Impact of temperature on the dust/gas partitioning of semi-volatile organic compounds in indoor environments

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Abstract. Semi-volatile organic compounds (SVOCs) are one of the ubiquitous families of indoor air pollutants. They can be found in the gas phase as well as in the adsorbed/absorbed phases including airborne particles and settled dust. The dust/gas partition coefficient, K_d, is the ratio of the SVOC concentrations in the settled dust and the gas phase at the equilibrium state thus is a key parameter for modeling the indoor transport and partitioning of SVOCs. Studies have shown that the value of K_d depends on the temperature, the organic fraction in dust, the dust size and density, etc. For indoor SVOC modeling in the context of climate change, the temperature effect on K_d should be addressed particularly. In the present study, a linear relationship between Log_{10} K_d and the inverse of temperature was derived for 18 SVOCs including polybrominated diphenyl ethers (PBDEs), polychlorinated biphenyls (PCBs), and polycyclic aromatic hydrocarbons (PAHs). K_d decreases by 91.8 to 99.6% when the temperature rises from 10 to 40 °C. The influence of temperature on K_d and the indoor concentration was estimated for three SVOCs using a validated mechanistic model. The dust phase concentration of the three SVOCs may vary by 1.5 orders of magnitude due to variations in K_d in a temperature range between 10 and 30 °C.

1 Introduction

Semi-volatile organic compounds are chemical indoor air pollutants that can be found in the gas phase, suspended particles, settled dust, and sink surfaces. SVOCs present potential health hazards, such as disrupting the endocrine system, influencing immune and reproductive functions and the development of the brain and nervous system [1]. The concentrations of SVOC in the adsorbed phases can be used to calculate its concentration in the gas phase, assuming that the equilibrium state is reached. The indoor dust/gas partition coefficient K_d is the ratio of the SVOC concentration in indoor settled dust and its respective in the gas phase. In most of the previous studies, K_d was calculated at 25°C. Wei et al. [2] summarized the empirical equations to calculate the particle/gas partition coefficient K_p, and K_d from the literature, then provided a distribution for these two parameters at 25°C. Although the influence of temperature on K_d has not been fully addressed, some studies showed that temperature had a significant influence on the outdoor soil/air partition coefficient (K_{sa}) for SVOCs [3], [4] and that indoor K_d was also temperature-dependent [5]. Pei et al. [6] derived the temperature dependence of K_d for three phthalates, i.e., DiBP, DnBP, and DEHP, by measuring their concentrations in dust and estimating their concentrations in the gas phase. Log_{10} K_d was linearly related to the inverse of temperature for the three phthalates. No study was found for other SVOCs, such as polybrominated diphenyl ethers (PBDEs), polychlorinated biphenyls (PCBs), and polycyclic aromatic hydrocarbons (PAHs). In the context of climate change, heat waves may lead to high indoor temperatures with increasing frequency and long duration. This may increase indoor SVOC concentrations, particularly for vulnerable dwellings that do not have cooling systems. To anticipate the climate change effect the present work was an impact analysis aiming to determine the temperature dependence of K_d for indoor SVOCs commonly detected in French dwellings.

2 Method

The indoor dust/gas partition coefficient is expressed by the following equation, assuming that an equilibrium partitioning is reached [5]:

$$K_d = \frac{f_{om\_d}}{\rho_d} \times K_{oa} \quad (1)$$

Where K_{oa} is the octanol-air partition coefficient; f_{om_d} is the fraction of organic matter in indoor settled dust; ρ_d is the density of indoor settled dust.

Some values of ρ_d and f_{om_d} from the literature are summarized in Tables 1 and 2. In this study, the dust density was assumed as 1.5 g.cm^{-3}, and the volume fraction of organic matter in dust was assumed as 0.2, which were approximately the medians of the values obtained from the literature.

Table 1. Values of indoor dust density from the literature

Dust density (g.cm^{-3})	Reference
2.5	Tian et al. [7]
1	Arfaeinia et al. [8]
2	Weschler and Nazaroff [5]
1.5	Shi and Zhao [9]
2	Hunt et al. [10]
2	Little et al. [11]
1	Weschler et al. [12]
0.938 (House Dust #2)	Liu and Folk [13]
0.661 (House Dust #6)	Liu and Folk [13]
1 (based on values from literature)	Salthammer and Schripp [14]

Table 2. Values of fraction of organic matter in indoor dust from the literature

Volume fraction of organic matter in indoor dust	reference

0.3	Shi and Zhao [9]
0.2	Weschler and Nazaroff [5]
0.2	Hunt et al. [10]
0.2	Little et al. [11]
0.2 (House Dust #2)	Liu and Folk [13]
0.12 (House Dust #6)	Liu and Folk [13]
0.35 (based on values from literature)	Salthammer and Schripp [14]

The study focused on PBDEs, PCBs, and PAHs prioritized in the First French Nationwide Campaign (CNL) for indoor air quality in dwellings [15]. The study of Li et al. [16] provided experimental values of K_{oa} at different temperatures for 7 PBDEs, 8 PCBs, and 3 PAHs, which were employed in the calculation of K_d using equation (1). Figure 1 presents the dependence of K_{oa} on temperature for one SVOC from each family: PCB118, phenanthrene, and PBDE99.

