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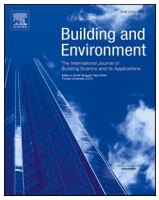

Novel classification criterion of indoor organic pollutants based on their relative abundances in house dust and indoor air

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ABSTRACT

Indoor organic pollutants are typically categorized into (very-)volatile, semi-volatile, and low-volatile organic compounds (VOCs, SVOCs, and LVOCs) for easier handling. Existing criteria have been found to be neither consistent nor precise in classifying many compounds, primarily because they have not captured the apparent differences between VOCs, SVOCs, and LVOCs: VOCs predominantly exist in the air, LVOCs mainly reside in reservoirs like house dust, and SVOCs serve as transitional compounds between them. Based on a systematic analysis of the relative abundance of compounds between house dust and indoor air (the two crucial transfer and storage media of indoor organic pollutants), a novel criterion was proposed in this study, i.e., VOCs: $\log K_{oa} < 6$, SVOCs: $6 \leq \log K_{oa} \leq 9.8$, and LVOCs: $\log K_{oa} > 9.8$ (K_{oa} is the octanol-air partition coefficient of compounds). In doing so, we developed a novel equation to estimate the dust-air partitioning quotient of compounds (K_d), incorporating for the first time the effects of K_{oa} and indoor conditions on K_d; and subsequently we determined the boundaries between VOCs, SVOCs, LVOCs based on the K_d equation and Monte Carlo simulations (to assess the combined effects of various indoor conditions). Consistence between classification results and literature evidences, as well as good agreement between estimates of the K_d equation and measured data retrieved from the literature, justified the proposed criterion. The novel criterion should facilitate the selections of most suitable methods for the chemical analysis, exposure assessment, and effective controls of organic pollutants in indoor environments.

1. Introduction

Organic compounds are an important factor that can degrade indoor air quality [1,2]. Pollutants in the air can more or less partition to various reservoirs including house dust, airborne particles, and surfaces, leading to diverse exposure pathways including inhalation of air and particles, ingestion of dust, and dermal sorption from air and surfaces [3,4]. Organic compounds are often classified as (very-)volatile, semi-volatile, and low-volatile organic compounds (VOCs, SVOCs, and LVOCs) [5–7]. Much of our understanding of human exposure and associated effects is based on measurements of compound concentrations in indoor air and dust, specifically in the air for VOCs, in both the air and dust for SVOCs, and in the dust for LVOCs [7]. Thus, the classification facilitates the selection of most suitable measures for chemical analysis and exposure assessment [8], which is particularly important for the increasing number of emerging pollutants whose indoor transport characteristics are highly uncertain [9].

Early in 1989, the World Health Organization proposed a classification criterion for indoor organic compounds based on their boiling points (BP): VVOC (< 0 °C to 50–100 °C), VOC (50–100 °C to 240–260 °C), SVOC (240–260 °C to 380–400 °C), and organic compounds associated with particulate organic matter (POM, > 380 °C) [10]. Note, VVOC is hereinafter merged into VOC since they are both dominating in the air, and POM is considered to be equivalent to LVOC. Because some compounds decompose before they boil (difficult to obtain their BP), other criteria are also proposed [11]. For example, the vapor pressure (V_p) [5]: VOC (> 10 Pa) and SVOC (10^{-9} to 10 Pa); the gas chromatographic retention time [12]: VOC (eluting before *n*-hexadecane) and SVOC (after *n*-hexadecane); and the carbon number [13]: VOC (< C_{16}) and SVOC (C_{16}–C_{22}). Unfortunately, some problems have been identified in the applications of these criteria [14]. First, different criteria may result in inconsistent classifications for some compounds [11]. For instance, 8:2 fluorotelomer alcohol (8:2 FTOH) can be classified as VOC

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Nomenclature

A_d	Area of dust-deposited surfaces (m^2)
C_a	Gas-phase concentration (μg/m^3)
C_d	Dust-phase concentration (μg/g)
C_p	Particle-phase concentration (μg/m^3)
$f_{om,d}$	Fraction of organic matter in dust (-)
$f_{om,p}$	Fraction of organic matter in particle (-)
H	Room height (m)
h_{md}	Mass transfer coefficient (m/s)
K_d	Dust-air partitioning quotient (m^3/μg)
$K_{d,e}$	K_d at equilibrium state (m^3/μg)
K_{oa}	Octanol-air partition coefficient (-)
$K_{oa,sl}$	SVOC-to-LVOC threshold of K_{oa} (-)
$K_{oa,vs}$	VOC-to-SVOC threshold of K_{oa} (-)
K_p	Particle-air partitioning quotient (m^3/μg)
K_s	Surface-air partitioning quotient (m)
K_{wa}	Water-air partitioning coefficient (-)
L_d	Dust mass per surface area (g/m^2)
M_d	Total mass of dust (g)
R_c	Removal rate of dust (s^{-1})
R_r	Resuspension rate of dust (s^{-1})
TSP	Concentration of particles (μg/m^3)
V_a	Total volume of indoor air (m^3)
v_d	Particle deposition velocity (m/s)
V_p	Vapor pressure (Pa)
β_d	Dust-air relative abundance (-)
β_p	Particle-air relative abundance (-)
β_s	Surface-air relative abundance (-)
ρ_d	Dust density (μg/m^3)

