



## Review

## SVOC partitioning between the gas phase and settled dust indoors

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## ABSTRACT

Semivolatile organic compounds (SVOCs) are a major class of indoor pollutants. Understanding SVOC partitioning between the gas phase and settled dust is important for characterizing the fate of these species indoors and the pathways by which humans are exposed to them. Such knowledge also helps in crafting measurement programs for epidemiological studies designed to probe potential associations between exposure to these compounds and adverse health effects. In this paper, we analyze published data from nineteen studies that cumulatively report measurements of dustborne and airborne SVOCs in more than a thousand buildings, mostly residences, in seven countries. In aggregate, measured median data are reported in these studies for 66 different SVOCs whose octanol-air partition coefficients ( $K_{oa}$ ) span more than five orders of magnitude. We use these data to test a simple equilibrium model for estimating the partitioning of an SVOC between the gas phase and settled dust indoors. The results demonstrate, in central tendency, that a compound's octanol-air partition coefficient is a strong predictor of its abundance in settled dust relative to its gas phase concentration. Using median measured results for each SVOC in each study, dustborne mass fractions predicted using  $K_{oa}$  and gas-phase concentrations correlate reasonably well with measured dustborne mass fractions ( $R^2 = 0.76$ ). Combined with theoretical understanding of SVOC partitioning kinetics, the empirical evidence also suggests that for SVOCs with high  $K_{oa}$  values, the mass fraction in settled dust may not have sufficient time to equilibrate with the gas phase concentration.

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## 1. Introduction

Semivolatile organic compounds (SVOCs) found indoors include flame retardants, such as the polybrominated diphenyl ethers (PBDEs); pesticides, such as chlordane, chlorpyrifos, and diazinon; plasticizers, such as di(n-butyl) phthalate (DnBP), butylbenzyl phthalate (BBzP) and di(2-ethylhexyl) phthalate (DEHP); heat transfer fluids, such as the polychlorinated biphenyls (PCBs), which were also widely used as plasticizers; and combustion byproducts, such as benzo(a)pyrene (BaP), dioxins, and furans. Indoors, SVOCs can partition among several compartments, including the gas phase, airborne particles, settled dust, exposed inanimate surfaces, and even to the surfaces of the occupants themselves. Such partitioning affects the fate of indoor SVOCs and influences the pathways by which humans are exposed (Lioy, 2006; Xu et al., 2010). Recently, we summarized how a compound's octanol-air partition

coefficient,  $K_{oa}$ , might be used to estimate equilibrium partitioning indoors (Weschler and Nazaroff, 2008). The aim of the present study is to employ empirical data to critically evaluate the predictive potential of  $K_{oa}$  for quantifying SVOC partitioning between the gas phase and settled dust in indoor environments.

## 2. Methods

## 2.1. Estimating SVOC mass fractions in settled dust

We analyzed data from studies that reported simultaneously measured SVOC mass fractions in dust ( $X_{dust}$ , typically in units of  $\mu\text{g}$  of dust-associated SVOC per g of dust) and mass concentrations of airborne SVOCs. The latter included measurements of gas-phase concentrations, concentrations associated with airborne particles, or concentrations of gaseous and particulate airborne SVOCs combined. Overall, measured dust-air pairs were cumulatively available for 66 separate SVOCs, one or more of which were measured in more than a thousand distinct buildings, as collectively reported in nineteen studies. For each SVOC in each study, we used the measured median airborne concentration to compute a predicted equilibrium mass

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Nomenclature			
$C_g$	SVOC gas-phase concentration ( $\mu\text{g m}^{-3}$ )	$K_{oa}$	octanol-air partition coefficient, corresponding to mass of SVOC dissolved in octanol per volume of octanol normalized by the mass concentration of gaseous SVOC (—)
$C_p$	mass of SVOC sorbed to particles per unit volume of air ( $\mu\text{g m}^{-3}$ )	$K_p$	particle-air partition coefficient for SVOC, corresponding to mass of particle-sorbed SVOC per mass of particle normalized by the mass concentration of gaseous SVOC ( $\text{m}^3 \mu\text{g}^{-1}$ )
$(C_g + C_p)$	total SVOC airborne concentration ( $\mu\text{g m}^{-3}$ )	TSP	mass concentration of airborne particles ( $\mu\text{g m}^{-3}$ )
$f_{om\_dust}$	volume fraction of organic matter associated with settled dust (—)	$X_{dust}$	mass-fraction of SVOC in dust ( $\mu\text{g}$ of dust-associated SVOC per $\text{g}$ of dust)
$f_{om\_part}$	volume fraction of organic matter associated with airborne particles (—)	$X_{dust,meas}$	measured mass-fraction of SVOC in dust
$K_{dg}$	dust-air partition coefficient for SVOC ( $\text{m}^3 \text{mg}^{-1}$ ); $K_{dg} = K_{dust} / \rho_{dust}$	$X_{dust,pred}$	predicted mass-fraction of SVOC in dust
$K_{dust}$	dust-air partition coefficient for SVOC, corresponding to mass of dust-sorbed SVOC per volume of dust normalized by the mass concentration of gaseous SVOC (—)	$\rho_{dust}$	density of settled dust ( $\text{mg m}^{-3}$ )
		$\rho_{part}$	density of airborne particles ( $\text{mg m}^{-3}$ )

fraction in dust, which was then compared with the median measured mass fraction in dust. (In a few cases, as detailed in the footnotes to Tables 1a–c, we used proxies because the medians of measured values were not reported.)

We define  $K_{dg}$  as the equilibrium coefficient that describes an SVOC's partitioning between settled dust and the gas phase. More specifically, it is the ratio of the mass fraction in dust ( $\mu\text{g}$  of dust-borne SVOC per  $\text{g}$  of dust) to the gaseous SVOC concentration ( $\text{ng}$  of gas-phase SVOC per  $\text{m}^3$  of air) and so has dimensions of volume/mass ( $\mu\text{g}/\text{g} \div \text{ng}/\text{m}^3 = \text{m}^3 \text{mg}^{-1}$ ). As defined here, it is analogous to but not identical to  $K_{dust}$ , a parameter described in our recent review (Weschler and Nazaroff, 2008, Eq. 3.11). The parameter  $K_{dust}$  is dimensionless, being defined as the ratio of the SVOC concentration in dust (e.g.,  $\text{ng SVOC}/\text{m}^3$  dust) to the gas-phase SVOC concentration. These two partitioning coefficients are related through the expression  $K_{dust} = K_{dg} \times \rho_{dust}$ , where  $\rho_{dust}$  is the density of dust. We use the parameter  $K_{dg}$  in this paper to conform to the units in which SVOC abundances in dust and air are commonly reported.

With one exception, the  $K_{oa}$  values used in this work were determined using the SPARC online calculator, September 2009 release w4.5 (Hilal et al., 2004; <http://ibmcl2.chem.uga.edu/sparc/>). There were difficulties calculating  $K_{oa}$  for pentachlorophenol using release w4.5; for this compound only, we used the value we had previously calculated with release w4.0. (See Table 3 of Weschler and Nazaroff, 2008.)

For equilibrium conditions, the ratio,  $K_{dg}$ , of an SVOC's mass fraction in dust,  $X_{dust}$ , to its gaseous concentration,  $C_g$ , is expected to be directly proportional to the octanol-air partition coefficient,  $K_{oa}$ , and to the fraction of the dust that is organic matter,  $f_{om\_dust}$ ; it is inversely proportional to the dust density (Pankow, 1994, 1998; Finizio et al., 1997; Cousins and Mackay, 2001; Xiao and Wania, 2003; Weschler and Nazaroff, 2008):

$$K_{dg} = \frac{X_{dust}}{C_g} = \frac{f_{om\_dust} \times K_{oa}}{\rho_{dust}} \quad (1)$$

Equation (1) is a theoretical relationship. In addition to assuming that equilibrium conditions prevail, it assumes that the equilibrium presence of an SVOC in dust is dominated by its absorption in dust's organic matter and that—for the purpose of describing the extent of sorption—octanol is a good chemical model for dustborne organic matter.

