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Procedia Engineering 121 (2015) 1697 – 1704

**Procedia  
Engineering**[www.elsevier.com/locate/procedia](http://www.elsevier.com/locate/procedia)

9th International Symposium on Heating, Ventilation and Air Conditioning (ISHVAC) and the 3rd International Conference on Building Energy and Environment (COBEE)

## A Simple VOC Prioritization Method to Determine Ventilation Rate for Indoor Environment Based on Building Material Emissions

Wei Ye <sup>a,b,\*</sup>, Doyun WON <sup>c</sup>, and Xu Zhang <sup>d</sup>

*a State Key Laboratory of Pollution Control and Resource Reuse, Tongji University, Shanghai 200092 P. R. China*

*b College of Environmental Science and Engineering, Tongji University, Shanghai 200092, P. R. China*

*c NRC Construction, National Research Council Canada, Ottawa, Ontario, Canada*

*d School of Mechanical Engineering, Tongji University, Shanghai 200092, P. R. China*

### Abstract

Building material emissions could be the major indoor air pollution source in low-occupant-density spaces, e.g., a private office. Lowest Concentration of Interest (LCI) schemes can be used to predict ventilation requirements based on building material emissions. However, it is not practical to obtain emission information on hundreds of chemicals with LCIs. 28 building materials selected from the NRC database were subjected to emission modelling, resulting in 101 VOCs as a starting VOC pool. A method was proposed to generate VOC priority lists. Three priority lists were obtained based on three LCI schemes, i.e., AFSSET, AgBB and EU-LCI, and each consisted of 17 - 21 VOCs, i.e., about 10% of the total substances in the schemes. This paper demonstrated the role of indoor VOCs in determining ventilation requirements and illustrated a way to predict the ventilation rate based on a simplified list of VOCs.

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Peer-review under responsibility of the organizing committee of ISHVAC-COBEE 2015

**Keywords:** AFSSET; AgBB; EU-LCI; Emission; Source control

\* Corresponding author. Tel.: +86-21-65984243; fax: +86-21-65983605.

E-mail address: [weiye@tongji.edu.cn](mailto:weiye@tongji.edu.cn)

## 1. Introduction

Volatile organic compounds (VOCs) in indoor air have attracted people's attention for more than 50 years, resulting in extensive research and regulations on material emissions to reduce their impact on human health. However, they are still a major source of pollutants that compromise the indoor air quality in our daily lives [1].

The effort to reduce the risk of human exposure to indoor VOCs generally falls into three parts, including source control, ventilation and air cleaning. Each solution has its role in lowering the indoor VOC concentrations. Nevertheless, there are technical and social barriers associated with these means. First, emission source control on building materials and products has been proposed and developed for more than two decades mainly in developed countries [1]. For most of the developing countries, introducing a simplified labeling scheme could be one of the solutions to begin with, but which substances should be targeted are still in question [2] as hundreds are targeted in a labeling scheme such as AgBB in Germany [3]. Second, once the materials and products have been placed indoors, ventilation is most frequently used to dilute emitted VOCs. It has been known that VOC emitted from building materials, instead of occupants, could be the major emission source in low-occupant-density spaces, e.g., a private office or a residence. Therefore, ventilation rate should be at least modified to incorporate VOCs emissions to maintain healthy environment in low-occupant-density buildings [4, 5]. And it is also relevant to ask what substances should be focused on to determine the ventilation rate. Third, in addition to ventilation, there are other mechanisms that change the indoor air concentrations, including the un-controlled reaction between ozone and VOCs and the controlled reaction that occur in air cleaning devices. Prioritizing VOCs for their relevance to IAQ would also be beneficial for understanding and/or utilizing both mechanisms.

The so-called Lowest Concentration of Interest (LCI) concept has been widely developed and practiced in Europe since 1997. LCIs are health-based values that could be used to evaluate material emissions after 28 days from a single product in a laboratory chamber test and, thus, serve as part of the labeling scheme to enforce source control [6]. At present, LCIs are commonly applied in product safety assessment in EU. Because current LCI schemes usually consist of hundreds of substances [3, 6, 7], a reduced list of LCIs is likely to be helpful for more practical application.