and SVOC based on the BP criterion (BP = 113 °C [15]) and V_p criterion (V_p = 1.6 Pa [15]), respectively. Second, existing criteria are not precise for some compounds though their classifications are consistent. Particularly, some pollutants being consistently classified as VOC have been found to behave like SVOCs indoors (with meaningful amount in both the air and reservoirs), e.g., furaneol ($C_6H_8O_2$, BP = 216 °C, V_p = 31 Pa) [4] and hexanoic acid ($C_6H_{12}O_2$, BP = 203 °C, V_p = 14 Pa) [16,17] (BP and V_p were obtained from US EPA CompTox Chemicals Dashboard v2.4.1: https://comptox.epa.gov/dashboard/).

Gas-reservoir partitioning of organic compounds is typically governed by the volatility: lower volatility often corresponds to greater amount in reservoirs [5]. Thus, VOCs are often considered as compounds with negligible amount in reservoirs (mainly exist in the air), LVOCs are exactly the opposite (mainly exist in reservoirs), and SVOCs are compounds with comparable amount in the air and reservoirs. However, the above criteria are all defined based on the basic properties of organic compounds (BP, V_p, etc.) instead of their relative abundance in the air and reservoirs, which is the apparent differences between VOCs, SVOCs and LVOCs. To facilitate the consistent and precise classification of indoor organic compounds, it is desirable to propose a novel criterion based on their reservoir-gas relative abundance in indoor environments.

In this study, indoor air and house dust are selected as the main focus because they are the two most frequently-used media for assessing the pollution levels and human exposure of organic pollutants in the indoor environment [18–21]. Since the dust-air relative abundance (β_d) of indoor compounds is affected by both the compound properties and environmental conditions (see details in Section 2.1), the β_d-based criterion is expected to vary significantly among indoor environments. Thus, an equation incorporating the effects of compound properties and indoor conditions on β_d will be established at first. Subsequently, the novel criterion will be derived based on the principle that the classification shall be consistent in different indoor environments (i.e., conditions of $\beta_d \ll 1$ and $\beta_d \gg 1$ always stand for VOCs and LVOCs, respectively). In particular, the variations of β_d in different indoor environments (associated with the combined effects of various indoor parameters) will be quantified by performing Monte Carlo simulations with the distributions of each indoor parameter.

2. Materials and methods

2.1. Method principle and key challenges

The dust-air relative abundance (β_d) of a certain compound can be determined by comparing its whole-house amount in the dust to that in the air, i.e.,

$$\beta_d = \frac{M_d \cdot C_d}{V_a \cdot C_a} = \frac{A_d}{V_a} \cdot L_d \cdot \frac{C_d}{C_a} \approx \frac{1}{H} \cdot L_d \cdot K_d \cdot 10^6 \quad (1)$$

where C_a (μg/m^3, compound mass per air volume) and C_d (μg/g, compound mass per dust mass) are compound concentrations in the air and dust, respectively; V_a (m^3) is the total volume of indoor air; M_d (g, = $A_d \bullet L_d$) is the total mass of dust; A_d (m^2) is the total area of dust-deposited surfaces; L_d (g/m^2, dust mass per surface area) is the dust loading; K_d (m^3/μg, = $C_d/C_a/10^6$) is the dust-air partitioning quotient of the compound; and the factor of 10^6 accomplishes the unit conversion (1 g = 10^6 μg). Assuming that dust is primarily deposited on horizontal surfaces like floors [22], the ratio of V_a to A_d can be approximate to the room height (H, m) and thus β_d equals the product of $1/H$, L_d, and K_d, i.e., the rightmost term of Eq. (1).