The present work explores how well equation (1) predicts actual, empirically determined partitioning of SVOCs between the

gas phase and settled dust indoors. Equation (1) can be rearranged to calculate a predicted mass fraction of a given SVOC in dust:

$$X_{dust,pred} = \frac{f_{om\_dust} \times K_{oa} \times C_g}{\rho_{dust}} \quad (2)$$

In the present work, for each SVOC in each study, we computed an  $X_{dust,pred}$  value, using the SVOC's  $K_{oa}$  at 298 K and its measured or inferred median gas-phase concentration,  $C_g$ . In doing so, we assumed that  $f_{om\_dust}$  was 0.2 and that  $\rho_{dust}$  was  $2.0 \times 10^6 \text{ g m}^{-3}$  based on the measurements reported in Hunt et al. (1992). In some cases, it was necessary to determine gas-phase concentrations from measured particle-phase ( $C_p$ ) or total airborne ( $C_g + C_p$ ) concentrations. To do this, we estimated the equilibrium constant that describes partitioning of an SVOC between airborne particles and the gas phase,  $K_p$ , as follows (Weschler and Nazaroff, 2008):

$$K_p = \frac{f_{om\_part} \times K_{oa}}{\rho_{part}} \quad (3)$$

Here,  $K_p$  represents the sorbed mass of SVOC on airborne particles per particle mass normalized by the gaseous mass concentration of the SVOC. In evaluating  $K_p$ , we assumed that the volume fraction of organic matter associated with airborne particles ( $f_{om\_part}$ ) was 0.4 (Fromme et al., 2005) and that the density of airborne particles was  $1 \times 10^6 \text{ g m}^{-3}$  (Turpin and Lim, 2001). In the one case where the particle phase SVOC,  $C_p$ , was measured, the gas phase concentration was estimated using this relationship:

$$C_g = \frac{C_p}{TSP \times K_p} \quad (4)$$

where TSP is the average indoor mass concentration of airborne particles, assumed to be  $20 \mu\text{g}/\text{m}^3$ . In cases in which the total airborne SVOC concentration,  $C_g + C_p$ , had been measured, the gas-phase concentration was estimated using this relationship:

$$C_g = \frac{C_p + C_g}{1 + (TSP \times K_p)} \quad (5)$$

where again, for evaluation, we assumed  $TSP = 20 \mu\text{g}/\text{m}^3$ .

We used data from all published studies we found in which simultaneous SVOC mass fractions in dust and airborne SVOC concentrations were measured contemporaneously in multiple indoor environments; the study sites happened to be mainly residences.

**Table 1a**

Measured median gaseous ( $C_g$ ) and median settled dust concentrations ( $X_{\text{dust,meas}}$ ) of SVOCs along with predicted settled dust concentrations ( $X_{\text{dust,pred}}$ ) based on equilibrium partitioning.<sup>a</sup>

Site	SVOC	$\log(K_{\text{oa}})$	$C_g$ measured ( $\text{ng m}^{-3}$ ) <sup>b</sup>	$X_{\text{dust,meas}}$ ( $\mu\text{g g}^{-1}$ )	$X_{\text{dust,pred}}$ ( $\mu\text{g g}^{-1}$ )	Reference
25 residences, West Midlands, UK	$\alpha$ -HBCD	12.4	0.032	0.32	8.0	Abdallah et al., 2008 <sup>c</sup>
	$\beta$ -HBCD	12.4	0.016	0.094	4.0	
	$\gamma$ -HBCD	12.4	0.105	0.69	26	
24 residences, Kuwait	phenanthrene	7.51	2.8	0.021	0.0091	Gevao et al., 2007 <sup>d</sup>
	pyrene	8.06	0.35	0.019	0.0040	
	fluoranthene	8.42	0.41	0.011	0.011	
	chrysene	9.93	0.06	0.0077	0.051	
	benzo(a)anthracene	9.98	0.02	0.0065	0.019	
	benzo(a)pyrene	10.5	0.06	0.073	0.18	
	benzo(b)fluoranthene	10.8	0.14	0.057	0.95	
benzo(k)fluoranthene	10.9	0.09	0.064	0.77		
10 residences, Toronto, CAN	PCB 28 and 31	8.09	0.58	0.0073	0.0071	Harrad et al., 2009 <sup>e</sup>
	PCB 52	8.62	0.61	0.0072	0.025	
	PCB 101	9.51	0.11	0.0088	0.036	
	PCB 118	10.0	0.035	0.0087	0.038	
	PCB 138	10.5	0.017	0.0095	0.055	
	PCB 153	10.4	0.021	0.0099	0.054	
	PCB 180	11.3	0.0038	0.0068	0.068	
38 residences, Wisconsin, USA	BDE-47	10.5	0.20	0.52	0.58	Imm et al., 2009 <sup>f</sup>
	BDE-99	11.8	0.037	0.61	2.14	
	BDE-100	11.8	0.016	0.12	0.91	
59 residences, Ottawa, CAN	MeFOSE	7.5	1.49	0.113	0.0045	Shoeb et al., 2005 <sup>g</sup>
	EtFOSE	7.8	0.74	0.138	0.0047	
10 residences, Brisbane, AU	BDE-47	10.5	0.025	0.056	0.072	Toms et al., 2009 <sup>h</sup>
	BDE-99	11.8	0.032	0.087	1.84	
62 residences, Ottawa, CAN	BDE-17	9.39	0.0061	0.001	0.0015	Wilford et al., 2004; Wilford et al., 2005 <sup>i</sup>
	BDE-28	9.39	0.011	0.003	0.0027	
	BDE-47	10.5	0.066	0.30	0.19	
	BDE-99	11.8	0.015	0.43	0.86	
	BDE-100	11.8	0.0042	0.073	0.24	

<sup>a</sup> Parameter definitions:  $K_{\text{oa}}$ —octanol-air partition coefficient, determined using SPARC online calculator release w4.5 (September 2009);  $C_g$  measured—measured median gaseous SVOC concentration;  $X_{\text{dust,meas}}$ —measured median mass fraction of the SVOC in settled dust;  $X_{\text{dust,pred}}$ —mass fraction in settled dust predicted from measured  $C_g$  using equation (2).

<sup>b</sup> In each of these studies, airborne concentrations were measured using a passive sampling technique that is more responsive to gas-phase species than to particle-bound species. The measurement results are interpreted here as direct measurements of gas-phase concentrations,  $C_g$ .

<sup>c</sup> Medians used in the present paper were extracted from Table SI-5 of the reference.

<sup>d</sup> Medians used in the present paper were extracted from Tables 2 and 3 of the reference.

<sup>e</sup> Medians used in the present paper were extracted from Tables 2 and 3 of the reference.

<sup>f</sup> Geometric means; values for  $X_{\text{dust,meas}}$  were extracted from Table 1; values for  $C_g$  were calculated from the "PUF" values in Table 1 assuming a uniform sampling rate of 2.5 m<sup>3</sup>/day and a sampling period of 30 days for a total sampled volume of 75 m<sup>3</sup>.

<sup>g</sup> Shoeb et al. (2005) did not report median values from their study; geometric means, as reported in Table 4 of the reference, are used here as proxies.

<sup>h</sup> Medians used in the present paper were extracted from Table 1 of the reference.

<sup>i</sup> Medians used in the present paper were extracted from Table 1 of Wilford et al. (2004) for  $C_g$  and Table 1 of Wilford et al. (2005) for  $X_{\text{dust,meas}}$ .

**Table 1b**

Measured median airborne particle ( $C_p$ ) and settled dust concentrations of SVOCs along with predicted settled dust concentrations based on equilibrium partitioning.<sup>a</sup>

Site	SVOC	$\log(K_{\text{oa}})$	$C_p$ measured ( $\text{ng m}^{-3}$ )	$C_g$ inferred ( $\text{ng m}^{-3}$ )	$X_{\text{dust,meas}}$ ( $\mu\text{g g}^{-1}$ )	$X_{\text{dust,pred}}$ ( $\mu\text{g g}^{-1}$ )	Reference
61 apartments, Berlin, DE	pyrene	8.06	0.26	280	0.67	3.2	Fromme et al., 2004a <sup>b</sup>
	fluoranthene	8.42	0.34	160	0.96	4.3	
	chrysene	9.93	0.24	3.5	0.55	2.9	
	benzo(a)anthracene	9.98	0.04	0.52	0.29	0.50	
	benzo(e)pyrene	10.4	0.51	2.4	0.40	6.3	
	benzo(a)pyrene	10.5	0.18	0.76	0.27	2.3	
	benzo(b)fluoranthene	10.8	0.25	0.45	0.54	3.1	
	benzo(k)fluoranthene	10.9	0.085	0.12	0.37	1.1	
	benzo(g,h,i)perylene	11.0	0.26	0.30	0.35	3.2	
	indeno(1,2,3-cd)pyrene	11.4	0.24	0.12	0.33	3.0	
	coronene	11.7	0.14	0.039	0.16	1.8	
	dibenzo(a,h)anthracene	11.9	0.07	0.011	0.05	0.88	

<sup>a</sup> Parameter definitions:  $K_{\text{oa}}$ —octanol-air partition coefficients, determined using SPARC online calculator release w4.5 (September 2009);  $C_p$  measured—measured median SVOC concentration in airborne particles;  $C_g$  inferred—inferred median gas-phase concentration based on  $C_p$  measured and equilibrium partitioning theory;  $X_{\text{dust,meas}}$ —measured median mass fraction of the SVOC in settled dust;  $X_{\text{dust,pred}}$ —mass fraction in settled dust predicted from  $C_g$  inferred using equation (2).

