Supporting Information for

A rapid micro chamber method to measure SVOC emission and transport model parameters

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Content

Table S1: Plasticizers used in the chamber experiments and their chemical properties

Full Name	**Short Name**	**CAS RN**	**Molecular Weight (g/mol)**	**Saturation Vapor Pressure (Pa) at 298 K[1, 2]**	**Saturation Vapor Pressure (μg/m³) at 298 K[1, 2]**	**Octanol-air Partition Coefficient (log(K_{oa}))[3, 4]**
Dimethyl phthalate	DMP	131-11-3	194.2	3.6×10^{-1}	28842	7.5
Diisobutyl phthalate	DiBP	84-69-5	278.3	9600×10^{-6}	1076	9.6
Di-n-butyl phthalate	DnBP	84-74-2	278.3	6700×10^{-6}	751	9.8
Di(2-ethylhexyl) phthalate	DEHP	117-81-7	390.6	16×10^{-6}	2.5	12.9
Di(2-ethylhexyl) terephthalate	DEHT	6422-86-2	390.6	2.7×10^{-6}	0.4	12.5
Diisononyl phthalate	DINP	28553-12-0	418.6	2.3×10^{-6}	0.4	14.0

Table S2: Characteristics of emission source materials used in the chamber experiments[5, 6]

Source Material ID	**Source Material Name**	**Source Material Description**	**Plasticizers in Source Material**	**C_0 (wt%)**
GreenVF	Vinyl flooring (green)	Polyvinyl chloride (PVC)	DEHP	23.3
RedVF	Vinyl flooring (red)		DiBP	4.6
			DnBP	3.8
TM-b	Backpack material	Polyester with PVC coating	DEHT	7.9
			DINP	4.2

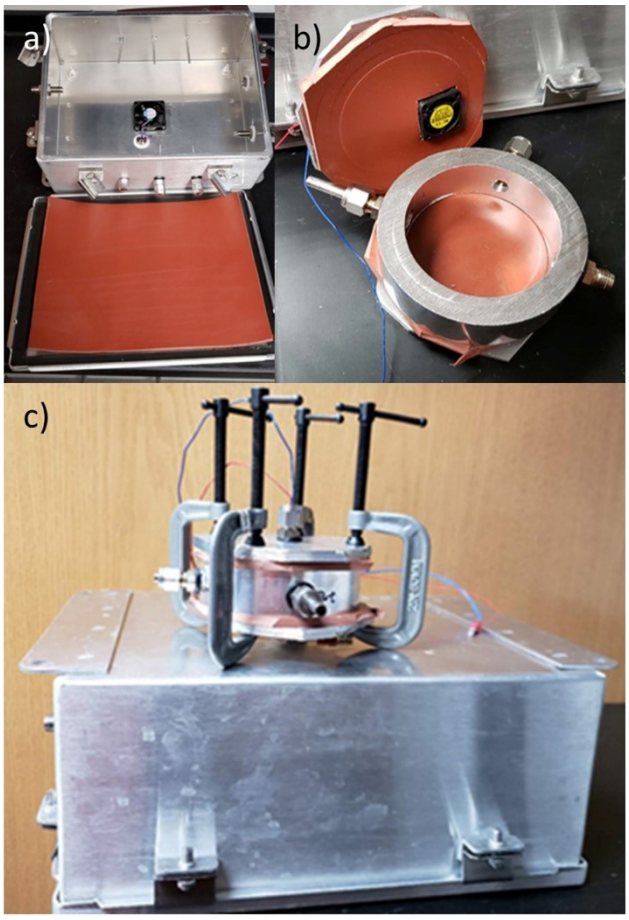

Figure S1. Photos of a) the interior of the macro chamber, b) the interior of the micro chamber, and c) size comparison of the micro (top) and macro (bottom) chamber.

Section S1: Details on Analytical Method

To analyze the aluminum rods, thermal desorption (TD) coupled with gas chromatography-flame ionization detection (GC-FID) or with gas chromatography-mass spectrometry (GC-MS) was used.

The sorbent tubes were desorbed for 30 mins at 300°C with a Helium flow rate of 50 mL/min, and a cold trap temperature of 5°C. Flash heating of the cold trap to 320°C transferred the analyte through the valves at 250°C and the transfer line at 255°C to the GC.