According to the definitions given in Introduction, VOCs are compounds with $\beta_d \ll 1$, LVOCs are compounds with $\beta_d \gg 1$, and β_d's of SVOCs are relatively moderate. Thus, if H and L_d are known, a critical K_d dividing VOCs and SVOCs can be obtained by substituting a sufficiently small β_d (e.g., 0.1) into Eq. (1), and another critical K_d dividing SVOCs and LVOCs can be obtained with a sufficiently great β_d (e.g., 10). However, H and L_d are inherently variable among houses, e.g., Johnson et al. [23] found that L_d varied over 2 orders of magnitude (0.04 ~ 2.33 g/m^2) in 488 houses. Hence, the two critical K_d's are also expected to vary significantly in different indoor environments, greatly impeding their use in classifying indoor organic compounds. Furthermore, K_d is not suitable for use as the critical metric since it is affected by not only the compound properties (e.g., V_p and octanol-air partition coefficient (K_{oa}) [24]) but also the indoor environmental conditions (e.g., L_d [25,26] and residence time of dust [27]). This problem can be simplified by using an equation explicitly describing the relationship between K_d and its dependent variables (especially indoor conditions). However, such equation is not available now, which is considered to be the key challenge of the present study and thus will be established below. A list of K_d equations reported in the literature is provided in Section S1 (S denotes the Supplementary Material).

2.2. Novel equation for estimating K_d

In 2015, Shi and Zhao [22] developed a mechanistic model to estimate C_d by assuming that organic compounds in house dust was accumulated mainly due to the sorption of compounds from the air and the deposition of compound-laden airborne particles, while removed by the resuspension and cleaning of dust. The correlation between model estimates (y) and 66 measured data (x) was very close to the $y = x$ line (y = 0.93x + 0.09, R^2 = 0.73), verifying the model performance. Therefore, the novel equation for estimating K_d was developed on the basis of Shi

and Zhao's model. Accordingly, the mass balance equation of a certain compound in house dust can be expressed by,

$$\frac{\mathrm{d}(M_d C_d)}{\mathrm{d}t} = h_{md}A_d\left(C_a - \frac{C_d}{K_{d,e}\cdot 10^6}\right) + v_d A_d C_p - R_r M_d C_d - R_c M_d C_d \quad (2)$$

where h_{md} (m/s) is the air-to-dust mass transfer coefficient; R_r (s^{-1}) is the resuspension rate of dust; R_c (s^{-1}) is the removal rate of dust due to cleaning activities; $K_{d,e}$ (m^3/μg) is the dust-air partitioning coefficient of the compound at equilibrium; v_d (m/s) is the deposition velocity of airborne particles; and C_p (μg/m^3) is the compound concentration associated with airborne particles, which can be calculated by [28]:

$$C_p = K_p\cdot \mathrm{TSP}\cdot C_a \quad (3)$$

where TSP (μg/m^3, particle mass per air volume) is the mass concentration of airborne particles; and K_p (m^3/μg) is the particle-air partitioning quotient of the compound, which can be estimated by the model proposed in our previous study [29] (see details in Section S2).

Li et al. [27] found that dust-air partitioning of compounds had reached the steady state in indoor environments. At the steady state, the left term of Eq. (2) will be equal to zero, i.e., $\mathrm{d}(M_d C_d)/\mathrm{d}t = 0$, and thus the equation of C_d can be derived as,

$$C_d = \frac{h_{md}C_a + v_d\cdot K_p\cdot \mathrm{TSP}\cdot C_a}{h_{md}/(K_{d,e}\cdot 10^6) + (R_r + R_c)L_d} \quad (4)$$

Subsequently, the equation of K_d can be obtained by $K_d = C_d/C_a/10^6$ (m^3/μg), i.e.,

$$K_d = K_{d,e}\left(1 + \frac{v_d}{h_{md}}K_p\cdot \mathrm{TSP}\right)\left[1 + \frac{(R_r + R_c)L_d}{h_{md}}K_{d,e}\cdot 10^6\right]^{-1} \quad (5)$$

Eq. (5) can also be expressed in the logarithmic form that is more frequently used [24],

$$\log K_d = \log K_{d,e} + \log\left(1 + \frac{v_d}{h_{md}}K_p\cdot \mathrm{TSP}\right) - \log\left[1 + \frac{(R_r + R_c)L_d}{h_{md}}K_{d,e}\cdot 10^6\right] \quad (6)$$

As described in Section S2, the equation of K_p is rather complex, which may complicate the use of Eq. (6). Fortunately, we find that the K_p term ($v_d/h_{md}\bullet K_p\bullet$TSP) has insignificant effects on the estimations of K_d. As shown in Figure S1, the difference between the estimations of Eq. (6) when TSP = 0 (i.e., neglecting the K_p term) and those when TSP = 60 μg/m^3 (typical TSP in indoor environments[27]) is less than 0.05 (the typical range of log K_d is –6 ~ –1 as shown in Fig. 1). Thus, Eq. (6) can be simplified as,

$$\log K_d = \log K_{d,e} - \log\left[1 + \frac{(R_r + R_c)L_d}{h_{md}}K_{d,e}\cdot 10^6\right] \quad (7)$$