<sup>b</sup> The sampling technique measured only the mass concentration of SVOC associated with airborne particles,  $C_p$ . For airborne concentrations, the medians reported here represent the arithmetic averages of the medians reported in Table 1 of Fromme et al. (2004a) for two subsamples of nonsmoking versus smoking households sampled in 2000 ( $n = 58$ ). The respective number of smoking and nonsmoking households was not reported. The dust samples are from households sampled in 2000 ( $n = 61$ ), with medians as reported in Table 2 of Fromme et al. (2004a).

**Table 1c**Measured median airborne ( $C_g + C_p$ ) and settled dust concentrations of SVOCs along with predicted settled dust concentrations based on equilibrium partitioning.<sup>a</sup>

Site	SVOC	log ( $K_{oa}$ )	$C_g + C_p$ meas (ng m <sup>-3</sup> )	$C_g$ inferred (ng m <sup>-3</sup> )	$X_{dust, meas}$ ( $\mu\text{g g}^{-1}$ )	$X_{dust, pred}$ ( $\mu\text{g g}^{-1}$ )	Reference
4 residences, W. Midlands, UK	TBBP-A	12.7	0.016	0.00043	0.031	0.19	Abdallah et al., 2008 <sup>c</sup>
12 houses, Michigan, USA	BDE-17	9.39	0.16	0.16	0.020	0.039	Batterman et al., 2009 <sup>d</sup>
	BDE-28	9.39	0.15	0.14	0.034	0.035	
	BDE-47	10.5	1.5	1.2	2.6	3.6	
	BDE-71	10.5	0.12	0.10	0.16	0.28	
	BDE-99	11.8	0.78	0.14	5.1	8.0	
	BDE-100	11.8	0.17	0.031	1.5	1.8	
	BDE-153	13.1	0.029	0.0003	0.16	0.36	
	BDE-154	13.1	0.024	0.0002	0.28	0.30	
20 houses, Salinas, CA, USA	chlorpyrifos	9.43	1.9	1.9	0.049	0.50	Bradman et al., 2007; Bradman, 2009 <sup>e</sup>
	diazinon	9.64	1.8	1.7	0.021	0.76	
	chlorthal-dimethyl	9.71	1.8	1.7	0.031	0.89	
30 apartments, Berlin, DE	DMP	7.52	406	406	1.5	1.3	Fromme et al., 2004b; Weschler et al., 2008 <sup>f</sup>
	DEP	8.21	670	669	6.1	10.9	
	DiBP	9.62	574	555	38	232	
	DnBP	9.83	1076	1021	47	690	
	BBzP	11.6	19	4.6	29	180	
	DEHP	12.9	128	2.0	703	1575	
34 residences, S. Bavaria, DE	BDE-28	9.39	0.00421	0.0041	0.00025	0.0010	Fromme et al., 2009 <sup>g</sup>
	BDE-47	10.5	0.00939	0.0076	0.0091	0.022	
	BDE-66	10.5	0.00031	0.00025	0.00019	0.00073	
	BDE-99	11.8	0.00265	0.00047	0.013	0.027	
	BDE-100	11.8	0.00054	0.000096	0.0025	0.0056	
	BDE-153	13.1	0.00027	0.0000027	0.0027	0.0033	
	BDE-154	13.1	0.00020	0.0000020	0.0016	0.0025	
218 residences, Arizona, USA	chlorpyrifos	9.43	8.0	7.8	0.16	2.1	Gordon et al., 1999 <sup>h</sup>
	diazinon	9.64	4.6	4.4	0.13	1.9	
41 houses, Sapporo, JPN	BHT	7.83	550	550	2.4	3.7	Kanazawa et al., 2010 <sup>i</sup>
	DEP	8.21	61	61	0.35	0.98	
	DiBP	9.62	75	73	2.4	30	
	DnBP	9.83	200	190	22	128	
	TBEP	9.31	23	23	164	4.6	
	DEHP	12.9	147	2.3	1200	1808	
129 houses, North Carolina, USA	$\gamma$ -chlordane	8.93	1.5	1.5	0.031	0.13	Morgan et al., 2004 <sup>j</sup>
	$\alpha$ -chlordane	9.09	0.89	0.88	0.022	0.11	
	chlorpyrifos	9.43	6.2	6.1	0.14	1.6	
	pentachlorophenol	9.20 <sup>b</sup>	1.5	1.5	0.060	0.24	
	diazinon	9.64	2.0	2.0	0.018	0.85	
	DnBP	9.83	234	222	5.6	150	
	chrysene	9.93	0.10	0.094	0.17	0.080	
	benzo(a)pyrene	10.5	0.08	0.065	0.18	0.19	
	benzo(b)fluoranthene	10.8	0.13	0.084	0.30	0.57	
	benzo(g,h,i)perylene	11.0	0.13	0.070	0.18	0.75	
	indeno(1,2,3-cd)pyrene	11.4	0.09	0.030	0.16	0.75	
	<i>cis</i> -permethrin	11.9	0.58	0.077	1.0	6.3	
	<i>trans</i> -permethrin	11.9	0.36	0.048	0.63	3.9	
	3,5,6-TCP	8.77	1.94	1.93	0.096	0.11	
	127 houses, Ohio, USA	$\gamma$ -chlordane	8.93	0.36	0.36	0.012	
$\alpha$ -chlordane		9.09	0.26	0.26	0.011	0.032	
chlorpyrifos		9.43	1.7	1.6	0.052	0.44	
pentachlorophenol		9.20 <sup>b</sup>	2.1	2.1	0.060	0.34	
2-isopropyl-6-methyl-4-pyrimidinol		9.64	0.53	0.51	0.014	0.22	
diazinon		9.64	0.97	0.94	0.020	0.41	
DnBP		9.83	249	236	5.2	159	
3,5,6-TCP		8.77	0.63	0.63	0.041	0.037	
13 daycare facilities, North Carolina, USA	heptachlor	8.39	5.4	5.4	0.019	0.13	Morgan et al., 2004 <sup>j</sup>
	$\gamma$ -chlordane	8.93	0.79	0.78	0.067	0.066	
	PCB 52	8.62	0.51	0.50	0.008	0.021	
	$\alpha$ -chlordane	9.09	0.51	0.51	0.043	0.062	
	chlorpyrifos	9.43	3	2.9	0.14	0.79	
	pentachlorophenol	9.20 <sup>b</sup>	1.2	1.2	0.081	0.18	
	PCB 101	9.51	0.08	0.08	0.0043	0.025	
	diazinon	9.64	2.3	2.2	0.065	0.96	
	DnBP	9.83	380	361	14	244	
	chrysene	9.93	0.090	0.084	0.23	0.072	
	benzo(b)fluoranthene	10.8	0.109	0.071	0.50	0.48	
	benzo(g,h,i)perylene	11.0	0.10	0.054	0.28	0.58	
	<i>cis</i> -permethrin	11.9	0.11	0.015	0.81	1.2	
3,5,6-TCP	8.77	0.93	0.93	0.066	0.055		