The GC-FID has a constant pressure of 12 psi, resulting in a flow rate of 10 mL/min at 320°C and equipped with a 30 m RTX-1 column (0.53 mm id, 0.25 µm film thickness, Restek, Bellefonte, PA), and operated at a 33:1 split ratio. The GC-MS has a constant pressure resulting in a flow rate of 2 mL/min at 320°C, and was equipped with a 0.25 mm ID GC column and operated at a 3:1 split ratio. The temperature program for GC-FID was held at 50°C for 1 min, ramp at 10°C/min until reaching 280°C, then ramp at 20°C/min to reach 320°C, and hold at 320°C for 5 min. The entire program lasted 31 minutes.

The temperature program for GC-MS was as follows: The temperature was held at 50°C for 1 min, ramped up at 35°C/min until reaching 320°C, and then held at 320°C for 10 min. The entire program lasted 19 minutes. GC-MS analyses were performed in full scan mode and technical information is summarized in Table S3. For GC-MS analysis, an RTX-5 column (30 m length, 0.25 mm inner diameter, 0.25 µm thickness) was used.

Section S2: Additional QA/QC

The material of the fan used in both chambers is plastic. Liquid extractions of fan material were conducted and none of the target SVOCs were detected. The background levels of both chambers with fans but without source materials were assessed under experimental conditions and following the experimental protocols, and the concentrations of the target SVOCs were found to be below detection limits.

Additional information about the plasticizer sampling method with TD tubes can be found in Wu et al. (2016)[7], including breakthrough tests and an inter-laboratory study.

Table S3: GC-MS retention times (t_R), with quantifying and qualifying ions for phthalates

Short Name	t_R (min)	Quantifying ion	Qualifying ions
DEHP	10.08	149	167, 279
DEHT	11.04	261	149, 167
DINP	10.2~12.4	293	149, 127
D4-DEHP	10.08	154	171, 183

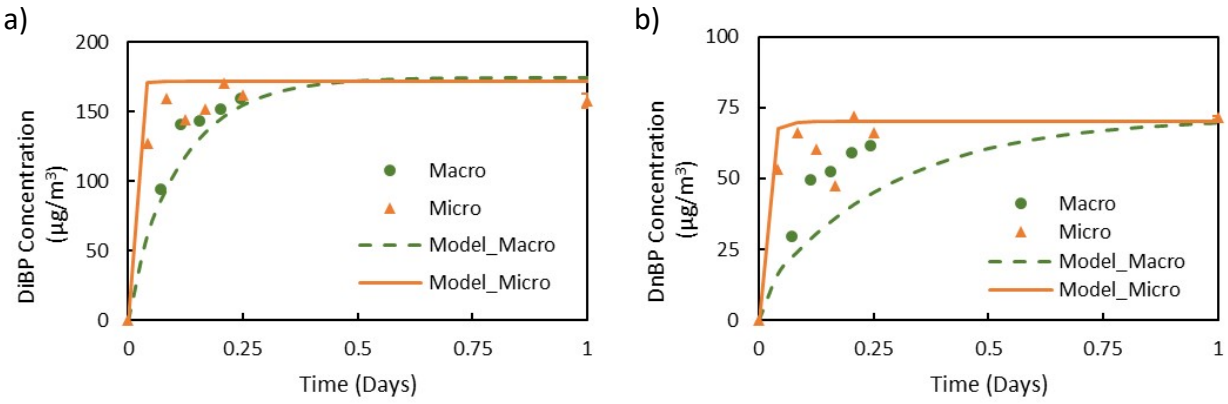

Figure S2. Close-up of the gas-phase concentrations of a) DiBP and b) DnBP over time in the macro chamber and in the micro chamber shown in Figure 3 in the main manuscript. Dots and triangles refer to measured gas-phase concentrations in the macro and micro chamber, respectively, while the lines are DustEx model predictions.