Furthermore, $K_{d,e}$ is often predicted in existing studies using the equation proposed by Weschler and Nazaroff [19]: log $K_{d,e}$ = log K_{oa} + log $f_{om,d}$ – log ρ_d ($f_{om,d}$ is the fraction of organic matter in dust and ρ_d is the dust density). The values of $f_{om,d}$ and ρ_d are often fixed as 0.2 and 2 × 10^{12} μg/m^3, respectively [19], yielding the equation for predicting $K_{d,e}$ based solely on K_{oa},

$$\log K_{d,e} = \log K_{oa} - 13 \quad \text{or} \quad K_{d,e} = K_{oa}\cdot 10^{-13}\ (m^3/\mu g) \quad (8)$$

Consequently, Eq. (7) can be rewritten as,

$$\log K_d = \log K_{oa} - 13 - \log\left[1 + \frac{(R_r + R_c)L_d}{h_{md}}K_{oa}\cdot 10^{-7}\right] \quad (9)$$

Eq. (9) is the final form of the novel K_d equation, which exhibits the dependence of K_d on both the compound property (K_{oa}) and indoor parameters (R_r, R_c, L_d, and h_{md}).

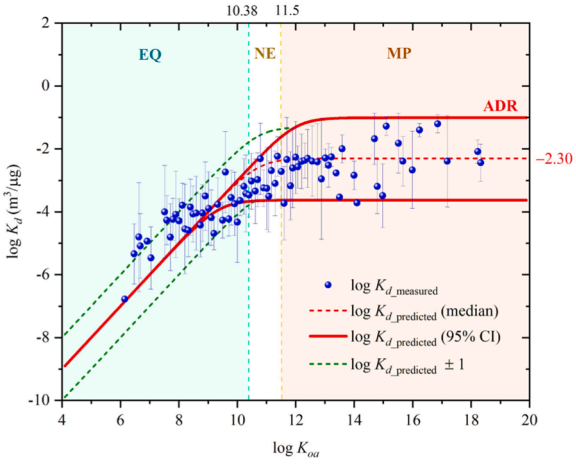

Fig. 1. Comparison between measured data of log K_d and estimates of Eq. (9). Points/bars: means/standard deviations of measured data; Red-solid curves: 95 % CI of estimates (acceptable deviation range, ADR); Red-dash curve: median of estimates; Green-dash curves: median of estimates ± 1 (ADR defined by Li et al. [27]); Vertical dash lines: thresholds of log K_{oa} dividing dust-air partitioning into three domains (EQ: equilibrium, NE: nonequilibrium, MP: maximum partition, defined by Li et al. [27]).

2.3. Boundaries between VOCs, SVOCs, and LVOCs

The equation for calculating the relative abundance of a compound in house dust and indoor air (β_d) can be updated by combining Eq. (1) with Eq. (9), i.e.,

$$\beta_d = \frac{1}{H}\cdot\left(\frac{10^7}{K_{oa}\cdot L_d} + \frac{R_r + R_c}{h_{md}}\right)^{-1} \text{ or } \log\beta_d = -\log H - \log\left(\frac{10^7}{K_{oa}\cdot L_d} + \frac{R_r + R_c}{h_{md}}\right) \quad (10)$$

As stated in Introduction, VOCs are mainly existed in the air (with negligible amount in dust, i.e., $\beta_d \ll 1$) while SVOCs have comparable abundance in both the air and dust. Thus, a sufficiently small β_d can be used as the threshold for dividing VOCs and SVOCs. Because the measuring errors of compound concentrations are often in the order of 10 % [21,30,31], the threshold of β_d is set to be 0.1, which yields the equation for calculating the boundary between VOCs and SVOCs (designated as $K_{oa,vs}$),

$$K_{oa,vs} = \frac{10^7}{L_d}\left(\frac{10}{H} - \frac{R_r + R_c}{h_{md}}\right)^{-1} \text{ or } \log K_{oa,vs} = 7 - \log L_d - \log\left(\frac{10}{H} - \frac{R_r + R_c}{h_{md}}\right) \quad (11)$$

Conversely, the threshold of β_d for dividing SVOCs and LVOCs should be significantly greater than 1, which is set to be 10 (corresponding to the inverse of 0.1). Then, the boundary equation between SVOCs and LVOCs ($K_{oa,sl}$) can be obtained,

$$K_{oa,sl} = \frac{10^7}{L_d}\left(\frac{1}{10H} - \frac{R_r + R_c}{h_{md}}\right)^{-1} \text{ or } \log K_{oa,sl} = 7 - \log L_d - \log\left(\frac{1}{10H} - \frac{R_r + R_c}{h_{md}}\right) \quad (12)$$

2.4. Indoor parameters, data sources and Monte Carlo simulations

Indoor parameters: According to Eqs. (9), (11), and (12), five indoor parameters (L_d, H, R_r, R_c, and h_{md}) are required for the calculations of K_d, $K_{oa,vs}$ and $K_{oa,sl}$. In addition, the distributions of these parameter are required in the following Monte Carlo simulations, which are all assumed to be lognormally distributed in this study. Details of these indoor parameters are listed in Table 1 (more specific information is

Table 1
Summary of indoor parameters used in the calculations (lognormal distribution is assumed for each parameter, details are presented in Section S3).