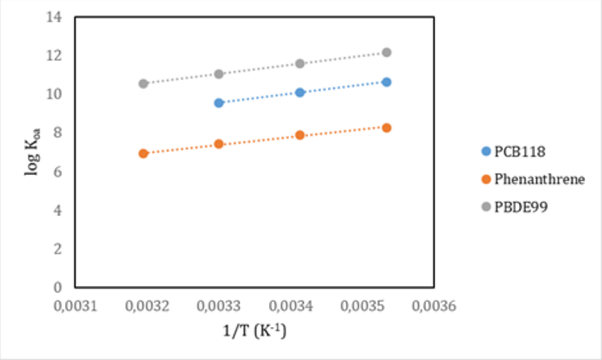


Figure 1. Effect of temperature on octanol/air partition coefficient for PCB118, phenanthrene, and PBDE99.

Temperature was found to have an exponential impact on the particle/gas partition and soil/air partition, as indicated in the study of Wei et al. [17] for indoor airborne particles (equation (2)) and in the study of Hippelein and McLachlan [4] for outdoor soil (equation (3)).

$$log_{10} K_p = \frac{A}{T} + B \quad (2)$$

$$ln\, K_{sa} = \frac{C}{T} + D \quad (3)$$

Where A, B, C, and D are constants specific to the concerned SVOC.

By analogy to particle/gas partition and soil/air partition, the indoor dust/gas partition coefficient, K_d, can be expressed by:

$$log_{10} K_{d,T} = \frac{A^*}{T} + B^* \quad (4)$$

To calculate the two constants A^* and B^*, the different values of K_d at different temperatures calculated from K_{oa} using equation (1) were used.

To evaluate the impact of temperature on indoor SVOC concentrations, a case study was conducted. The case study considered a daycare center of 199.3 m^3. An SVOC model [18] was applied to three SVOCs: PBDE99, phenanthrene, and PCB118. Two K_d values at 10 and 30°C were considered as they were representative of a common indoor temperature range, while all the other parameters are fixed at constant values for simulations of different temperature scenarios. The average air change rate in the daycare center in operation was 0.71 h^{-1}, and the total suspended particles was 625 $\mu g.m^{-3}$. The other input parameters to characterize mass transfer are presented in Table 3.

Table 3. Input parameters for SVOC simulations

SVOC	Surface/gas partition coefficient, K_s (m)	Emission parameter	Particle/gas partition coefficient, $Log_{10} K_p$ ($m^3.\mu g^{-1}$) [2]
PBDE99	3294 (for cotton) [19]	$y_0 = 10^{-3}$ $\mu g.m^{-3}$ [20]	-1.29
Phenanthrene	28 (for carpet) [21]	Specific emission rate in gas phase = 31.3 $\mu g.h^{-1}$ In particle phase= 4.66 $\mu g.h^{-1}$ [20]	-3.96
PCB118	10 (assumed $=K_{oa}$) [5]	0.1 $\mu g.h^{-1}$ [22]	-2.62

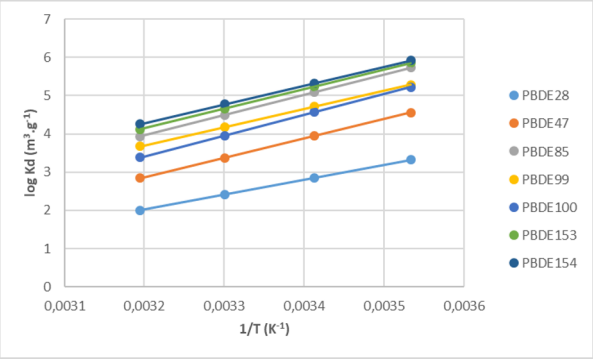
3 Results and discussion

The equations relating K_d to temperature are obtained by linear regression. Figure 2 illustrates the case of PBDEs, PCBs, and PAHs. The equations and the coefficients of determination R^2 are presented in Table 4. K_d was calculated at three temperatures (10, 20, and 30°C) for PCBs, and at four temperatures for PBDEs and PAHs (10, 20, 30, and 40°C).