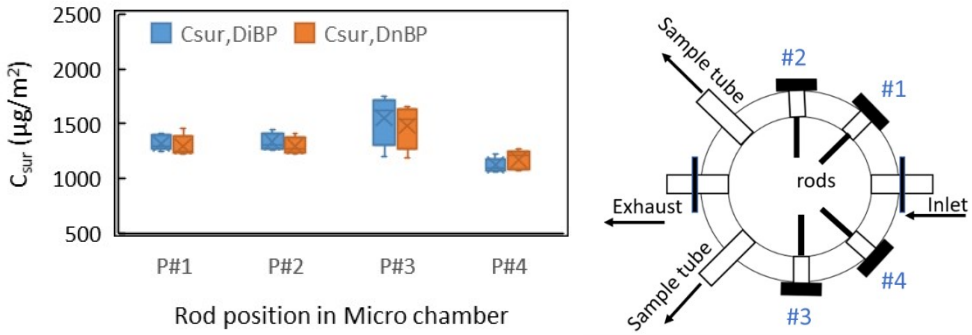

Figure S3. Surface concentrations on aluminum rods (positions 1-4) in the micro chamber at steady state. Blue bars are DiBP surface concentrations and yellow bars are DnBP surface concentrations. The order of rod positions is counter-clockwise from the inlet. The surface concentration in each position was measured four times at steady state except for position #1, which has six measurements.

Table S4: Model parameters used to predict the gas-phase concentration profiles and the surface (rod) concentrations profiles in the macro chamber and the micro chamber

	Volume V (m³)	**Air Change Rate λ (1/h)**	**Source Surface Area S_m (m²)**	**Sink (Wall) Surface Area S_{sur} (m²)**	**Rod Surface Area (m²)**	**Sink-to-Source Surface Area Ratio**
Macro Chamber	7.7×10^{-3}	0.96	6.4×10^{-2}	2.2×10^{-1}	3.1×10^{-3}	3.4:1
Micro Chamber	1.2×10^{-4}	158	9.1×10^{-3}	6.1×10^{-3}	5.7×10^{-4}	0.7:1

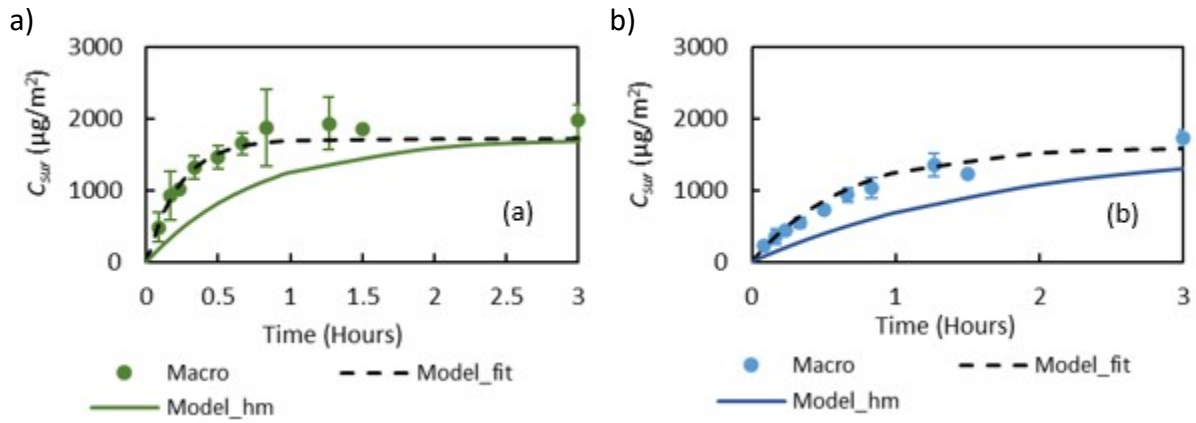

Figure S4. Comparison of the surface concentrations of a) DiBP and b) DnBP on aluminum rod surfaces in the macro and micro chambers during the first 3 hours of the experiment. Dots and triangles refer to measured concentrations on the rods in the macro and micro chamber, respectively, while the green and blue lines are DustEx model predictions. The dashed lines represent the fitted curve used to calculate h_s.

Table S5: Parameters used for plasticizer exposure assessment with the DustEx online tool