Parameters	Geometric Mean (GM)	Geometric Standard Deviation (GSD)	95 % Confidence Interval (Lower to Upper Bounds)
L_d (g/m^2)	0.311	2.73	0.043 ~ 2.33
H (m)	2.40	1.12	1.92 ~ 3.00
R_r (10^{-07} s^{-1})	1.39	3.70	0.255 ~ 7.41
R_c (10^{-07} s^{-1})	0.613	2.80	0.231 ~ 2.31
h_{md} (10^{-04} m/s)	3.89	1.97	1.03 ~ 7.78

provided in Section S3). Note, when determining the distributions of L_d, H, R_r, and R_c, Layton and Beamer [32] was regarded as the key reference because their results were summarized from measurements of over 200 residences in the US and Netherlands.

Data sources: To evaluate the performance of Eq. (9) (novel K_d equation), a total of 1794 K_d values of 139 compounds were collected from the measurements of 60 articles, as listed in Table S2 (see the selection criteria in Section S4). Note, the collected data may be far from exhaustive because we are not intended to perform a systematic review of K_d of indoor organic pollutants, but the number of these data shall be adequate for the evaluation. In addition, K_{oa} is the key parameter reflecting the dependence of K_d on compound properties. K_{oa} values of the target compounds are listed in Table S2 and these values were determined by the method provided in Section S4.

Monte Carlo Simulations: Estimates of Eqs. (9), (11), and (12) are likely to be variable in different indoor environments because variable indoor parameters are involved in these equations. Thus, Monte Carlo simulations were performed to obtain the distributions of their estimates (K_d, $K_{oa,vs}$, and $K_{oa,sl}$) by running the calculations 10,000 times (found to be sufficient to obtain stable distributions) with the values of each parameter randomly selected from their distributions listed in Table 1. The 2.5th and 97.5th quantiles of the outputs were selected as their upper and bottom bounds, respectively, which were then defined as the 95 % CI of estimated K_d, $K_{oa,vs}$, and $K_{oa,sl}$.

3. Results and discussion

3.1. Performance of novel K_d equation

Comparisons between collected data and estimates of Eq. (9) are shown in Fig. 1 as a function of log K_{oa}. For the convenience of illustration, collected data was grouped into 78 clusters, with an interval of 0.1 for log K_{oa} values, in the figure. For example, the mean value and standard deviation of log K_d values with log $K_{oa} \in$ [7.95, 8.05) were depicted as a point and an error bar, respectively (x-coordinate of the point was set as the mean log K_{oa} of these log K_d values). The median and 95 % CI of the estimated log K_d were plotted as the red-dash and red-solid curves in Fig. 1, respectively.

It can be seen that, as the increase of log K_{oa}, log K_d tends to linearly increase at first, then gradually deviate from the line, and finally reach a maximum value. This pattern is consistent with the findings of Li et al. [27], i.e., dust-air partitioning can be divided into three domains: equilibrium (EQ, log K_d is linearly related to log K_{oa}), nonequilibrium (NE, log K_d is non-linearly related to log K_{oa}), and maximum partition (MP, log K_d reaches its maximum and is independent of log K_{oa}). These domains are divided by two thresholds of log K_{oa}: EQ (log $K_{oa} <$ 10.38), NE (10.38<log $K_{oa} <$ 11.5), and MP (log $K_{oa} >$ 11.5). As shown in Fig. 1, our K_d equation also follows the above division: median log K_d is independent of indoor parameters when log $K_{oa} <$ 10.38 while becomes independent of log K_{oa} when log $K_{oa} >$ 11.5. Additionally, Li et al. [27] also proposed a K_d equation: $\log K_{d,\mathrm{Li}} = \log K_{oa} + \log f_{om,p} - 12 - \log(1 + 2.09\times10^{-10} f_{om,p} K_{oa})$ ($f_{om,p} = 0.4$). As depicted in Figure S2, the relative deviations between estimates of Li's equation and median estimates of Eq. (9) are less than 20 %, indicating good agreement between two equations. Compared to Li's equation, the advantage of Eq. (9) is that it can describe the effects of indoor parameters on dust-air partitioning (especially in NE and MP domains).