Because LCIs were derived mainly based on risk assessment and closely related to building material (and products) emissions, LCIs can be adopted to predict required ventilation rate (RVR) from a health perspective for low-occupant-density spaces in which building materials could be the majority of the emission sources [5]. Moreover, by examining each VOC that contributes to determining the ventilation rate, a priority list of VOCs that have the most influence on determining the ventilation rate can be obtained. In this paper, 101 VOCs emitted from building materials were analyzed for this purpose. The building material emission data were adopted from the NRC database [8]. A method to obtain a VOC priority list was proposed based on both the emissions and indoor air quality thresholds (LCIs). This LCI-based priority list focuses on health effects and could potentially help engineers to estimate ventilation requirements for offices and residences from the health perspective.

## 2. Methods

### 2.1. VOC emission sources and scenarios

The 28 emission sources used in this study was adopted from the NRC database [8], for the following reasons: 1) the selected materials represent a variety of building material usage, including ceiling, wall, floor and furniture materials, and also covering both residential and commercial usage; 2) all selected materials could be considered approximately as single-layer, uniform, therefore, screening-level emission estimation method based on internal diffusion coefficient and initial material-phase concentration could be applied to determine emission rates [9]; 3) all the selected materials were analyzed by GC/MS for VOC emissions and a subset of materials were also analyzed for low molecular aldehydes with HPLC [10]. A total of 101 different VOCs were detected and these VOCs were treated as the starting VOC "pool".

## 2.2. LCI references

IAQ reference values for VOCs are available in the form of threshold values for individual pollutants (e.g., chronic reference exposure level by the California government). By estimating the emission rate of a specific VOC, the RVR value for this particular VOC can be determined based on an IAQ reference value [4]. Furthermore, the so-called leading VOCs that are most likely to determine the ventilation rate could be obtained based on various individual IAQ references [5]. However, the combined effects of different pollutants are difficult to obtain since the weight of each VOC to the outcome (the ultimate ventilation rate) is not known.

Meanwhile, IAQ reference values can also be adopted to predict required ventilation as a composite index rather than an individual index if there is a criterion for the sum of multiple compounds (Eq. 1 and 2) [5]. The advantage of using a composite index to determine RVR is that each VOC would have its own weight to the outcome influenced by multiple VOCs and, potentially, VOCs with bigger weights could be acquired as priority chemicals. Examples of such composite index are the lowest concentrations of interest (LCI) adopted in the material emissions evaluation scheme such as AFSSET, AgBB and EU-LCI. The descriptions of these LCI references are summarized in Table 1.

Table 1. Selection and description of indoor air quality references.

No.	LCIs	References	Published year	Brief descriptions	Number of compounds common to VOCs emitted from the materials selected from NRC database
1	AFSSET	[7]	2009	LCI values for 165 substances, France	63
2	AgBB	[3]	2012	LCI values for 176 substances, Germany	50
3	EU-LCI	[6]	2013	Interim LCI values for 82 substances and another 95 substances to be derived, EU	33

A reference value can serve as a weight and each VOC has a ratio  $R_{i,j}$  defined as Eq. (1)

$$R_{i,j} = \frac{y_j}{I_j}, i = 1, 2, L, n; j = 1, 2, L, m \quad (1)$$

where  $R_{i,j}$  is the ratio of gas-phase concentration to Lowest Concentration of Interest value for the  $j$ -th compound emitted from the  $i$ -th building material, dimensionless;  $y_j$  is the gas-phase concentration for the  $j$ -th compound,  $\mu\text{g}\cdot\text{m}^{-3}$ ;  $I_j$  is the Lowest Concentration of Interest (LCI) value for the  $j$ -th compound, which is typically obtained by dividing occupational exposure limits by a safety factor (100 or 1000),  $\mu\text{g}\cdot\text{m}^{-3}$ ;  $n$  and  $m$  are the number of the materials and all selected compounds, respectively.

The main difference between an individual index and a composite index is that the composite index has a criterion for sum of all the compounds. That is, the sum of all  $R_j$  shall not exceed the value of 1 as Eq. (2)

$$R_i = \sum_{j=1}^m R_{i,j} \leq 1 \quad (2)$$

where  $R_i$  is the summation of all the  $R_{i,j}$ s for the  $i$ -th building material, dimensionless. Obtaining a ventilation rate that meets Eq. (2) is the main concept of using material emissions data to determine ventilation rate [5].