Residence:			
Room volume (m^3)	50		
Ventilation rate (1/h)	0.5		
Product/emission:	**DnBP**	**DEHP**	**DEHT**
Product surface area (m^2)	20		
Product volume (*assuming thickness of 0.005 m*) (m^3)	0.1		
Concentration of the substance in the product (g/cm^3), see Table S2	C_0/100% * ρ_{PVC} = 3.8%/100% * 1.5 g/cm^3 = 0.057 g/cm^3	C_0/100% * ρ_{PVC} = 23.3%/100% * 1.5 g/cm^3 = 0.350 g/cm^3	C_0/100% * ρ_{PVC} = 7.9%/100% * 1.5 g/cm^3 = 0.119 g/cm^3
Dust:			
Organic matter content dust (fraction)	0.2 (default)		
Dust loading (g/m^2)	0.3 (default)		
Density of dust (g/cm^3)	2 (default)		
Elimination rate from indoor environment (per year)	5 (default)		
Substance properties:	**DnBP**	**DEHP**	**DEHT**
Substance K_{oa} (10Log)	9.6	12.9	13
Molecular weight (g/mol)	278	391	391
K_{ma} (estimated based on y_0 measured in this study, Table 1) (10Log)	8.9	11.2	11.4
Mass transfer coefficient for surfaces (m/h)	1	0.89	0.89
Transdermal permeability coefficient, calculated based on Weschler and Nazaroff[8] (m/h)	3.9	4.6	4.3
Indoor surfaces/sinks:	**DnBP**	**DEHP**	
Surface area dust (m^2)	10 (min. value)		
Total surface area for sorption (m^2)	160		
Surface/air partitioning -> Surface/air partition coefficient (this study)	18	1410	1800
Airborne particulate matter:			
Air concentration particulate matter ($\mu g/m^3$)	20 (default)		
Density airborne particulate matter (g/cm^3)	1 (default)		
Mass transfer coefficient airborne particles (m/h)	100 (default) (range: 1-1000)		
Organic matter content (fraction)	0.4 (default)		
Exposed population:	**Child (default)**	**Adult (default)**	
Dust ingestion rate (mg/day)	100	50	

Inhalation rate (m^3/day)	9	36
Body weight (kg)	8	70
Skin surface area (m^2)	0.5	2
Simulation:		
Simulation duration (days)	365 (default)	
Exposure frequency (per year)	365 (default)	
Start of exposure (day)	0 (default)	
Exposure duration on day of exposure (hours)	24 (default)	
Exposure:		
Oral absorption fraction	1 (default)	
Inhalation absorption fraction	1 (default)	

Table S6: DustEx tool results for DnBP, DEHP and DEHT concentrations after 365 days

	Concentration in Compartments (g/m^3)		
	DnBP	DEHP	DEHT
Gas Phase Air Concentration	3.3×10^{-5}	6.8×10^{-7}	1.4×10^{-7}
Particle Bound Air Concentration	1.1×10^{-6}	2.9×10^{-5}	6.4×10^{-6}
Dust Concentration	2.5×10^{4}	6.4×10^{3}	1.3×10^{3}
Product Concentration	5.7×10^{4}	3.5×10^{5}	1.2×10^{5}
Surface Concentration	1.3×10^{5}	5.0×10^{6}	1.2×10^{6}