**Table 1c** (continued)

Site	SVOC	$\log(K_{oa})$	$C_g + C_p$ meas ( $\text{ng m}^{-3}$ )	$C_g$ inferred ( $\text{ng m}^{-3}$ )	$X_{\text{dust, meas}}$ ( $\mu\text{g g}^{-1}$ )	$X_{\text{dust, pred}}$ ( $\mu\text{g g}^{-1}$ )	Reference
16 daycare facilities, Ohio, USA	$\gamma$ -chlordane	8.93	0.26	0.25	0.013	0.022	Morgan et al., 2004 <sup>j</sup>
	PCB 52	8.62	0.49	0.48	0.007	0.020	
	$\alpha$ -chlordane	9.09	0.18	0.18	0.011	0.022	
	chlorypyrifos	9.43	2.1	2.0	0.17	0.54	
	pentachlorophenol	9.20 <sup>b</sup>	1.3	1.3	0.036	0.21	
	PCB 101	9.51	0.10	0.10	0.0061	0.032	
	2-isopropyl-6-methyl-4-pyrimidinol	9.64	0.54	0.52	0.017	0.23	
	PCB 95	9.60	0.10	0.10	0.006	0.039	
	diazinon	9.64	0.96	0.93	0.040	0.41	
	DnBP	9.83	318	302	15	204	
	chrysene	9.93	0.072	0.067	2.4	0.057	
	3,5,6-TCP	8.77	0.71	0.707	0.058	0.042	
	bisphenol-A	13.1	0.92	0.010	0.28	11	
	9 residences, Texas, USA (spring)	propoxur	7.83	27.8	27.8	0.25	
chlorypyrifos		9.43	7.6	7.4	0.30	2.0	
p,p'-DDE		9.63	1.0	0.97	0.10	0.41	
diazinon		9.64	1.4	1.4	0.064	0.59	
p,p'-DDT		10.1	1.8	1.7	0.12	1.9	
cis-permethrin		11.9	0.7	0.09	0.47	7.6	
trans-permethrin		11.9	0.9	0.12	0.82	9.8	
6 residences, Texas, USA (summer)	propoxur	7.83	26.1	26.1	0.74	0.18	
	chlorypyrifos	9.43	23.7	23.2	0.56	6.2	
	p,p'-DDE	9.63	1.0	0.97	0.11	0.41	
	diazinon	9.64	3.5	3.4	0.072	1.5	
	p,p'-DDT	10.1	1.2	1.1	0.14	1.3	
	trans-permethrin	11.9	0.7	0.09	3.1	7.6	
80 residences, Maryland, USA	chlorypyrifos	9.43	6.7	6.6	0.355	1.8	Pang et al., 2002 <sup>l</sup>
120 houses, Cape Cod, Massachusetts, USA	DEP	8.21	590	589	5.0	9.6	Rudel et al., 2003 <sup>m</sup>
	methyl paraben	7.88	2.9	2.9	0.98	0.022	
	o-phenylphenol	8.75	71	71	0.28	4.0	
	pentachlorophenol	9.20 <sup>b</sup>	1.6	1.6	0.79	0.25	
	DiBP	9.62	61	59	1.9	25	
	DnBP	9.83	220	209	20	141	
	4-nonylphenol	9.97	110	102	2.6	96	
	octylphenol	10.0	8.6	8.0	0.13	8.1	
	monoethoxylate						
	nonylphenol	10.9	17	10	3.4	81	
	monoethoxylate						
	DEHA	11.3	9	3.5	6.0	69	
	DEHP	12.9	77	1.2	340	947	
30 residences, 75 rooms, Bavaria, DE	pentachlorophenol	9.2	2.4	2.4	1.1	0.38	Schnelle-Kreis et al., 2000 <sup>n</sup>

<sup>a</sup> Parameter definitions:  $K_{oa}$ —octanol-air partition coefficient, determined using SPARC online calculator release w4.5 unless otherwise noted;  $C_g + C_p$  meas—measured median airborne concentration combining both gaseous and particle-phase species;  $C_g$  inferred — inferred from measured  $C_g + C_p$  using equilibrium partitioning theory;  $X_{\text{dust, meas}}$ —measured median mass fraction of the SVOC in settled dust;  $X_{\text{dust, pred}}$ —mass fraction in settled dust predicted from inferred  $C_g$  using equation (2).

<sup>b</sup>  $K_{oa}$  for pentachlorophenol calculated using SPARC online calculator release w4.0.

<sup>c</sup> Median for  $C_g + C_p$  meas calculated using values in Table SI-7 for house codes 2–5; median for  $X_{\text{dust, meas}}$  calculated using values in Table SI-6 for house codes 2, 3, 11 and 12; despite the different house codes, these are paired samples from the same houses.

<sup>d</sup> Data represent our analysis of published “Supplementary Information,” Tables 2–4. Batterman et al. (2009) separately measured the gas and particle phases, and the sum is reported here as  $C_g + C_p$  meas. We deem that the experimental approach to separately collect particle and gas-phase species is subject to artifacts, and we therefore infer the gas-phase concentration from the measured total airborne level rather than rely on the measured gas-phase result directly. In some houses, replicate measurements were made; these were averaged before determining the median, using half the minimum detection level to replace values below the quantification limit. Hence, results reported here represent the median house values from the 12-house sample.

<sup>e</sup> Medians used in the present paper were extracted from Table 3 (revised) in the corrigendum (Bradman, 2009) of results published by Bradman et al. (2007).

<sup>f</sup> We used data reported in Table 1 of Weschler et al. (2008), which in turn reports results from Fromme et al. (2004b). Species were sampled on PUF cartridges and are assumed here to represent the sum of gaseous plus particulate species. Medians were computed directly from the detailed data.

<sup>g</sup> Medians used in the present paper were extracted from Table 3 of the reference.

<sup>h</sup> Medians used in the present paper were extracted from Table 7 of the reference.

<sup>i</sup> Airborne concentration measurements from Table 5 of Kanazawa et al. (2010) were interpreted to represent the sum of gaseous plus particulate species concentrations. Dust mass-fractions were medians from “multi-surface” samples (Kanazawa et al., Table 6).

<sup>j</sup> Medians used in the present paper were extracted from the detailed tables presented in Appendix I (North Carolina) and Appendix J (Ohio) of Morgan et al. (2004). All species are reported for a given group of buildings whenever “indoor air” and “indoor floor dust” median concentrations are each above the reported “method detection limit.”

<sup>k</sup> Medians used in the present paper were extracted from Table 5 ( $C_g + C_p$  meas) and 6 ( $X_{\text{dust, meas}}$ ) of the reference.

<sup>l</sup> Medians used in the present paper were extracted from Table 3 of the reference.

<sup>m</sup> Medians used in the present paper were extracted from Tables S1 ( $C_g + C_p$  meas) and S2 ( $X_{\text{dust, meas}}$ ) in the Supporting Information of the reference.

<sup>n</sup> Medians used in the present paper were extracted from Table 1 of the reference.

## 2.2. Uncertainties in the estimation procedure

To properly interpret the results that follow, it is useful to have a sense of how well or poorly the various parameters in equation

(2) can be estimated. We begin with  $K_{oa}$ , since it is at the heart of the discussion and has the largest potential uncertainty. We have compared  $K_{oa}$  values calculated using SPARC with  $K_{oa}$  values measured for a series of PAHs (Ha and Kwon, 2010), a series of

PBDEs (Harner and Shoeib, 2002), two perfluorinated surfactants (Shoeib et al., 2004), several organochlorine pesticides (Shoeib and Harner, 2002) and a series of PCBs (Harner and Bidleman, 1996). Altogether, the comparison spans 30 SVOCs. Calculated and corresponding measured values are presented in the supporting information, Table S1. For most of the tabulated compounds, the agreement is good. Overall, the absolute value of the difference between the calculated and measured log ( $K_{oa}$ ) values averages 0.39, corresponding to a factor of 2.5 in  $K_{oa}$  values. For 90% of the species, the absolute difference was less than 0.8, corresponding to a factor of 6.3. Only for BDE-153, BDE-154, and benzo(a)anthracene, species with relatively high values of log ( $K_{oa}$ ), do the  $K_{oa}$  values predicted by SPARC differ from the measured value by more than 10 $\times$ . For some compounds,  $K_{oa}$  may be in error owing to limitations in the algorithms and data embedded in SPARC. In such cases, predicted levels in dust would also be off by an amount proportional to the error in  $K_{oa}$ .

For SVOCs for which  $C_g$  has been measured passively and for SVOCs with log ( $K_{oa}$ ) < 10, the uncertainty in  $C_g$  is essentially that associated with measurement errors. For SVOCs with log ( $K_{oa}$ ) > 10, substantial levels are expected to be associated with airborne particles as compared with the gas phase. When it was necessary to estimate gas-phase concentrations from measured particle-phase or total airborne concentrations, we used an equilibrium parameter,  $K_p$ , “typical” indoor airborne particle concentrations, as well as estimates of  $f_{om\_part}$  and  $\rho_{part}$  as detailed in equations (4) and (5). Since  $K_{oa}$  is used to estimate  $K_p$  (see equation (3)) errors in  $K_{oa}$  will lead to proportional errors in  $C_g$  when the particle phase dominates airborne SVOCs.

Measured values for  $f_{om\_dust}$  range from 0.05 to 0.95, with  $f_{om\_dust}$  increasing as the size of the dust decreases (see Morawska and Salthammer, 2003). Fergusson et al. (1986) measured  $f_{om\_dust}$  values between 0.26 and 0.57 in eleven homes in Christchurch, NZ. Mølhave et al. (2000) report a median value of 0.33 for dust samples collected in seven Danish offices. The analysis in Weschler et al. (2008) indicates that the fraction of organic matter in settled dust is typically smaller than that in airborne particles, consistent with a larger fraction of mineral particles and fibers found in settled dust as compared to airborne particles. In the present analysis we assumed that  $f_{om\_dust}$  was 0.2. We acknowledge that this value is near the lower range of what has been reported for dust samples. However, in the case of the 19 studies that form the basis for this analysis we feel that the dust was often collected in a manner that did not exclude as much of the larger-sized inorganic material as has been the case for many of the reported measurements of  $f_{om\_dust}$ . Given the available evidence, it seems likely that for certain studies,  $f_{om\_dust}$  may be as much as a factor of two larger than what we have assumed here.