## 2.3. A simplified method to determine ventilation rate based on material emissions

To maximize the impact of emission characteristic of different materials on the required ventilation rate, each selected material was subjected to ventilation rate study individually (28 scenarios) to meet the criterion of Eq. (2). Therefore, a simplified characteristic ventilation rate method, which doesn't take multiple material coexisting into account [4], was revised to determine the ventilation rate and was shown in Eq. (3)

$$N_i = \frac{1}{V} \sum_{j=1}^m \frac{F_{i,j} A_i}{I_j} = \frac{1}{V} \sum_{j=1}^m \frac{E_{i,j}}{I_j} \quad j = 1, 2, L, n \quad (3)$$

where  $F_{i,j}$  and  $E_{i,j}$  are the emission factor and emission rate of the  $j$ -th compound emitted from the  $i$ -th material and can be estimated by a screening-level method based on the NRC database [9],  $\mu\text{g}\cdot\text{m}^{-2}\cdot\text{h}^{-1}$  and  $\mu\text{g}\cdot\text{h}^{-1}$ , respectively;  $A_i$  is the emission area of the  $i$ -th material,  $\text{m}^2$ ;  $N_i$  is the required ventilation rate for the  $i$ -th material based on all the possible VOCs,  $\text{h}^{-1}$ ; and  $V$  is the volume of the room,  $\text{m}^3$ .

The main goal is to obtain the relative weight of each compound to the determined ventilation rate instead of acquiring an actual ventilation rate. Therefore, the loading ratio (the ratio of emission area to the room volume) is irrelevant in this study. However, to demonstrate the calculation process, a private office was used as a standard room and was subject to emission-based ventilation rate study. The loading ratio in all scenarios was set to  $1 \text{ m}^2\cdot\text{m}^{-3}$ .

#### 2.4. A method to generate a VOC priority list for determining ventilation rate

By plugging Eq. (1) into Eq. (3), the  $R_{i,j}$  values can be expressed as Eq. (4)

$$R_{i,j} = \frac{y_j}{I_j} = \frac{E_{i,j}}{I_j N_i V}, i = 1, 2, \dots, n; j = 1, 2, \dots, m \quad (4)$$

The weight of the each  $R_{i,j}$  on determining the ventilation rate  $N_i$  can be given by

$$P_{i,j} = \frac{R_{i,j}}{\sum_{j=1}^m R_{i,j}}, i = 1, 2, \dots, n; j = 1, 2, \dots, m \quad (5)$$

where  $P_{i,j}$  is the weight of the  $j$ -th compound in determining the ventilation rate  $N_i$  based on the emissions from the  $i$ -th material, fractional.

Thus, the average weight of the  $j$ -th compound on determining all the  $N_i$ s can be given as

$$W_j = \frac{\sum_{i=1}^n P_{i,j}}{n}, j = 1, 2, \dots, m \quad (6)$$

where  $W_j$  is the average weight of the  $j$ -th compound in determining the ventilation rate based on the emissions from all the available materials individually, fractional.

Let  $M = \{W_{j=a_1}, W_{j=a_2}, \dots, W_{j=a_{m-1}}, W_{j=a_m}\}$ , where  $W_{j=a_1} \geq W_{j=a_2}, \dots, W_{j=a_{m-1}} \geq W_{j=a_m}$  and the subscript  $a_m$ s are sequential numbers.

A parameter called ‘‘average ventilation rate ratio’’,  $R_{VR}(k)$ , is defined as follows:

$$R_{VR}(k) = \frac{\sum_{j=a_1}^k W_j}{\sum_{j=1}^m W_j} \geq \text{critical value} \quad (7)$$

where  $a_1$  and  $k$  are the first and last sequential number for VOCs that belong to the group of priority VOCs, dimensionless;  $\sum_{j=a_1}^k W_j$  is the summation of the  $k$   $W_j$ s in total for priority VOCs, dimensionless;  $\sum_{j=1}^m W_j$  is the summation of all the  $W_j$ s, dimensionless; and  $R_{VR}(k)$  is a cumulative percentile and represents the ratio of the average ventilation rate determined by partial list of priority VOCs to the average ventilation rate from all the scenarios

determined by all the possible VOCs in each scenario, fractional. Therefore, by setting a critical value for  $R_{VR}$ , the  $k$  VOCs that represent a priority list to determine ventilation rate can be found.