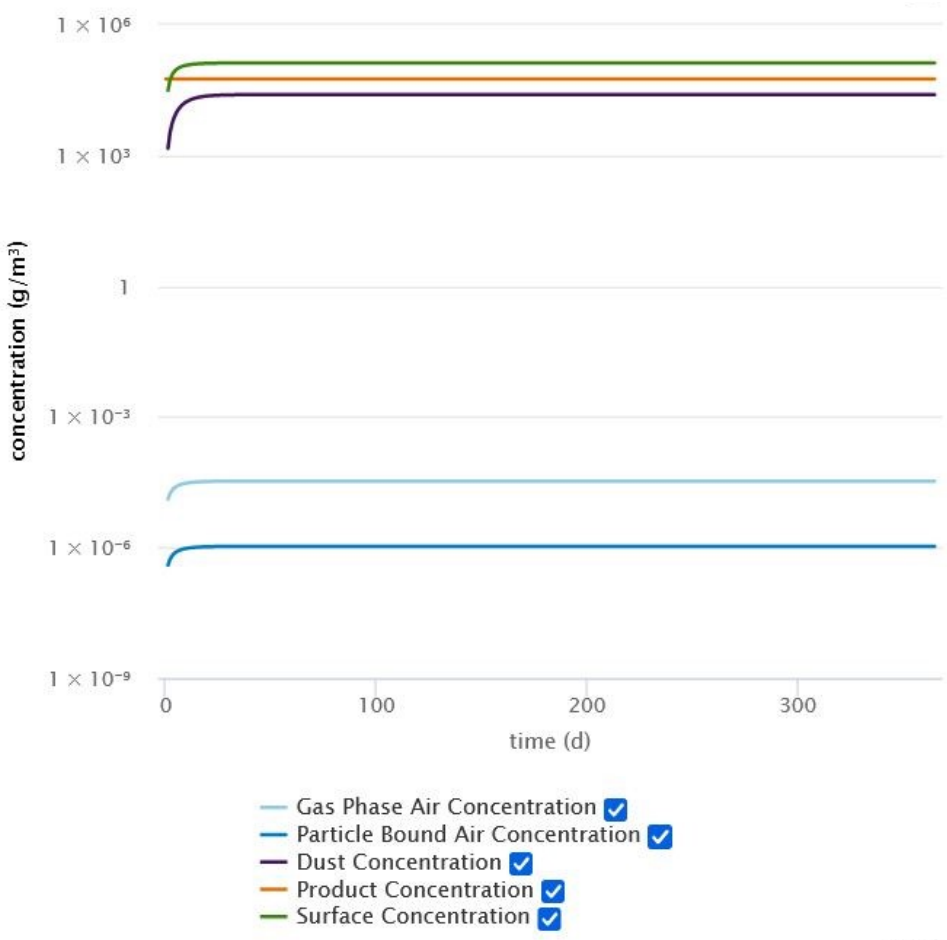

Figure S5: Concentrations of DnBP in indoor compartments as calculated by the DustEx tool after 365 days.

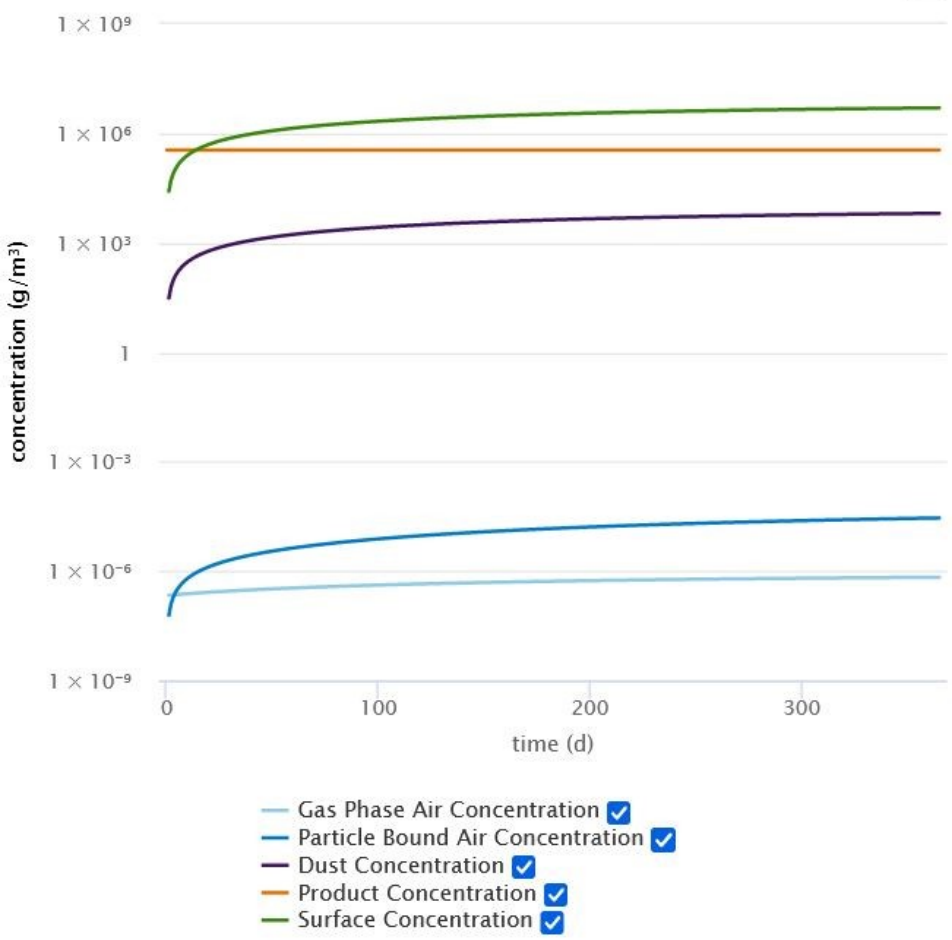

Figure S6: Concentrations of DEHP in indoor compartments as calculated by the DustEx tool after 365 days.