The density of dust solids is expected to be in the range (1–2.5)  $\times 10^6$  g m $^{-3}$ ; we assumed that  $\rho_{dust}$  was  $2.0 \times 10^6$  g m $^{-3}$  based on the measurements reported in Hunt et al. (1992). They collected dust samples from 16 homes; these were taken from vacuum cleaner bags and were sieved (<1 mm) prior to the determination of their density by a flotation technique. The “float solution” had a density of 1.9 g/cm $^3$ . The researchers found that 47% of the mass of their dust samples had a density > 1.9; 43% of the mass had a density < 1.9 and 10% of the mass was “missing”. A density of  $2.0 \times 10^6$  g m $^{-3}$  is consistent with the composition of typical dust (and density of its constituents) as reported by Morawska and Salthammer (2003).

In summary, the larger uncertainties in equation (2) are judged to be in  $K_{oa}$  and  $C_g$ , with lesser uncertainties in  $f_{om\_dust}$  and  $\rho_{dust}$ . The set of SVOCs included in this study possess a range of  $K_{oa}$  values that is very much larger than any of the uncertainties in parameter values.

### 3. Results and discussion

#### 3.1. Measured air and dust concentrations

Table 1 summarizes the median measured air and dust concentrations from the studies used in the present analysis. Also tabulated for each of the SVOC entries are the log ( $K_{oa}$ ) values (as calculated with SPARC), corresponding gas-phase concentrations (measured or inferred) and predicted dust mass fraction. The  $K_{oa}$  values for the various SVOC species span a large range—more than five orders-of-magnitude ( $10^{7.5}$ – $10^{13.1}$ ). Regarding  $C_g$ , the studies used in the present analysis have been divided into three categories:

Table 1a. These studies used passive sampling to measure the mass concentrations of gaseous SVOCs (Wilford et al., 2004, 2005; Shoeib et al., 2005; Gevao et al., 2007; Abdallah et al., 2008; Harrad et al., 2009; Imm et al., 2009; Toms et al., 2009). In these cases, the predicted mass fraction in dust was calculated directly (using equation (2)) from the median gas-phase concentration for the set of buildings in which measurements were reported.

Table 1b. One study measured mass concentrations of SVOCs only associated with airborne particles (Fromme et al., 2004a). In this case, for each SVOC, we estimated  $C_g$  from its median airborne particle concentration ( $C_p$ ) using equation (4). The predicted mass fraction in dust was then calculated using the resulting inferred gas-phase concentration and applying equation (2).

Table 1c. These studies measured the sum of the mass concentrations of gaseous and particulate-phase SVOCs in air (Mukerjee et al., 1997; Gordon et al., 1999; Schnelle-Kreis et al., 2000; Pang et al., 2002; Rudel et al., 2003; Fromme et al., 2004b, using data reported in Weschler et al., 2008; Morgan et al., 2004; Abdallah et al., 2008; Batterman et al., 2009; Bradman et al., 2007; Bradman, 2009; Fromme et al., 2009; Kanazawa et al., 2010). In these cases, we calculated  $C_g$  using equation (5). The predicted mass fraction in dust was then calculated using equation (2) and this inferred gas-phase concentration. Note that for compounds with log ( $K_{oa}$ ) less than 10, there is little difference between the measured “total” air concentration,  $C_g + C_p$ , and the inferred gas-phase concentration,  $C_g$ .

#### 3.2. Dust sampling methods

In addition to using different methods to sample SVOCs in air, the studies that form the basis of the present analysis used different methods to sample the settled dust. Batterman et al. (2009) and Schnelle-Kreis et al. (2000) vacuumed dust onto pre-cleaned and pre-weighed filters. Bradman et al. (2007), Morgan et al. (2004), Mukerjee et al. (1997) and Pang et al. (2002) used an HVS3 dust sampler (as described in Roberts et al., 1991). Rudel et al. (2003) vacuumed dust into cellulose extraction thimbles. Abdallah et al. (2008) and Harrad et al. (2009) vacuumed dust into a nylon sock. Fromme et al. (2004a,b) took fine dust from the space between the inner and outer layers of vacuum cleaner bags. Kanazawa et al. (2010) sampled dust from a paper bag affixed to a vacuum cleaner. Imm et al. (2009), Fromme et al. (2009), Gevao et al. (2007), Gordon et al. (1999), Shoeib et al. (2005), Toms et al. (2009), and Wilford et al. (2004, 2005) took dust from vacuum cleaner bags, canisters, or the containers of central vacuum systems. Furthermore, some but not all of these studies sieved the dust samples prior to analysis. When sieving has occurred, the typical cut-points have been between 50 and 150  $\mu$ m diameter. It is anticipated that these

different methods of collecting and processing the dust may result in systematic differences among the subsequent measurements (Butte and Heinzow, 2002; Liou et al., 2002; Morawska and Salthammer, 2003), but only a few studies have investigated this concern. The present section is intended to alert the reader to this issue, citing articles that are illustrative of certain points. It is not intended to be an exhaustive examination of the topic.

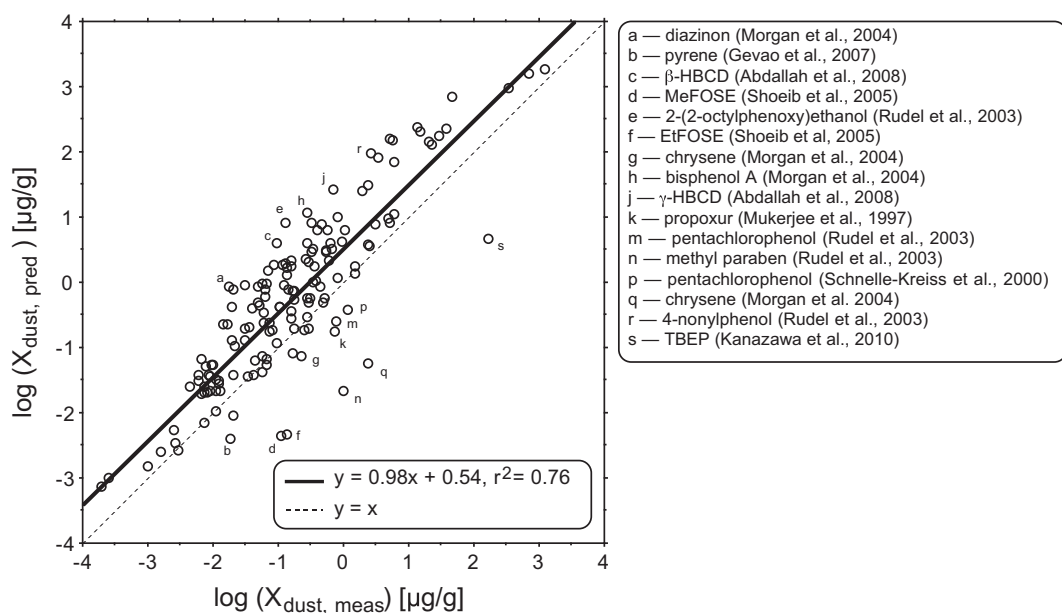
Dust samples taken from vacuum cleaner bags or from the canisters of central vacuum systems are adventitious samples that tend to come from multiple rooms. The surfaces “vacuumed” are those judged by the residents to require cleaning. Different residences may use different types and brands of vacuum cleaners. Room air repeatedly passes through the vacuum cleaner bag and previously collected dust as the “vacuum” is turned on and off. In contrast, dust samples collected by researchers are planned; the vacuumed surfaces have been specifically selected by the investigators; and sampling often occurs in only one or two rooms. In the HVS3 sampler, dust is diverted to a collection vessel; air does not pass through the collected dust.

Colt et al. (1998, 2008) have published results from two studies comparing SVOCs measured in samples taken from used vacuum cleaner bags with SVOCs measured in dust collected using the HVS3 sampler. In the 1998 article, HVS3 sampling was conducted in multiple rooms of 15 residences and dust samples from vacuum cleaner bags were taken from these same residences. Ten of the targeted SVOCs were detected in five or more homes and among these compounds the median levels were generally similar; a paired *t*-test showed no significant differences. In the 2008 study, HVS3 sampling was limited to a single room in each of 45 residences. In this study the authors again found that the median mass-fractions were similar between the two methods; the Spearman correlation coefficients were  $\geq 0.60$  for most analytes; for two SVOCs, there were meaningful differences, but, in each case, they had been detected in six or fewer of the 45 homes. Taken together these two studies indicate that, although there are differences between the household vacuum cleaner method and the HVS3

method, the agreement between mass fractions of SVOC measured in the respective dust samples is generally good.

