

It is important to quantify the gas phase/particulate phase partitioning because when passive sampling is employed to measure SCCPs since passive sampling does not collect the particulate fraction. Sampling at temperatures less than 283.1 K has significant consequences when only gas phase SCCP measurements are made and may lead to lower observed concentrations compared to the actual concentrations. This is particularly true for passive sampling, where the particulate fractions of SCCPs are not measured.

Active versus passive sampling

SCCP concentrations were measured in parallel using active and passive sampling techniques over a 12-month period in 2013. The observations are presented in Fig. 2. The active and passive samplers were co-located at the Aspendale site within 5 metres from each other. The active samples were collected at monthly periods, and the passive samples were collected over three 3-monthly periods one 6-monthly period and one 12-monthly period.

The active samples are converted to atmospheric concentrations using:

$$C_A = \frac{N_{PUF}}{Ft} \quad (1)$$

where C_A = atmospheric concentration of SCCPs from the active sample (ng m^{-3}), N_{PUF} = SCCP mass on the sampler (ng sampler^{-1}), t = time (days), F = volumetric flow rate through the active sampler, m^3 per day where the volume is at STP.

As the active and passive samples were collected over the same time period and at the same location, it is possible to use this data to determine the absorption rate of SCCPs by the passive samplers, a quantity not readily available from theoretical considerations. The absorption rate was calculated from (2) as suggested in a previous study.^[6]

$$R_{PUF} = \frac{N_{PUF}}{C_A t} \quad (2)$$

where R_{PUF} = absorption rate of SCCPs by the PUF disk ($\text{m}^3 \text{day}^{-1}$), N_{PUF} = SCCP mass on the sampler (ng sampler^{-1}), C_A = atmospheric concentration of SCCPs from the active sample (ng m^{-3}), t = time (days).

The absorption rates were calculated for the 3 and 6 monthly sampling periods and the results averaged give an uptake rate of $3.4 \pm 1.2 \text{ m}^3 \text{day}^{-1}$, where the uncertainty is the standard error of the mean. Table S3 gives passive uptake rates for SCCPs calculated from this and a previous study. The estimation from the study in China, Japan and South Korea is $4.2 \text{ m}^3 \text{day}^{-1}$, and is not significantly different from this study^[6]. In another study^[3], the uptake rate is established as $17.1 \text{ m}^3 \text{day}^{-1}$; about a factor of 4 higher than the other two studies. However, in that study^[3] the active concentration C_A was assumed, rather than measured over the period of passive sampling. Therefore, the estimate is less well constrained because of the uncertainty of using an estimated rather than measured concentration in the uptake estimate.

Contamination study

During this study sampling was conducted inside 10 dwellings. The question arose whether SCCPs were present in the pump exhaust. For the samples collected indoors, where the pump exhausted directly in the room, any SCCPs in the pump exhaust had the potential to increase the SCCPs mass on the filter/PUF sampler.

In order to quantify any possible increase in SCCPs concentration due to the exhaust, a sampling procedure using four POPs samplers, was carried out in March 2010 at the Aspendale site in suburban Melbourne.

Fig. S1 shows the arrangement of the four samplers. Sampler 1, a blank, was located about 30 metres from samplers 2 and 3 (Fig. S1). The pump exhaust from sampler 2 was directed to the inlet of sampler 3. The exhaust was placed close to the inlet but not physically connected to it, so that air could flow into the sampler in a normal way. Thus ambient air could also be sampled. This ensured that sampler 3 was sampling a mixture of pump exhaust and ambient air. Sampler 2 was sampling ambient air, as was sampler 4, which was located about 50 metres from samplers 2 and 3. The blank was left in the sampler for the 7-day period, but the pump was not turned on.

Table S4 shows the results of the sampling procedure designed to measure any effect on SCCPs concentration due to the exhaust from the sampling pump. Table 4 shows that at $<0.06 \text{ ng m}^{-3}$ the blank is low, but not zero. It shows, in Table 4, that at the blank is low, and less than 1% of the sample concentrations. The SCCPs concentration measured on the ambient plus exhaust sample was 10.5 ng m^{-3} compared to 15.7 ng m^{-3} measured on the co-located ambient sample. The fourth sampler measured 11.1 ng m^{-3} in ambient air, a concentration close to that measured on the ambient plus exhaust sample. These results show that there was no increase in concentration due to contamination from the pump exhaust, even when the sampler was directly sampling exhaust from a co-located sampler. The result in the ambient plus exhaust sample is consistent with $\frac{1}{3}$ of the volume sampled being exhaust and $\frac{2}{3}$ of the volume sampled being ambient air with a SCCP concentration of 15.7 ng m^{-3} as observed by the co-located sampler. The concentrations of the SCCPs measured inside and outside of the 10 dwellings can then be assumed to be entirely free of contamination from exhaust from the sampling pump.