To quantify the degree of agreement between Eq. (9) and collected data, we firstly defined the region bounded by the red-solid curves in Fig. 1 (95 % CI of the estimated log K_d) as the acceptable deviation range (ADR) of Eq. (9). As shown, most points in MP domain are within the ADR; but on the contrary, most points in EQ domain are out of the ADR. This is because Eq. (9) becomes independent of indoor parameters in EQ domain and thus the corresponding ADR becomes very narrow (even converges to a line), which indicates that the above ADR requires redefinition. Li et al. [27] defined the ADR of their K_d equation as the region bounded by a deviation of ± 1 log unit from the estimated log K_d (because their equation could only generate a single log K_d value for each compound). This ADR was considered to be reasonable since measured K_d values of many compounds varied over 2 orders of magnitude (e.g., log K_d of di-2-ethylhexyl phthalate (DEHP) varied from –2.34 to 0.27 according to the results of Sukiene et al. [33], REF #40 in Table S2). Thus, a novel ADR for evaluating our K_d equation was defined by combining the 95 %CI ADR with the ±1 ADR, i.e., the maximum region bounded by red-solid curves and green-dash curves in Fig. 1. Green-dash curves were plotted with the values with deviations of ± 1 log unit from median estimates of Eq. (9). Noted that the new ADR still cannot cover the measuring errors of all the data points because the error bars of some points in Fig. 1 span over 2 or even 3 log units. Nevertheless, 85.9 % of the mean data points (EQ: 73.5 %, NE: 100 %, MP: 93.9 %) were within the ADR and 69.4 % of the individual data point (EQ: 63.2 %, NE: 70.8 %, MP: 77.7 %, as listed in Table S2) were within the ADR. The high match rates between the ADR and collected data imbued strong confidence in the novel K_d equation.

Overall, the above results give convinced support on the performance of the novel K_d equation and the reasonability of the values/distributions of indoor parameters listed in Table 1, which is the essential basic of the classification criterion derived below.

3.2. Classification criterion based on K_{oa} of organic compounds

Theoretically, the classification of indoor organic compounds can be implemented based on log $K_{oa,vs}$ and log $K_{oa,sl}$ defined in Eqs. (11) and (12), i.e., VOCs (log $K_{oa} <$ log $K_{oa,vs}$), SVOCs (log $K_{oa,vs} \leq$ log $K_{oa} \leq$ log $K_{oa,sl}$), and LVOCs (log $K_{oa} >$ log $K_{oa,sl}$). However, the classification can vary significantly in different houses because $K_{oa,vs}$ and $K_{oa,sl}$ are the functions of variable indoor parameters according to Eqs. (11) and (12). Therefore, Monte Carlo simulations were performed to quantify the variation ranges of $K_{oa,vs}$ and $K_{oa,sl}$ associated with the combined variation of indoor parameters. The results indicated that 95 % CI of log $K_{oa,vs}$ was 6.02 ~ 7.72 (median: 6.88) and 95 % CI of log $K_{oa,sl}$ was 8.04 ~ 9.75 (median: 8.90), which were considered to be the variation ranges of log $K_{oa,vs}$ and log $K_{oa,sl}$ in most ($\geq$ 95 %) indoor environments.

According to the principle that compounds being classified as VOCs shall always meet the condition of $\beta_d < 0.1$ (mainly exist in the air in most indoor environments), the criterion of VOCs should be set as the bottom bound of log $K_{oa,vs}$ (6.02). In contrast, the criterion of LVOCs should be set as the upper bound of log $K_{oa,sl}$ (9.75) because LVOCs are defined as compounds always meeting the condition of $\beta_d > 10$. Beyond these ranges, compounds will be classified as SVOCs. For the convenience of applications, the two thresholds of log K_{oa} were rounded as 6.0 and 9.8, respectively, becoming slightly stricter than the original thresholds (< 6.02 and > 9.75). Thus, the classification criterion of indoor organic compounds based on their log K_{oa} values was settled as: VOCs (log $K_{oa} <$ 6), SVOCs (6 $\leq$ log $K_{oa} \leq$ 9.8), and LVOCs (log $K_{oa} >$ 9.8).

We also performed Monte Carlo simulations for Eq. (10) to quantify the variation ranges of log β_d, as shown in Fig. 2. The red-solid curves

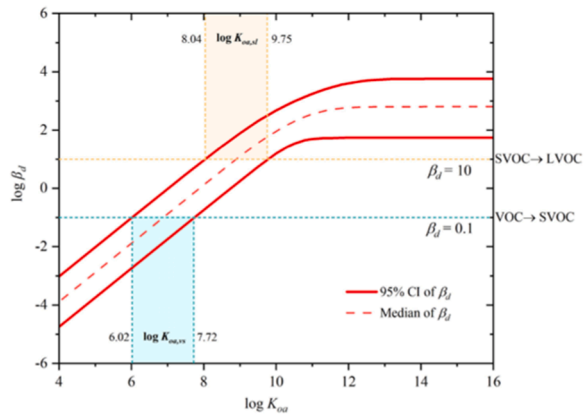

Fig. 2. Variation range of β_d as a function of log K_{oa} obtained by Monte Carlo simulation. Cyan-horizonal line: $\beta_d = 0.1$ (boundary between VOCs and SVOCs); Yellow-horizonal line: $\beta_d = 10$ (boundary between SVOCs and LVOCs).