### 3. Results and discussions

#### 3.1. Preliminary VOC priority lists

Figure 1 shows the cumulative percentiles of  $R_{VR}$  calculated for all 28 scenarios based on the three LCI references. The critical values of  $R_{VR}$  were set to be 0.50, 0.80 and 0.90. And  $R_{VRs}$  were: 1) for AFSSET,  $R_{VR}(6)=0.52 > 0.50$ ,  $R_{VR}(15)=0.82 > 0.80$ ,  $R_{VR}(21)=0.90 \geq 0.90$ ; 2) for AgBB,  $R_{VR}(5)=0.54$ ,  $R_{VR}(12)=0.82$ ,  $R_{VR}(17)=0.91$ ; 3) for EU-LCI,  $R_{VR}(7)=0.56$ ,  $R_{VR}(13)=0.81$ ,  $R_{VR}(18)=0.91$ .

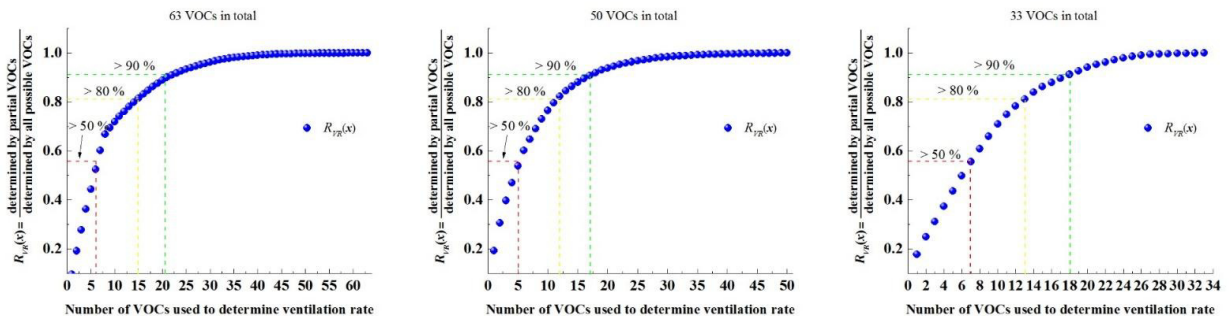


Fig. 1. The cumulative results of  $R_{VR}$  calculated for all 28 scenarios ( $m=28$ ) based on the three LCI references (a) AFSSET; (b) AgBB; (c) EU-LCI.

With AgBB as an example,  $R_{VR}(5)=0.54$  means that 5 VOCs contributed to 54 % of the required ventilation rates determined by all 50 VOCs in all 28 scenarios on average. And  $R_{VR}(17)=0.91$  indicates that the determined ventilation rates would be close to 91 % “accurate” on average if 17 VOCs are selected.

Table 2 summarizes the VOC priority lists for determining ventilation rate based on LCI references with VOCs in descending order for  $R_{VR}$  values. The priority classes were determined based on the three critical values of the average ventilation rate ratio,  $R_{VR}$ . On average, by selecting 5~7 VOCs (priority class I), the determined ventilation rate could be determined on a ~50% accuracy compared to the required ventilation rate determined by all possible VOCs. And by selecting 12~15 VOCs (priority class I+II), the determined ventilation rate could be on a ~80% accuracy. Also, by selecting 17~21 VOCs (priority class I+II+III), the determined ventilation rate could be on a ~90% accuracy. Therefore, by choosing approximately 10% of the substances on a LCI reference list, the determined ventilation rate would be reasonably close to the value from all VOCs (i.e., 90% accuracy).

However, it should be noted that the VOC priority lists are different for different LCI references. In total, 33 VOCs were included in the three priority lists in Table 3. Hexanal,  $\alpha$ -pinene,  $\beta$ -pinene and 1-nonanal and decanal are the only five substances included in all three lists. The discrepancies among the three lists are partially due to the following two reasons: 1) some VVOCs (very volatile organic compounds), such as butanal, acetone, formaldehyde and acetaldehyde, are not required in the AgBB evaluation scheme, but are included in AFSSET. Also, while acetaldehyde and butanal are included in EU-LCI, formaldehyde and acetone are excluded from EU-LCI).

Table 2. VOC priority lists for determining ventilation rate based on LCI references. VOCs are given in descending order for their contribution to the  $R_{VR}$  value..