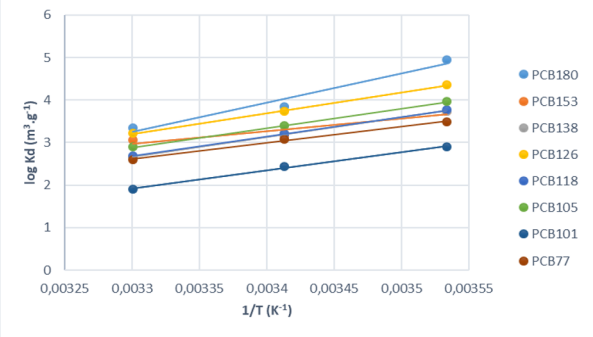
Table 4. Empirical equations of K_d ($m^3.g^{-1}$) ($x = \frac{1}{T}$, $y = \log_{10} K_d$)

	COSV	Equation	R^2
PBDEs	PBDE28	y = 3885,1x - 10,408	1
	PBDE47	y = 5063,4x - 13,338	1
	PBDE85	y = 5323,9x - 13,081	1
	PBDE99	y = 4750,7x - 11,502	1
	PBDE100	y = 5453,3x - 14,045	1
	PBDE153	y = 5125,4x - 12,255	1
	PBDE154	y = 4927,8x - 11,493	1
PCBs	PCB180	y = 6887,5x - 19,473	0,9604

	PCB153	y = 2980,1x - 6,8573	0,8792
	PCB138	y = 4626,7x - 12,601	0,9983
	PCB126	y = 4891,6x - 12,933	0,9983
	PCB118	y = 4588,2x - 12,45	0,9999
	PCB105	y = 4589,2x - 12,257	0,9997
	PCB101	y = 4282,9x - 12,214	0,9971
	PCB77	y = 3810x - 9,9585	0,9939
PAHs	Fluorene	y = 4279,2x - 14,445	0,989
	Phenanthrene	y = 3977,8x - 12,615	0,9913
	Pyrene	y = 4271,2x - 12,39	0,9895



(a)



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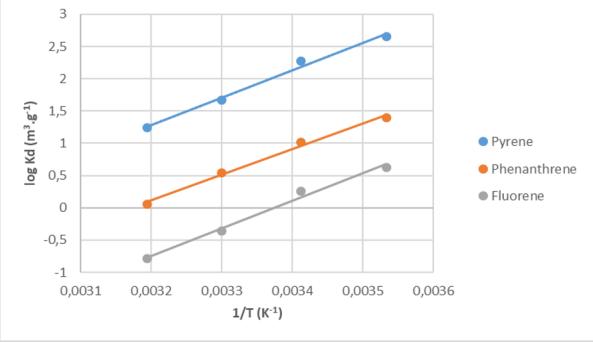
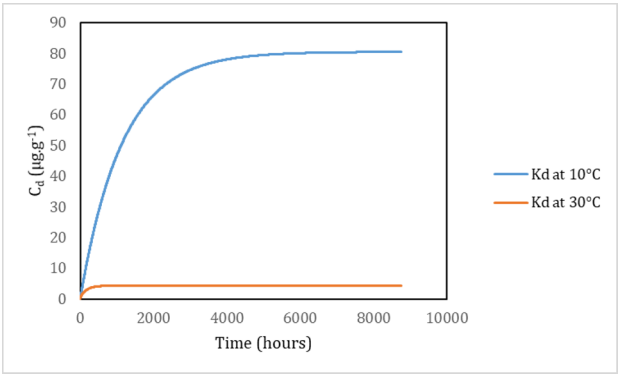


(c)

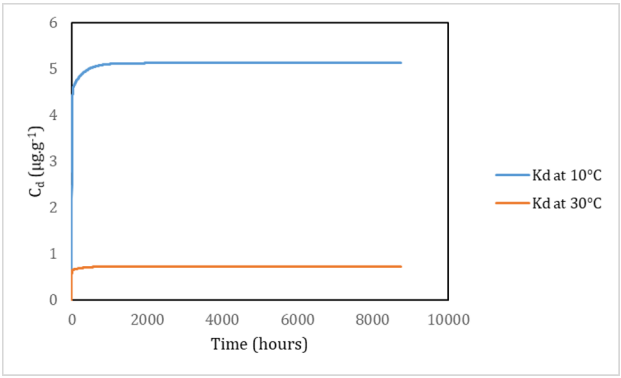
Figure 2. Effect of temperature on dust/gas partition coefficient K_d ($m^3.g^{-1}$) for (a) PBDEs, (b) PCBs, and (c) PAHs.

Temperature was found to have a significant influence on the dust/gas partition coefficient. K_d dropped by one to two orders of magnitude for PAHs, PBDEs, and PCBs when the temperature rises from 10 to 40°C.