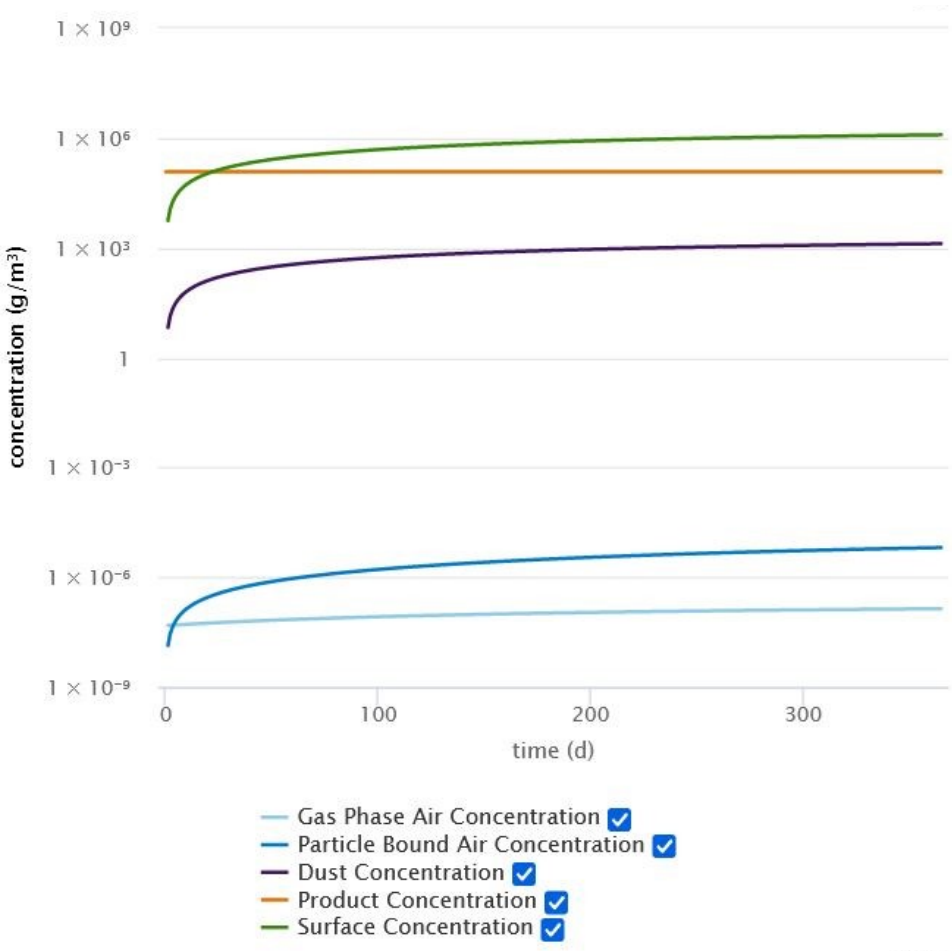

Figure S7: Concentrations of DEHT in indoor compartments as calculated by the DustEx tool after 365 days.

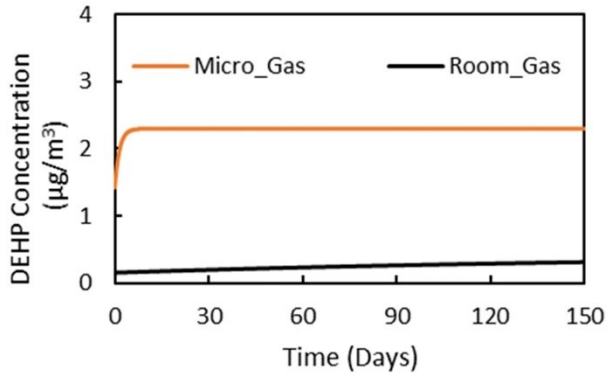

Figure S8: DEHP gas-phase concentrations predicted by the DustEx model for a simulated room and for the micro chamber.

Table S7: DustEx tool results for estimated exposure to DnBP, DEHP and DEHT for children and adults

	Absorbed Dose (g/(kg BW d))					
	DnBP (child)	DnBP (adult)	DEHP (child)	DEHP (adult)	DEHT (child)	DEHT (adult)
Inhalation gas phase	3.7×10^{-5}	1.7×10^{-5}	5.6×10^{-7}	2.6×10^{-7}	1.1×10^{-7}	5.2×10^{-8}
Inhalation particle phase	1.2×10^{-6}	5.4×10^{-7}	1.6×10^{-5}	7.5×10^{-6}	3.6×10^{-6}	1.6×10^{-6}
Dermal absorption from air	1.9×10^{-4}	8.8×10^{-5}	3.5×10^{-6}	1.6×10^{-6}	6.5×10^{-7}	3.0×10^{-7}
Dust ingestion	1.5×10^{-4}	8.7×10^{-6}	2.4×10^{-5}	1.4×10^{-6}	4.9×10^{-6}	2.8×10^{-7}
Total	3.8×10^{-4}	1.1×10^{-4}	4.5×10^{-5}	1.1×10^{-5}	9.3×10^{-6}	2.3×10^{-6}

