

3 RESULTS

The role of particles is important because SVOCs are attached to them. Figure 2 shows the percent removal of outdoor particles by filtration is greater than by ventilation. These results reflect the total particle mass removed from the three size bins modeled. Filtration dominates regardless of the outdoor air fraction modeled, but it is particularly important when the outdoor air fraction is within the typical range of 0.1 to 0.4. Total ventilation rate (outdoor air + recirculated air) of the space was 4 h^{-1}.

VOCs and SVOCs are removed from the modeled space by ventilation, filtration, and losses to indoor surfaces. Figure 3 shows the percent removal of pollutant by ventilation relative to the total removal by all processes. As the fraction of outdoor air increases from 0.05 to 1, a higher percentage of VOCs and SVOCs are removed by ventilation because more air is being moved through the indoor space, carrying indoor pollutants with it. For VOCs with a low $\log(K_{oa})$ <9, nearly all indoor pollutants are removed by ventilation because very little of the VOCs are attached to particles. This is true regardless of the fraction of outdoor air supplied to the room. For SVOCs with a high $\log(K_{oa})$ >11, Figure 3 shows that ventilation is not the dominant process of removal when the fraction of outdoor air is in the typical range of 0.1 to

0.3. This is because most of the SVOCs are attached to particles such that they are more readily removed by filtration. Net losses to indoor surfaces are minor even for SVOCs with high K_{oa}, accounting for <10% of the removal. For SVOCs with moderate to high log(K_{oa}) between 9 and 11, both ventilation and filtration are important removal processes.

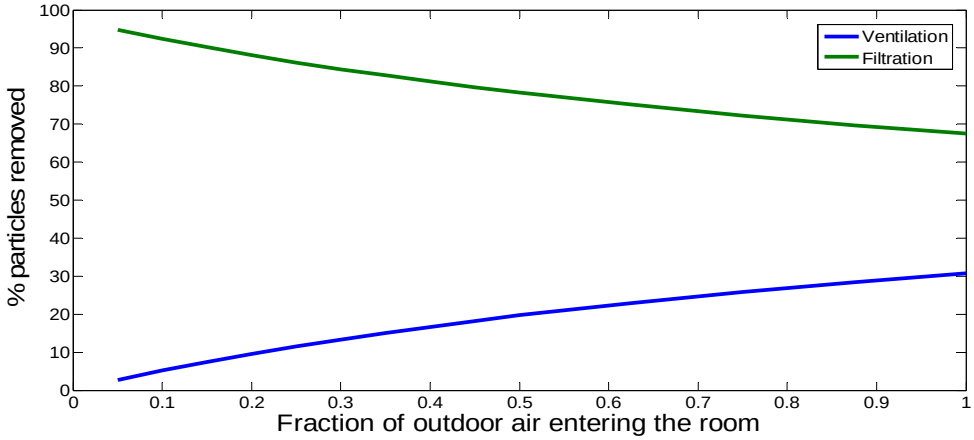


Figure 2. Percentage of outdoor air particles removed by ventilation and filtration as a function of outdoor air fraction.

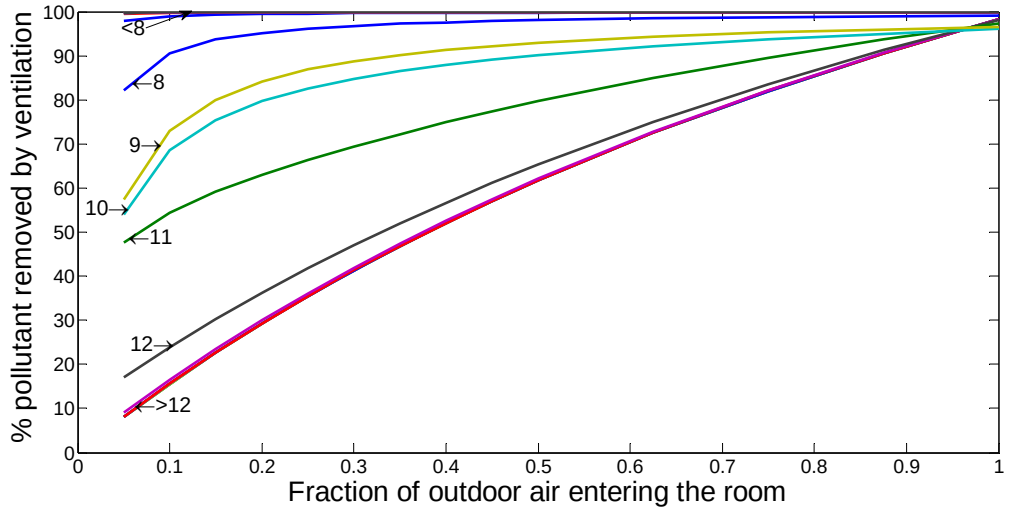


Figure 3. Percentage of VOCs and SVOCs, as characterized by their log(K_{oa}) values, that would be removed by ventilation. Results are shown for fraction of outdoor air to total supply air ranging from 0.05 to 1. Note: log(K_{oa}) is labeled in the figure.