Allen et al. (2008) compared, for 20 homes, mass fractions of PBDEs measured in dust samples collected from vacuum cleaner bags with those collected by researchers who vacuumed dust into a cellulose thimble attached to the cleaner’s suction tube. The researchers collected dust exclusively from floor surfaces in two rooms – bedrooms and the main living area; the samples were analyzed separately. In all cases, the dust samples were sieved ( $<500\ \mu\text{m}$  diameter) prior to analysis. Comparing vacuum bags with researcher collected dust from the bedrooms, the correlation coefficient, *r*, was 0.39, 0.40 and 0.77 for the sum of the penta-, octa-, and deca-congeners, respectively. The authors speculated that the researcher-collected dust may have had systematically higher levels of PBDEs than the vacuum cleaner bags since the researchers focused on rooms likely to contain sources of PBDEs.

When researchers collect dust, some sample only from floor surfaces, while others specifically avoid floor surfaces. One of the 19 studies listed in Table 1 has collected dust from both floor and non-floor surfaces (Kanazawa et al., 2010). Only results from the non-floor samples (“multi-surface samples”) have been used in the present analysis. However, the Kanazawa et al. study provides an opportunity to compare SVOC mass fractions in dust samples from floor- and non-floor surfaces. For most of the SVOCs targeted in this study, there was little difference between floor and non-floor samples. However, the mass-fractions of DiBP, BBzP and TBEP were significantly higher in floor dust as compared with non-floor dust. DiBP and BBzP are used as plasticizers in vinyl flooring, while TBEP is present in floor care products. In these instances, it appears that the SVOC content of the dust was enhanced by SVOCs present in the surface onto which dust had settled. Dust sampled from PVC flooring plasticized with DEHP has been shown to be enriched in DEHP relative to dust sampled from other surfaces, possibly because of contact transfer (Clausen et al., 2004). This finding is illustrative of a broader point: SVOCs can become associated with dust by mechanisms other than sorption from the air (see also Section 3.5.2).



**Fig. 1.** Scatterplot of the logarithm of the predicted mass fraction in dust,  $\log(X_{\text{dust, pred}})$ , against the corresponding logarithm of the measured mass fraction in dust,  $\log(X_{\text{dust, meas}})$ . The predictions assume equilibrium partitioning between the gas phase and settled dust (equation (2)). Each data point represents the median value for one SVOC measured in a set of buildings as reported in one of the 19 studies we have reviewed. The solid line presents the result of a least-squares regression, treating each data point with equal weight. The dashed line shows the correlation predicted by equation (2). Each data point that deviates by more than  $10\times$  compared with the regression line is labeled with an identifier code for which the corresponding SVOC and study is listed in the key.

### 3.3. Predicted vs. measured SVOC mass fractions in dust

Fig. 1 depicts predicted levels of SVOCs in dust,  $\log(X_{\text{dust,pred}})$ , plotted against the corresponding measurement results,  $\log(X_{\text{dust,meas}})$ . Outliers are identified by chemical name and

study. Table 2 presents the chemical name, CAS number, chemical classification and common indoor origin or use of the 66 SVOCs plotted in this figure. If equilibrium partitioning were to prevail, as described by equation (1), such a plot should display a linear relationship with unit slope. We find that the predicted

**Table 2**  
Chemical name, CAS number, classification and common indoor origin or use of SVOCs included in this study.

Chemical	CAS No.	Classification	Origin or use
BBzP (butyl benzyl phthalate)	85-68-7	Phthalate	Plasticizer
BDE-17 (2,2',4-tribromodiphenyl ether)	147217-75-2	PBDE	Flame retardant
BDE-28 (2,4,4'-tri...)	41318-75-6	PBDE	Flame retardant
BDE-47 (2,2',4,4'-tetra...)	5436-43-1	PBDE	Flame retardant
BDE-66 (2,3',4,4'-tetra...)	187084-61-5	PBDE	Flame retardant
BDE-71 (2,3',4',6-tetra...)	189084-62-6	PBDE	Flame retardant
BDE-99 (2,2',4,4',5-penta...)	60348-60-9	PBDE	Flame retardant
BDE-100 (2,2',4,4',6-penta...)	189084-64-8	PBDE	Flame retardant
BDE-153 (2,2',4,4',5,5'-hexa...)	68631-49-2	PBDE	Flame retardant
BDE-154 (2,2',4,4',5,6'-hexa...)	207122-15-4	PBDE	Flame retardant
benzo(a)anthracene	56-55-3	PAH	Combustion byproduct
benzo(a)pyrene	50-32-8	PAH	Combustion byproduct
benzo(b)fluoranthene	205-99-2	PAH	Combustion byproduct
benzo(e)pyrene	192-97-2	PAH	Combustion byproduct
benzo(g,h,i)perylene	191-24-2	PAH	Combustion byproduct
benzo(k)fluoranthene	207-08-9	PAH	Combustion byproduct
BHT (butylated hydroxy toluene)	128-37-0	Phenol	Antioxidant
bisphenol-A	80-05-7	Phenol	Residual monomer
$\alpha$ -chlordane	5103-71-9	Chlorocarbon	Pesticide
$\gamma$ -chlordane	5566-34-7	Chlorocarbon	Pesticide
chlorpyrifos	2921-88-2	Organophosphate	Pesticide
chlorthal-dimethyl (dimethyl tetrachloroterephthalate)	1861-32-1	Chlorocarbon	Pesticide
chrysene	218-01-9	PAH	Combustion byproduct
coronene	191-07-1	PAH	Combustion byproduct
p,p'-DDE	72-55-9	Chlorocarbon	Pesticide
p,p'-DDT	50-29-3	Chlorocarbon	Pesticide
DEHA (di(2-ethylhexyl) adipate)	103-23-1	Adipate	Plasticizer
DEHP (di(2-ethylhexyl) phthalate)	117-81-7	Phthalate	Plasticizer
DEP (diethyl phthalate)	84-66-2	Phthalate	Plasticizer
diazinon	333-41-5	Organophosphate	Pesticide
dibenzo(a,h)anthracene	53-70-3	PAH	Combustion byproduct
DiBP (di(isobutyl) phthalate)	84-69-5	Phthalate	Plasticizer
DMP (dimethyl phthalate)	131-11-3	Phthalate	Plasticizer
DnBP (di(n-butyl) phthalate)	84-74-2	Phthalate	Plasticizer
EtFOSE (N-ethyl perfluoro-octane sulfonamidoethanol)	1691-99-2	Perfluorocarbon	Stain repellent, surfactant
fluoranthene	206-44-0	PAH	Combustion byproduct
$\alpha$ -HBCD ( $\alpha$ -hexa-bromocyclododecane)	23774-70-1	Bromocarbon	Flame retardant
$\beta$ -HBCD ( $\beta$ -hexa...)	23774-70-1	Bromocarbon	Flame retardant
$\gamma$ -HBCD ( $\gamma$ -hexa...)	23774-70-1	Bromocarbon	Flame retardant
heptachlor	76-44-8	Chlorocarbon	Pesticide
indeno(1,2,3-cd)pyrene	193-39-5	PAH	Combustion byproduct
2-isopropyl-6-methyl-4-pyrimidinol	2814-20-2	Other	Degradation product (diazinon)
MeFOSE (N-methylperfluoro-octane sulfonamidoethanol)	24448-09-7	Perfluorocarbon	Stain repellent, surfactant
methyl paraben (methyl 4-hydroxybenzoate)	99-76-3	Paraben	Fungicide
4-nonylphenol	104-40-5	Phenol	Surfactant
nonylphenol monoethoxylate	27986-36-3	Alkylphenol ethoxylate	Surfactant
octylphenol monoethoxylate	1322-97-0	Alkylphenol ethoxylate	Surfactant
PCB 28 (2,4,4'-trichlorobiphenyl)	7012-37-5	PCB	Many historic uses
PCB 31 (2,4',5-tri...)	16606-02-3	PCB	Many historic uses
PCB 52 (2,2',5,5'-tetra...)	35693-99-3	PCB	Many historic uses
PCB 95 (2,2',3,5',6-penta...)	38379-99-6	PCB	Many historic uses
PCB 101 (2,2',4,5,5'-penta...)	37680-73-2	PCB	Many historic uses
PCB 118 (2,3',4,4',5-penta...)	31508-00-6	PCB	Many historic uses
PCB 138 (2,2',3,4,4',5'-hexa...)	35065-28-2	PCB	Many historic uses
PCB 153 (2,2',4,4',5,5'-hexa...)	35065-27-1	PCB	Many historic uses
PCB 180 (2,2',3,4,4',5,5'-hepta...)	35065-29-3	PCB	Many historic uses
pentachlorophenol	87-86-5	Chlorocarbon	Preservative, biocide
cis-permethrin	52645-53-1	Pyrethroid	Pesticide
trans-permethrin	51877-74-8	Pyrethroid	Pesticide
phenanthrene	85-01-8	PAH	Combustion byproduct
o-phenylphenol	90-43-7	Phenol	Fungicide
propoxur	114-26-1	Carbamate	Pesticide
pyrene	129-00-0	PAH	Combustion byproduct
TBBP-A (tetrabromobisphenol A)	107719-55-1	Bromocarbon	Flame retardant
TBEP (tris(2-butoxyethyl) phosphate)	78-51-3	Organophosphate	Plasticizer, flame retardant
3,5,6-TCP (3,5,6-trichloro-2-pyridinol)	6515-38-4	Other	Degradation product (chlorpyrifos)



values do correlate with those measured ( $r^2 = 0.76$ ) with a slope close to unity (0.98) and an intercept of 0.54. The intercept indicates that, on average, the predicted SVOC mass fractions in dust are 3.5 times larger ( $=10^{0.54}$ ) than the measured values. It is conceivable but unlikely that contributions to this discrepancy could result from an assumed value for the fraction of organic matter in dust that is too large or from an assumed value for the density of dust that is too small. However, as discussed below, other known factors might explain the observed differences between predicted and measured SVOC mass fractions in dust.