represent the 2.5th and 97.5th quantiles (i.e., 95 % CI) of the simulated log β_d. According to the points of intersection between the 95 % CI curves and the cyan-horizonal line ($\beta_d = 0.1$), the threshold of log K_{oa} dividing VOCs and SVOCs was 6.02 ~ 7.72, which also yielded a criterion for VOCs as log $K_{oa} = 6.02$. Similarly, the threshold of log K_{oa} dividing SVOCs and LVOCs was determined to be 8.04 ~ 9.75 based on the yellow-horizonal line ($\beta_d = 10$), yielding a criterion for LVOCs as log $K_{oa} = 9.75$. Thus, consistent classification criterion was obtained by Monte Carlo simulations of Eq. (10) and those of the boundary equations of VOCs, SVOCs, and LVOCs (log $K_{oa,vs}$ and log $K_{oa,sl}$).

It is noteworthy that the above criterion agreed well with the results of Fahy et al. [34] though their focus was to assess the importance of multiphase chemistry relative to dust cleaning and ventilation in removing indoor chemicals. They found that (1) ventilation contributed > 90 % loss for compounds with log $K_{oa} < 6$ that mainly existed in the air, which was in high consistence with our criterion for VOCs (log $K_{oa} <$ 6); (2) dust cleaning was most efficient for compounds with log $K_{oa} > 10$ (cleaning contributed > 50 % loss and multiphase chemistry contributed the remaining loss), which was also in good agreement with our criterion for LVOCs that mainly existed in house dust (log $K_{oa} > 9.8$). Furthermore, Fig. 1 implied that K_d data was absent for compounds with log $K_{oa} < 6$ in existing studies, which might be attributed to their low concentrations in dust (i.e., their amount in dust was negligible) and thus was also considered as a positive evidence supporting the criterion for VOCs (log $K_{oa} < 6$). Moreover, as mentioned in "Introduction" section, some compounds like furaneol and hexanoic acid were classified as VOCs by existing criteria despite behaving like SVOCs indoors. This problem was found to disappear by using our criterion (SVOCs: $6 \leq$ log $K_{oa} \leq 9.8$): furaneol (log $K_{oa} = 8.0$) and hexanoic acid (log $K_{oa} = 6.43$) were classified as SVOCs instead of VOCs (log K_{oa} values were obtained from CompTox Chemicals Dashboard v2.4.1). Overall, the above discussions supported to some extent that our criterion could be helpful for the consistent and precise classifications of indoor organic compounds.

3.3. Implications, limitations, and further studies

Except for the classifications, the novel criterion can also guide the selections of most suitable methods for the chemical analysis, exposure assessment, and effective controls of indoor organic pollutants. For compounds with log $K_{oa} < 6$ (VOCs), indoor air is the only medium that matters. Thus, their analysis, exposure, and controls depend only on the measurements of C_a, the pathway via inhalation of air, and the ventilation and air purifiers, respectively. On the contrary, indoor air becomes an irrelevant medium for compounds with log $K_{oa} > 9.8$ (LVOCs), we need to focus on the measurements of C_d, the pathways related to reservoirs (ingestion of dust, inhalation of airborne particles, dermal sorption from surfaces), and the removal via dust/surface cleaning. Whereas for compounds with $6 \leq$ log $K_{oa} \leq 9.8$ (SVOCs), their analysis, exposure, and controls require to consider diverse media including both the air and house dust (as well as other reservoirs), which are rather complicated but are necessary for comprehensiveness.

Additionally, some assumptions were made in this study. First, dust compositions may vary among buildings with different indoor conditions (e.g., building locations, living habits, and housing ages). The effects of dust compositions on dust-air partitioning were not considered in the novel K_d equation. Many studies have investigated the correlations between indoor conditions and C_d via questionnaires coupled with statistical analysis or machine learning models [35]. Nevertheless, to the best knowledge of the authors, no equation explicitly describing these correlations is available now. How to incorporate the effects of dust compositions into the K_d equation warrants further studies. Second, the ratio of room volume (V_a) to the horizonal surface area (A_d, i.e., area of dust-deposited surfaces) was approximated as the room height (H) in Eqs. (1), (10)-(12), i.e., assuming that A_d equaled the floor area (A_f). However, A_d may be greater than A_f in some rooms such as classrooms and offices. Although the analysis in Section S2 indicate that the assumption of $A_d = A_f$ has insignificant effects on the two thresholds of log K_{oa} when A_d varies in the range of A_f/1.5 to 1.5A_f, further evaluations are still expected in the future with more comprehensive analysis and measurements. Third, when determining the two log K_{oa} thresholds, the critical β_d values were set to be 0.1 and 10 for the VOC-SVOC and SVOC-LVOC boundaries, respectively. The reason is that the distinction between VOCs and SVOCs may be unachievable if β_d is set to be less than 0.1 (similarly for SVOCs and LVOCs if β_d is greater than 10) because the measuring errors of gas- and dust-phase concentrations are often in the order of 10 % [20,30,31]. However, the reasonability of the selection of the two critical β_d values still requires further investigation and evaluation.