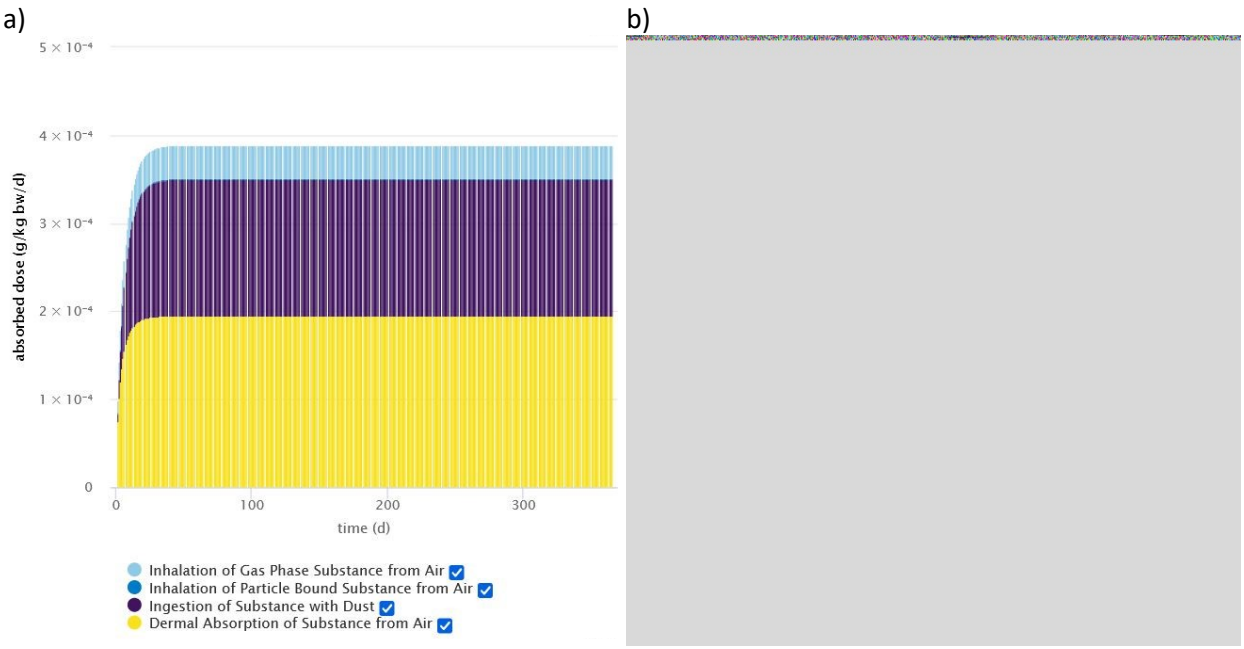

Figure S9: Absorbed dose of DnBP by adsorption pathway for a) a child and b) an adult as calculated by the DustEx tool for 365 days of exposure.