No.	Priority class	AFSSET (165 LCIs in total)		AgBB (176 LCIs in total)		EU-LCI (to be 177 LCIs in total)	
		CAS No.	Substance	CAS No.	Substance	CAS No.	Substance

1		64-19-7	Acetic acid	91-20-3	Naphthalene	66-25-1	Hexanal
2		80-56-8	$\alpha$ -Pinene	66-25-1	Hexanal	100-42-5	Styrene
3		91-20-3	Naphthalene	64-19-7	Acetic acid	112-31-2	Decanal
4	I ( $R_{VR} \geq 50\%$ )	123-38-6	Propanal	100-52-7	Benzaldehyde	110-62-3	Pentanal
5		4994-16-5	4-Phenyl-1-cyclohexene	108-95-2	Phenol	6846-50-0	Propanoic acid
6		50-00-0	Formaldehyde			80-56-8	$\alpha$ -Pinene
7					124-19-6	1-Nonanal	
8		66-25-1	Hexanal	80-56-8	$\alpha$ -Pinene	106-46-7	1,4-Dichlorobenzene
9		108-95-2	Phenol	104-76-7	2-Ethylhexanol	127-91-3	$\beta$ -Pinene
10		138-86-3	Limonene	4994-16-5	4-Phenyl-1-cyclohexene	108-38-3	<i>m</i> -Xylene
11	II ( $R_{VR} \geq 80\%$ )	104-76-7	2-Ethylhexanol	2548-87-0	trans-2-octenal	75-07-0	Acetaldehyde
12		108-38-3	<i>m</i> -Xylene	127-91-3	$\beta$ -Pinene	106-42-3	<i>p</i> -Xylene
13		124-19-6	1-Nonanal	111-15-9	2-Ethoxyethyl acetate	108-21-4	Isopropyl acetate
14		100-52-7	Benzaldehyde	18829-55-5	trans-2-Heptenal		
15		106-46-7	1,4-Dichlorobenzene				
16		112-31-2	Decanal				
17		106-42-3	<i>p</i> -Xylene	110-54-3	Hexane	123-72-8	n-Butanal
18		127-91-3	$\beta$ -Pinene	138-86-3	Limonene	95-63-6	1,2,4-Trimethylbenzene
19	III ( $R_{VR} \geq 90\%$ )	6846-50-0	Propanoic acid	110-62-3	Pentanal	98-86-2	Acetophenone
20		98-01-1	Furfural	124-19-6	1-Nonanal	99-87-6	<i>p</i> -Isopropyltoluene
21		108-88-3	Toluene	112-31-2	Decanal	124-13-0	Octanal
22		2548-87-0	trans-2-octenal				

### 3.2. Preliminary VOC priority lists

To investigate the effects of priority list selections on the ventilation requirements, 28 building materials selected from the NRC database were subjected to emission modelling and the required ventilation rates were determined by Eq. (3) using the emission data of the VOCs that are common to the priority lists. The results are shown in Figure 2 for VOCs on the priority list.

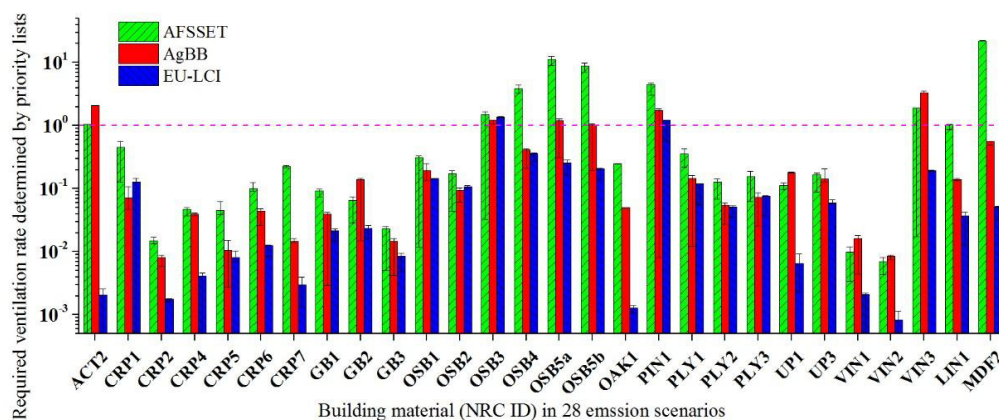


Fig. 2. Required ventilation rates determined for VOCs on the priority list (priority class I+II+III) for 28 emission scenarios. The positive and negative error bars were required ventilation rates predicted by (1) all the possible VOCs and (2) a sub-set of priority list VOCs (priority class I), respectively. The loading ratio in all 28 scenarios was set to 1 m<sup>2</sup>·m<sup>-3</sup>. The NRC ID could be found in Ref. [8].