#### 3.4. Kinetic considerations

As the value of  $K_{oa}$  increases, the approach to equilibrium partitioning occurs at a slower rate, and the mass fraction of an SVOC in settled dust may not have sufficient time to equilibrate with its gas-phase concentration or vice versa (Weschler and Nazaroff, 2008; Schripp et al., 2010). To examine this aspect of SVOC dynamics, we have plotted the data that forms the basis of Fig. 1 in a manner that isolates  $K_{oa}$ . More specifically, Fig. 2 displays a plot of  $\log(X_{dust,meas}/C_g)$ , versus  $\log(K_{oa})$ . Such a plot reveals whether the measured ratio of  $K_{dg}$  deviates in a systematic fashion from the equilibrium described in equation (1) as the value of  $K_{oa}$  increases. Note that this plot must be interpreted with caution. For many data pairs,  $C_g$ , a factor in the dependent variable, has been estimated using  $K_{oa}$ , the independent variable.

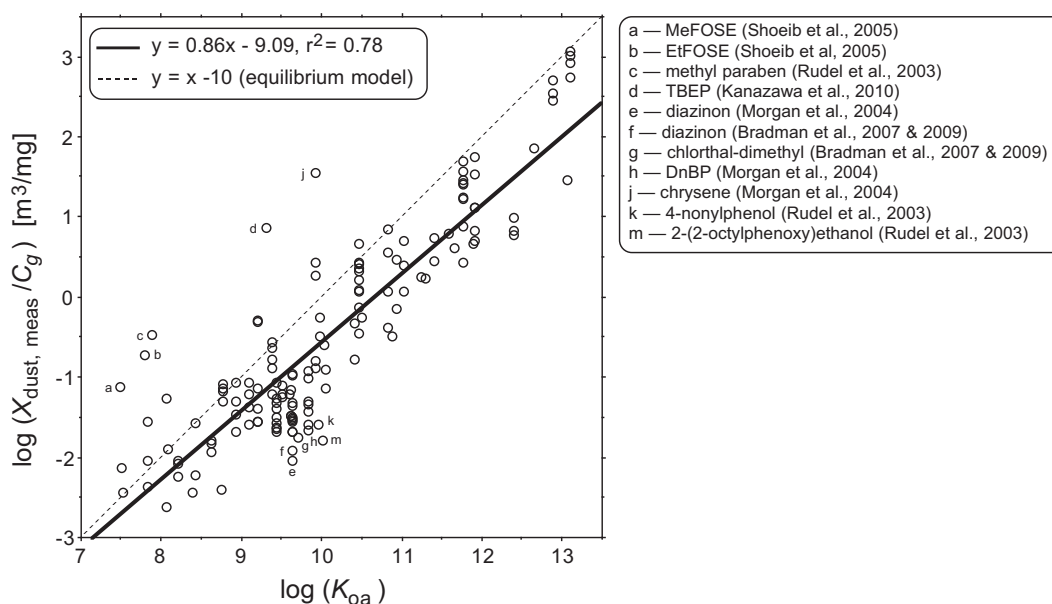
The dashed line in Fig. 2 shows the correlation predicted for equilibrium partitioning:  $y = x - 10$ . (The intercept, “-10”, is obtained from  $\log(f_{om,dust}/\rho_{dust})$  assuming that  $f_{om,dust}$  is 0.2 and  $\rho_{dust}$  is  $2.0 \times 10^9 \text{ mg m}^{-3}$ .) For high  $K_{oa}$  values, the measured SVOC levels in dust are systematically less than would be predicted by equilibrium. This finding suggests that, for typical indoor conditions, kinetic constraints on equilibration may meaningfully influence SVOC partitioning of species with high  $K_{oa}$  values (corresponding to very low volatilities). Given equilibrium predictions, the empirical evidence indicates that these high  $K_{oa}$  species tend to be underrepresented in dust relative to their abundance in air.

#### 3.5. Factors that influence partitioning between gaseous and dustborne SVOCs

##### 3.5.1. Differences between octanol and organic matter in dust

The relationship described by equation (1) is predicated on the assumption that the solubility of an SVOC in the organic matter present in dust is similar to its solubility in octanol. The validity of this assumption likely varies among different classes of chemicals. Table 3 presents the ratio of predicted-to-measured mass fractions for the more commonly measured SVOCs grouped by their chemical classification. For PCBs, agreement between predicted and measured values is reasonably good. The same is true for pentachlorophenol, the only chlorocarbon measured in three or more studies, as well as three other chlorocarbons that are not shown ( $\alpha$ - and  $\gamma$ - chlordane and 3,5,6-TCP). Two organophosphates, chlorpyrifos and diazinon, have been measured in multiple studies. Predicted values of chlorpyrifos tend to be an order of magnitude larger than measured values; for diazinon the discrepancy is even greater. For SVOCs that are classified as PAH, the predicted values tend to be within an order of magnitude of measured values; the agreement is better in the studies by Gevaio et al. (2007) and Morgan et al. (2004) than in the study by Fromme et al. (2004a). For SVOCs classified as PBDE, the agreement between predicted and measured mass fractions is quite good for each of the five studies in which they were measured, excepting BDE-99 in Toms et al. (2009). Three of these studies measured gas-phase concentrations using passive sampling (Wilford et al., 2004; Imm et al., 2009; Toms et al., 2009), whereas two measured total air concentrations (Batterman et al., 2009; Fromme et al., 2009) from which we have inferred gas-phase concentrations. For SVOCs classified as phthalates, the predicted values are within a factor of three of the measured values for three esters—DMP, DEP and DEHP. However, for the other three esters—DiBP, DnBP and BBzP—the predicted values are significantly larger than the measured values, with DnBP displaying the greatest discrepancy.

MeFOSE and EtFOSE are two perfluorinated sulfonamides (PFAS) included in Fig. 1 but not listed in Table 3 (since data on these species are available from only one study); their predicted mass



**Fig. 2.** Scatterplot of the logarithm of the ratio ( $X_{dust,meas}/C_g$ ) against the corresponding logarithm of  $K_{oa}$ . The  $K_{oa}$  values have been estimated using SPARC release 4.5 except for pentachlorophenol. (See Table 1.) The data are the same as plotted in Fig. 1. The solid line shows the results of a least-squares regression with each data point weighted equally. The dashed line shows the correlation predicted for equilibrium partitioning (equation (1)). Note that the ratio ( $X_{dust,meas}/C_g$ ) is equivalent to an experimental  $K_{dg}$ . Each data point that deviates by more than 10× compared with the regression line is labeled with an identifier code for which the corresponding SVOC and study is listed in the key.