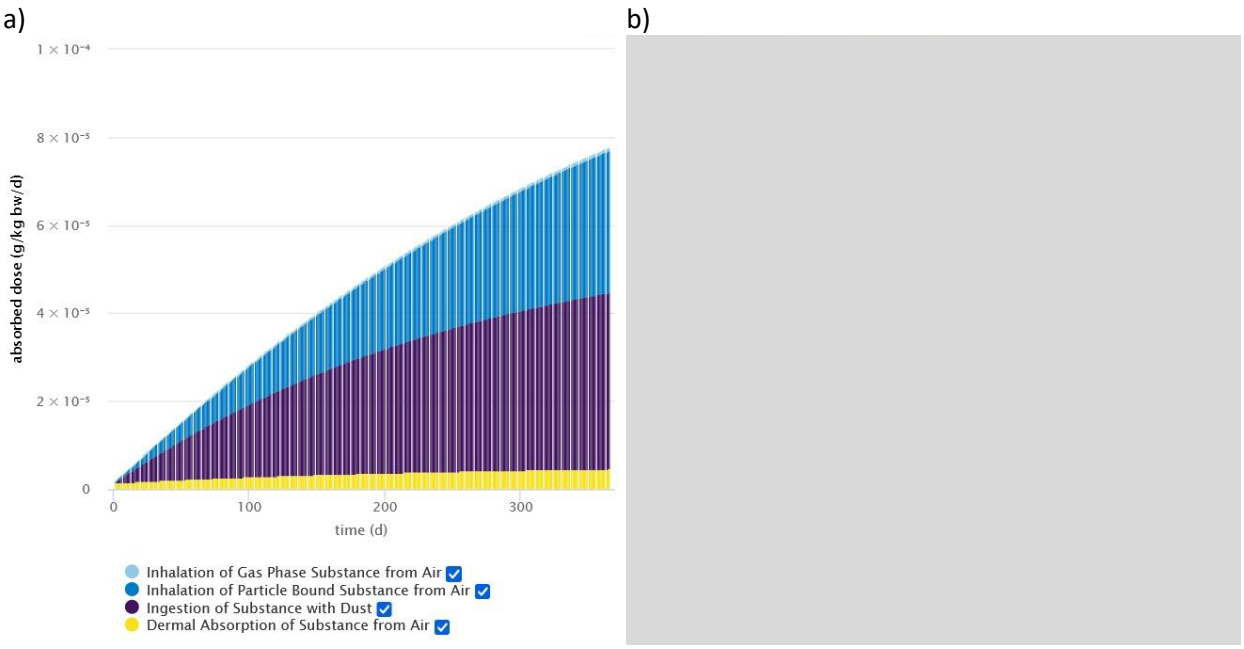

Figure S10: Absorbed dose of DEHP by adsorption pathway for a) a child and b) an adult as calculated by the DustEx tool for 365 days of exposure.

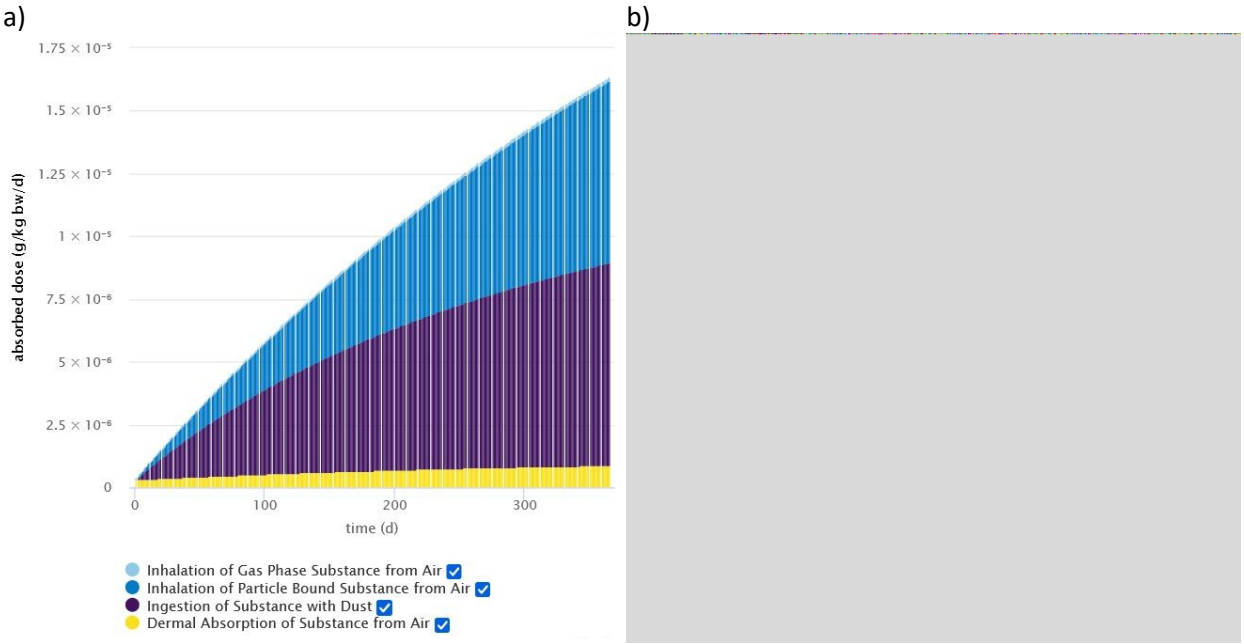

Figure S11: Absorbed dose of DEHT by adsorption pathway for a) a child and b) an adult as calculated by the DustEx tool for 365 days of exposure.

References

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