Three major observations can be made from Figure 2. First, the narrow range of error bars indicates that the priority list can be used to replace the whole LCI list for screening-level estimation of ventilation and potentially help the industry to conduct better source control on those VOCs that have been prioritized. Second, the determined ventilation rates predicted by AFSSET were the greatest for 22 (out of 28) scenarios. This is likely the results of the more stringent values by AFSSET. The most noticeable difference is that AFSSET is the only scheme that includes VVOCs (e.g., formaldehyde). Also, most of the LCIs provided by AFSSET tend to be smaller than the LCIs in AgBB or EU-LCI with a few exceptions such as naphthalene and phenol. Third, the determined ventilation rates vary in a range of six orders of magnitude for all available materials in the NRC database. The ventilation rates for most of carpets (CRP1

– CRP7) and gypsum wallboards (GB1 – GB3) are less than  $01 \text{ h}^{-1}$ , while ventilation rates for oriented strand boards (OSB1 – OSB5b) are great than  $1 \text{ h}^{-1}$ . This indicates that the emissions of the VOCs from oriented strand boards were approximately one order of magnitude higher than those from carpets or gypsum wallboards. Among all the scenarios, medium density fiberboard requires the highest ventilation rate ( $\sim 22 \text{ h}^{-1}$  based on AFSSET list). The main reason is that the estimated formaldehyde emissions was at a  $\sim 200 \mu\text{g}\cdot\text{m}^{-3}$  level, suggesting that engineered wood materials could result in high ventilation demand if formaldehyde emissions are taken into account. However, engineered wood materials may not be the only issue as natural wood materials can also lead to a high ventilation rate due to the emissions of terpenes (see PIN1 (pine) in Figure 2).

#### 4. Summary and limitations

It has been demonstrated that LCIs can be adopted to predict ventilation rate for offices based on building material emissions [4]. However, it is not practical to determine the ventilation rate based on hundreds of VOCs in the LCI schemes.

Three LCI schemes, i.e., AFSSET, AgBB and EU-LCI, as well as 28 building materials selected from the NRC database [8], were used to determine VOC priority lists in the process of estimating the required ventilation rate. 101 VOCs were included as a starting VOC “pool”. A method to generate a VOC priority list was proposed and three priority lists were obtained for three LCI schemes. Each list consisted of 17–21 VOCs, which are about 10% of the total substances in the LCI schemes. These priority lists represent the VOCs that have the most influence on determining ventilation rate.

The effects of priority list selections on the determined ventilation rate were investigated. The results showed that, among the three lists, AFSSET list led to the highest ventilation rate partially due to its relatively strict LCI values for VOCs. The determined ventilation rates for 28 scenarios (only one material in one scenario) were in a range of six orders of magnitude, indicating dramatic effects of building material selections on the ventilation requirements. And it is recommended to include some VVOCs (e.g., formaldehyde), especially for the ongoing EU-LCI, since the formaldehyde-contained medium density fiberboard led to the highest RVR.

Although it has been illustrated that the priority lists can be used to replace the whole LCIs to predict ventilation rate or provide information for source control, there are still limitations in this study. First, the materials tested in the NRC database were mainly from North America, while all three LCI schemes were originated in Europe. Therefore, the obtained VOC priority lists are more suitable for North America. Caution is required when they are used in the European context. Second, an identical material loading ratio was used for all materials, ignoring the differences in the loading ratio of different materials in an office. While this simplification is useful for comparing materials based on emission rate per area only, it likely led to the results that are different from the actual concentrations indoors. Material usage patterns that are typical in offices need to be developed. Additionally, as discussed in reference [9], there are uncertainties associated with the screening-level estimates of both the building material emissions and required ventilation rate. Overall, this paper showed the role of indoor VOCs in determining ventilation requirements and demonstrated a way to predict the ventilation rate based on a simplified list of VOCs.

#### Acknowledgements

The material emissions database by National Research Council Canada (NRC) is the outcome of two consortium projects, i.e., CMEIAQ I and II. The authors would like to thank the members of the consortiums and the technical advisory committees.

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