**Table 3**  
Ratio of predicted-to-measured median mass fractions for SVOCs in settled dust from different chemical classes and different studies.<sup>a</sup>

Chlorocarbon	Study A (NC:H, OH:H, NC:D, OH:D) <sup>b</sup>			Study B	Study C
pentachlorophenol	3.9, 5.6, 2.2, 5.8			0.32	0.33
Organophosphate	Study D	Study E	Study A (NC:H, OH:H, NC:D, OH:D) <sup>b</sup>	Study F (spring, summer)	Study G
chlorpyrifos	10	13	12, 8.5, 5.5, 3.5	6.7, 11	5.0
diazinon	36	15	49, 21, 15, 10	9.3, 21	
PAH	Study H		Study I	Study A (NC:H, NC:D, OH:D) <sup>b</sup>	
phenanthrene	0.44				
pyrene	0.21		4.8		
fluoranthene	0.97		4.4		
chrysene	6.6		5.3	0.47, 0.32, 0.02	
benzo(a)anthracene	2.9		1.7		
benzo(e)pyrene			16		
benzo(a)pyrene	2.4		8.3	1.1, –, –	
benzo(b)fluoranthene	17		5.7	1.9, 0.95, –	
benzo(k)fluoranthene	12		2.9		
benzo(g,h,i)perylene			9.1	4.3, 2.1, –	
indeno(1,2,3-cd)pyrene			9.1	4.6, –, –	
coronene			11		
dibenzo(a,h)anthracene			18		
PBDE	Study J	Study K	Study L	Study M	Study N
BDE-17			1.5	1.9	
BDE-28			0.90	1.0	4.1
BDE-47	1.1	1.3	0.63	1.4	2.4
BDE-66					3.8
BDE-71				1.8	
BDE-99	3.5	21	2.0	1.6	2.2
BDE-100	7.6		3.3	1.2	2.2
BDE-153				2.2	1.2
BDE-154				1.1	1.5
PCB	Study O			Study A (NC:D, OH:D) <sup>b</sup>	
PCB 28 & 31	1.0				
PCB 52	3.5			2.6, 2.8	
PCB 95				–, 6.4	
PCB 101	4.0			5.8, 5.2	
PCB 118	4.4				
PCB 138	5.8				
PCB 153	5.5				
PCB 180	9.9				
Phthalate	Study P	Study Q	Study A (NC:H, OH:H, NC:D, OH:D) <sup>b</sup>	Study B	
DMP	0.90				
DEP	1.8	2.8		1.9	
DiBP	6.1	13		1.3	
DnBP	15	5.8	27, 31, 18, 14	7.0	
BzBP	6.2				
DEHP	2.2	1.5		2.8	

<sup>a</sup> Sources: Study A – Morgan et al., 2004; Study B – Rudel et al., 2003; Study C – Schnelle-Kreis et al., 2000; Study D – Bradman et al., 2007; Bradman, 2009; Study E – Gordon et al., 1999; Study F – Mukerjee et al., 1997; Study G – Pang et al., 2002; Study H – Gevao et al., 2007; Study I – Fromme et al., 2004a; Study J – Imm et al., 2009; Study K – Toms et al., 2009; Study L – Wilford et al., 2004, 2005; Study M – Batterman et al., 2009; Study N – Fromme et al., 2009; Study O – Harrad et al., 2009; Study P – Fromme et al., 2004b; Weschler et al., 2008; Study Q – Kanazawa et al., 2010.

<sup>b</sup> NC = North Carolina; OH = Ohio; H = houses; D = daycare facilities.

fractions are ~ 25 to 30 times *smaller* than their measured mass fractions. Shoeib et al. (2005), who made these measurements in Canadian homes, analyzed their results in a manner similar to that employed here and reached a similar conclusion—that the mass fraction in dust and the gas-phase concentrations are correlated, but that  $K_{oa}$  significantly underpredicts the mass fraction of these perfluorinated compounds in settled dust. Shoeib et al. speculated that a possible reason for the divergence between observation and theory is a potentially large difference between the solubility of perfluorinated species in octanol and in the organic matter of dust.

### 3.5.2. Abrasion of material containing a particular SVOC

A second reason postulated by Shoeib et al. for the observed discrepancy between measured and predicted partitioning is that some of the PFAS compounds in dust may be present in PFAS-rich

particles derived from indoor abrasion or wear processes. Webster et al. (2009) have demonstrated such a phenomenon for BDE-209, a relatively nonvolatile PBDE. They found that in samples with high levels of BDE-209, the bromine was “was concentrated in widely scattered, highly contaminated particles.” Indeed, some SVOCs found in dust may well be incorporated in the matrix of individual dust particles having been generated through a fragmentation process rather than *sorbed* to organic matter in dust as would be expected for a gas-phase mediated transport process. Such circumstances could contribute toward explaining why certain data points lie significantly below the trend line in Fig. 1 or above the equilibrium line in Fig. 2. For example, TBEP (Kanazawa et al., 2010), labeled as an outlier in Figs. 1 and 2, is used as a plasticizer in floor-care products (Weschler, 1980) and may be enriched in particles generated by buffing or by other processes that induce floor-surface wear.

### 3.5.3. Other factors

Additional factors that can contribute to discrepancies on an order-of-magnitude scale have already been discussed: errors in the calculated value of  $K_{oa}$ , direct transfer of an SVOC from a surface to dust in contact with that surface (Clausen et al., 2004), and differences in dust sampling and processing.

We have identified several further factors that merit mention; however, these are generally expected to affect outcomes on a scale smaller than that of the larger deviations observed. (i) Active sampling to measure SVOCs in air often represents short-term determinations and may not be representative of long-term average concentrations. Passively measured gas-phase concentrations and dustborne SVOCs reflect conditions over longer time periods. The effective time scale over which dust particles effectively sample the gas phase would also vary with  $K_{oa}$ , with higher  $K_{oa}$  values corresponding to longer equilibration time scales (Weschler and Nazaroff, 2008). (ii) For SVOCs where the detection limit and measured values are similar, bias can result because higher-than-average outcomes are detected whereas lower-than-average results are not. (iii) The indoor temperature during sampling may be higher or lower than 298 K, the temperature at which  $K_{oa}$  has been calculated. The influence of this factor varies among chemical classes. (iv) Some of the organic matter in dust, such as cotton linters, may differ meaningfully from octanol in terms of sorption of gas phase SVOCs.

Yet another consideration, which may reduce discrepancies between predicted and measured values, is that some active dust-sampling protocols promote at least transient equilibration between gas-phase SVOCs and sampled dust. As air passes through a filter cassette or a vacuum cleaner bag, there is the opportunity for gas-phase SVOCs to equilibrate with levels in the captured dust. On the other hand, kinetic considerations suggest that there would be insufficient time for this process to meaningfully influence the results for SVOCs with high  $K_{oa}$  values.

### 3.6. Median values and individual values

Fig. 1 demonstrates that, using  $K_{oa}$ , the median value for the mass fraction of an SVOC in a collection of dust samples can be estimated reasonably well from its corresponding median gas-phase concentration and vice versa. The use of median values from a collection of measurements made in multiple residences tends to dampen the deviations from the values assumed in the present study for various factors in individual residences that could influence partitioning (e.g., temperature, fraction of organic matter, density, concentration of airborne particles). In contrast, we anticipate that the approach presented here would not be as successful in predicting partitioning between the gas phase and settled dust in individual residences where deviations from assumed norms are not blunted by emphasizing the central tendency, as we have done. In other words, the relationship shown in equation (1) might best be used as a screening tool for interpreting an ensemble of measurement results. Owing to the anticipated ranges of values for the factors that influence this relationship, one should not interpret the present study as providing strong justification to calculate individual SVOC concentrations in air from concentrations in dust (or vice versa) on a house-by-house basis.

## 4. Conclusions

Weschler et al. (2008) have shown that the mass fractions of various phthalate esters in airborne particles, calculated using either  $K_{oa}$  or the saturation vapor pressure, correlate with their measured mass fractions in settled dust. Such a relationship would be anticipated to hold for all SVOCs. Taken together, that earlier study and the present one provide evidence, based on extensive

and detailed measurements in actual indoor environments, that SVOCs in settled dust, in airborne particles and in the gas phase are correlated. Hence, if one of these is measured or otherwise determined in a collection of residences, then the other two can be estimated for that same collection of residences, at least in central tendency.

The immediate goal of this research has been to investigate the extent to which  $K_{oa}$  can be used to estimate partitioning of SVOCs between settled dust and the gas phase. The nineteen studies that form the basis of the present analysis have used different methods to collect and sieve the settled dust and different methods to sample SVOCs in air. Also, the assumptions underlying the estimation method appear to be more valid for some compounds than for others. Despite these limitations, the outlined approach works well. For example, of the 150 points plotted in Fig. 2, 55% lie within a factor of 3 of the regression model's predictions and 90% are within an order of magnitude. This analysis indicates that the thermodynamic parameter  $K_{oa}$ , which varies markedly among SVOC species, correlates strongly with indoor environmental partitioning. More broadly, estimates of the type presented in this study aid in understanding pathways that govern indoor SVOC dynamics, which can substantially influence indoor exposures and uptake of SVOCs by people (Lioy, 2006; Weschler and Nazaroff, 2008).

Overall, the findings of this study contribute to an emerging body of research on indoor SVOC dynamics, which can elucidate the processes that govern human exposure to SVOCs in indoor environments. In principle, such knowledge could support better characterization of exposures in epidemiological investigations and, if warranted, also provide a rational foundation for interventions aimed at reducing exposures.

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## Appendix. Supplementary material

Supplementary data associated with this article can be found in the online version, at doi:10.1016/j.atmosenv.2010.06.029.

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