Figure 3 shows the PBDE99, phenanthrene, and PCB118 concentrations in the dust phase, calculated based on two values of K_d at 10 and 30°C. The simulations indicate that when the K_d value at 10°C was used, the concentration of PBDE99 in dust, C_d, reached 80.5 $\mu g.g^{-1}$ at the steady state, while the steady-state concentration was 4.3 $\mu g.g^{-1}$ when the K_d value at 30°C was considered (Figure 3(a)). For phenanthrene, C_d drops from 5.12 to 0.73 $\mu g.g^{-1}$ when K_d decreases from 24.6 to 3.49 $m^3.g^{-1}$ at 10 and 30°C, respectively (Figure 3(b)). Figure 3(c) shows that C_d reaches 0.87 $\mu g.g^{-1}$ for K_d at 10°C, while it does not exceed 0.073 $\mu g.g^{-1}$ for K_d at 30°C. Therefore, a huge difference in SVOC dust phase concentration may result from the variation in indoor temperature.



(a)



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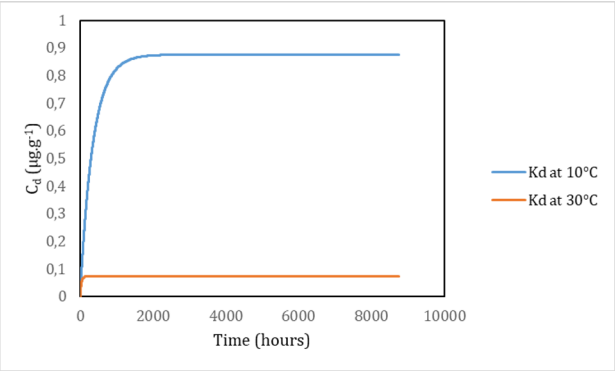
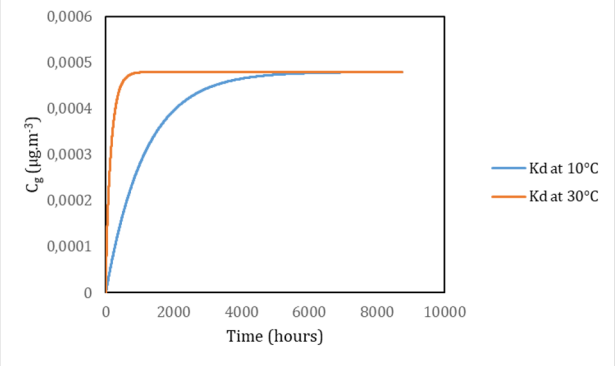


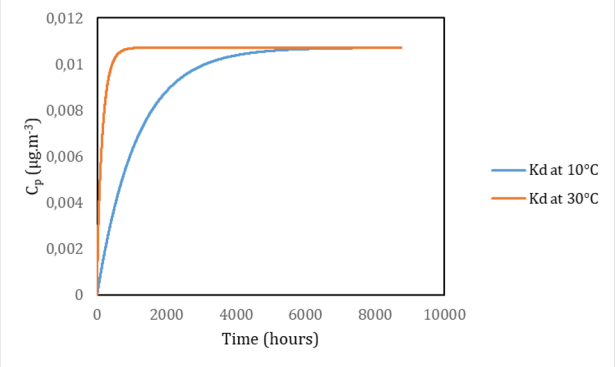
(c)

Figure 3. The dust phase concentration of (a) PBDE99, (b) phenanthrene, and (c) PCB118 considering two values of K_d at 10 and 30°C.

The variation of K_d does not present an influence on the steady-state SVOC concentration in the gas phase C_g and on suspended particle C_p. However, when K_d at a higher temperature was used, the transient time to reach the equilibrium state was shorter. Figure 4 shows the example of PBDE99.



(a)



(b)

Figure 4. PBDE99 concentrations considering K_d at 10°C and 30°C in (a) the gas phase and (b) the particulate phase.

4 Conclusion

In this study, the temperature dependence of the dust/gas partition coefficient K_d was developed. A linear relationship was proved between Log_{10} K_d and the inverse of temperature. The empirical equations were calculated for 18 SVOCs from three different families. K_d can drop by up to two orders of magnitude when the temperature rises from 10 to 40°C. The variation of K_d with temperature induces a significant decrease in the SVOC dust phase concentration, going up to more than 15 times considering a K_d variation from 10 to 30°C. Thus, under climate change conditions, SVOC indoor partitioning between the air and the settled dust may significantly change during the heat wave and cold wave periods, and induce huge changes in the SVOC concentrations in the settled dust. The SVOC concentrations in the gas and particle phase are not impacted by using the K_d value at high temperatures, but the equilibrium state is reached more quickly. Considering how temperature impacts other SVOC-related factors such as emission parameters and partition coefficients is important. Such considerations can lead to greater disparities in SVOC concentrations across all phases.

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