Furthermore, the K_{oa}-based criterion was derived based only on the dust-air relative abundance (β_d) of organic compounds. Other than house dust, airborne particles and indoor surfaces are also important reservoirs of compounds [1]. As presented in Section S5, airborne particles were found to be an unsuitable reservoir for the derivation of classification criterion since the threshold of log K_{oa} for dividing SVOCs and LVOCs could not be obtained based on the particle-air relative abundance (β_p, the condition of $\beta_p > 10$ cannot be reached in most indoor environments). Furthermore, for indoor surfaces, the derivations of K_{oa}-based criterion based on the surface-air relative abundance (β_s) were found to be unattainable because the equation describing the relationship between surface-air partitioning quotient (K_s), K_{oa}, and indoor parameters was still lacking. The K_s equation is likely to be much more complicated than the K_d equation because the surfaces themselves may be time-varying (due to the formation and growth of organic films on surfaces [36–39]) and the properties of surfaces are quite different from each other (e.g., walls versus carpets). Further studies are warranted to solve the surface-related problems and then quantify the deviations between the criterion based on β_d and those based on β_s. Nevertheless, the use of house dust as the only reservoir is considered to be reasonable because house dust, expect for indoor air, is one of the most frequently-used media in chemical analysis and exposure assessment of indoor organic pollutants (especially SVOCs and LVOCs) [18,20].

Finally, indoor organic compounds are composed of polar and weak/non-polar species. The novel K_d equation developed in this study may be only suitable for weak/non-polar compounds (mainly because the $K_{d,e}$-K_{oa} equation expressed in Eq. (8) assumes that compounds are absorbed in dust's organic matter [19]). Note that all the compounds listed in Table S2 belong to weak/non-polar species, indicating that weak/non-polar compounds are more frequently investigated in indoor sciences currently. For polar species like acids and amines, their dust-air partitioning may be more dependent on their water-air partitioning coefficient (K_{wa}, instead of K_{oa}), dust's water content (instead of organic matter), as well as pH of water content [17]. Thus, the K_{oa}-based

criterion is likely to be unable to precisely classify polar compounds, whose classification criterion (possibly depends on K_{wa}) require further studies (if reliable equation describing the effects of K_{wa}, water content and pH on K_d can be established).

4. Conclusions

A novel equation, which considered the effects of compound property (K_{oa}) and indoor environmental conditions, was developed to estimate the partitioning quotient (K_d) of organic compounds between house dust and indoor air. Estimates of the equation agreed well with measured data retrieved from previous studies. Based on the novel equation and Monte Carlo simulations (to quantify the combined effects of various indoor parameters), a novel criterion for classifying indoor organic compounds was proposed: VOCs (log $K_{oa} < 6$), SVOCs ($6 \leq \log K_{oa} \leq 9.8$), and LVOCs (log $K_{oa} > 9.8$). The first threshold (log $K_{oa} < 6$) corresponds to the definition that VOCs are compounds with negligible amount in house dust in most indoor environments (mainly exist in the air), whereas the last threshold (log $K_{oa} > 9.8$) corresponds to the definition that LVOCs are compounds with negligible amount in the air (mainly exist in house dust). Consistence between classification results and evidences reported in the literature confirmed the reliability of the proposed criterion. Overall, the novel criterion are expected to be helpful for the precise classification of indoor (weak/non-polar) organic compounds, which would further facilitate the chemical analysis, exposure assessment, and effective controls of indoor organic pollutants. Further studies may focus on the classification criterion of polar organic compounds like acids and amines.

CRediT authorship contribution statement

Xingyu Duan: Writing – original draft, Validation, Methodology, Investigation, Formal analysis. **Yujie Zhu:** Writing – review & editing, Methodology, Investigation. **Jianping Cao:** Writing – review & editing, Methodology, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

The supporting material includes empirical equations of reservoir-gas partitioning quotients retrieved from the literature (Section S1), discussions about model assumptions (Section S2), details of indoor environmental parameters (Section S3), equation evaluation (Section S4 and Table S2), and classification criteria related to airborne particles and indoor surfaces (Section S5).

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.buildenv.2024.112497.

Data availability

Data will be made available on request.

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