Intake fraction is a dimensionless exposure metric defined as the ratio of mass of pollutant inhaled per unit mass emitted. Intake fraction is simply defined as the source-strength normalized concentration (h/m^3) in indoor air (gas + particle) multiplied by the breathing rate (m^3/h). The average daily breathing rate of an adult is used in this calculation (Layton, 1993). Figure 4 shows that intake fraction is sensitive to the fraction of outdoor air for VOCs with low K_{oa}. This relationship is particularly important over the range of relevant outdoor air fraction from 0.1 to 0.3. But for SVOCs with high K_{oa}, intake fraction is not expected to change with the fraction of outdoor air. This is because the model predicts that as the removal rate by ventilation decreases, there is a compensating increase in removal of the pollutant by

filtration, as shown in Figure 2. Thus, there is essentially no change in exposure as the fraction of outdoor air varies.

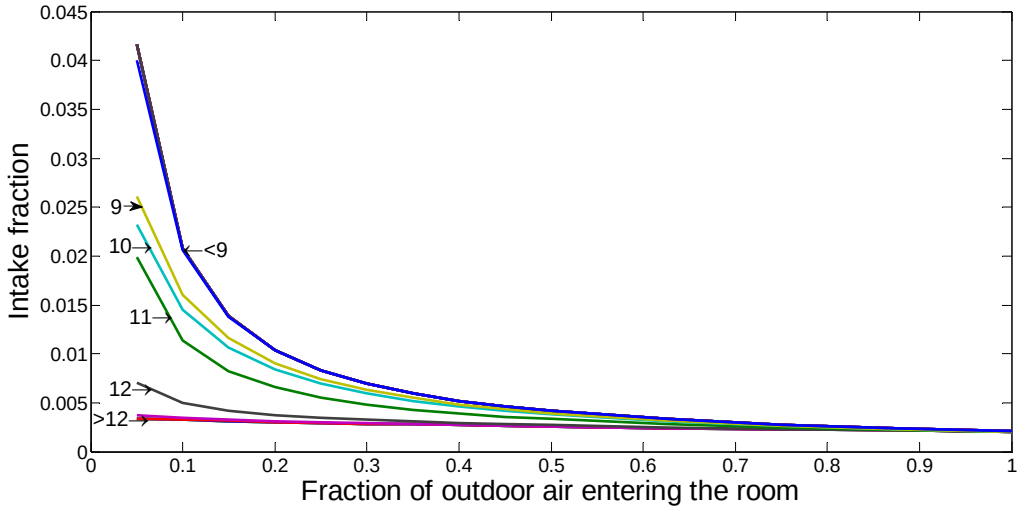


Figure 4. Intake fraction of VOCs and SVOCs with log(K_{oa}) ranging from <9 to >12 at different fractions of outdoor air. Note: log(K_{oa}) is labeled in the figure.

4 DISCUSSION

Our results suggest that VOC concentrations are sensitive to ventilation rates. A few studies report the impact of ventilation rate in commercial buildings on VOC concentrations. Hotchi et al. (2006) measured VOC concentrations in a big box retail store. An average 50% increase in concentrations of VOCs was seen when some air handling units in the building were turned off for load handling. Menzies et al. (1996) carried out a controlled double blind study in office buildings, where lower VOC concentrations were measured when ventilation rates were increased. Zuraimi et al. (2006) reported that shutting down the ventilation system caused an increase in VOC levels in office buildings in Singapore. Also, Hodgson et al. (2004), report that concentrations of pollutants with indoor sources decreased with increased ventilation, in studies carried out in a call center in the US.

Limitations

Currently our model limits the exit pathways of the SVOCs from indoor air, since we do not yet include cleaning and surface reactions as removal processes. Flow of consumables out of the buildings, such as clothes, trash, and other products will also alter the SVOC load indoors. Thus for SVOCs, the modeled results provide an upper bound on how well ventilation can perform in pollutant removal. We have not modeled chemical reaction pathways, which could be a significant removal mechanism for some VOCs and SVOCs such as terpenes and phthalates (Weschler, 2000). We do not account for SVOC and particle entry through infiltration into the building. Some types of commercial buildings such as some retail buildings can also have other direct air exchange with the outdoors through doors that are kept open. For the modeling of how ventilation rates affect SVOC exposures, we have also neglected indoor sources of particles.

Some of our conclusions are based on the assumption that minimum outdoor air fractions are typically in the range of 0.1 to 0.4, and total air supply rates are approximately 4 h^{-1}. For particles, we have assumed removal by a filter with moderately high removal efficiency relative to current typical practice. As real buildings deviate from these conditions, results

may differ. Many commercial buildings have different ventilation schedules during nights and weekends; however, we assume that the building is ventilated continuously at the same rate.

5 CONCLUSIONS

For VOCs and SVOCs with indoor sources, increased ventilation will be very helpful in controlling exposures when the $\log(K_{oa})$ is low (<9), and not helpful if the $\log(K_{oa})$ is large (>12). With intermediate values of K_{oa}, ventilation is moderately effective in reducing exposure. Some examples of pollutants with $\log(K_{oa})$ <9 include low molecular weight aldehydes such as formaldehyde, acetaldehyde and aromatics such as toluene. Some examples of pollutants with $\log(K_{oa})$ >12 include brominated flame retardants, higher molecular weight phthalates and pesticides. The need to control exposures to these compounds with indoor sources may determine minimum ventilation requirements in commercial buildings. The fugacity model is the best available tool; however, very limited data are available for validating the model.

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