Repeatability

During the period of this study, five samples were collected in duplicate to assess the repeatability of the results. The samples were collected over the same time periods by samplers located within one metre of each other, and are presented in Table S5. The repeatability was assessed as a Pearson correlation coefficient with a value of 0.93 which is significant at the 1% level for a single sided test.

Inter-comparison study

The extraction and chemical analysis of SCCPs is quite complex, and the techniques were newly developed in Australia therefore an inter-comparison was conducted with an established laboratory, the Norwegian Institute for Air Research, (NILU) Kjeller, Norway. To achieve this, four samples and two blanks were collected using two co-located PUF samplers over a period of about 7 days. Two samples and one blank were collected from each sampler. After sampling was complete the filters and PUF samples were stored at $-10\text{ }^{\circ}\text{C}$ until they were ready to be shipped to the laboratories for analysis. One set of two samples and one blank were sent to NMI where they were extracted and analysed with the techniques described previously. The other set of two co-located samples and blanks were sent to NILU where they were extracted and analysed using the techniques they have employed previously to analyse SCCPs.^[7, 8]

The data in Table S6, presented previously^[9], show the results of the inter-comparison. The blank concentrations were low compared with the samples. The concentrations of the samples analysed at NILU were 4.8 ng m^{-3} and 12.7 ng m^{-3} , while the corresponding results from NMI were 6.3 ng m^{-3} and 4.8 ng m^{-3} . The concentrations reported by NMI are reported as equivalent to 55.5% whereas the NILU results are for the total SCCPs concentration for the sample. The differences in the SCCPs concentrations include contributions due to differences in: sampling, storage, extraction and the analytical techniques used by the two laboratories. The results in Table S6 have differences greater than expected from the repeatability of a single laboratory as determined previously. The results in Table S6 are consistent with a previous inter-comparison^[2] where the ratios of concentrations of SCCPs determined by individual laboratories on an unknown SCCP mixture (when standards of individual SCCPs were provided) ranged from 0.7 to 4.1 times the target concentration and the CVs of results between laboratories was 56%. Overall, the SCCPs determined in this study are consistent with the international accepted standards for SCCP measurements. Table S7 presents the concentrations of SCCPs measured using active and passive sampling in Melbourne during 2013. Table S8 gives some details of the 10 dwellings employed to measure concentrations of SCCPs measured indoors and outdoors in Melbourne during summer 2009.

Table S9 provides the details of SCCP air concentrations from measurements in background, rural and urban/industrial sites and indoor environments which are cited in previous studies. Table S10 provides the details of SCCP soil and air concentrations in the Pearl River Delta, as used in this paper. Table S11 lists selected physical properties of some individual SCCPs.

Soil Moisture Values

Soil moisture values are taken from the Australian Bureau of Meteorology at www.bom.gov.au/water/landscape. Soil moistures are measured in % saturation at the root zone, 0 – 1 metre soil

depth. This study uses % soil moisture in correlations with various parameters and gas concentrations. The correlations are given in Table 2 of the main document. The soil moistures are employed for the particular sampling periods, and are the average values of six sites that were chosen to spatially represent the Melbourne area. The latitude and longitude of the six sites are shown in Table S12.

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Table S1. Physical characteristics of the 10 dwellings employed in the study

Dwelling	Attached Garage	Occupied	Age of dwelling years	Construction	Latitude degrees	Longitude degrees
1	No	No	49	Brick veneer	37.783	145.330
2	No	No	65	Double brick	37.897	145.076
3	No	Yes	16	Double brick	37.896	145.049
4	Yes	Yes	4	Weatherboard	38.167	145.191
5	No	No	7	Brick veneer	37.874	145.126
6	No	No	75	Double brick	37.889	145.005
7	No	No	76	Double brick	37.904	145.010
8	Yes	Yes	31	Brick veneer	38.024	145.109
9	No garage	Yes	75	Double brick	37.916	145.002
10	Yes	Yes	12	Brick veneer	37.902	145.011

Table S2. Percentage of SCCPs in gas and particulate phases

Concentrations of SCCPs in particles and gas are ng m^{-3} . NM, not measured; NG, not given

Season	Particle	PUF 1	Resin	PUF 2	Total gas	Total	Gas %	Particle %	Temp [⌘] K
Autumn [*]	1.01	NM	NM	NM	8.29	9.30	89	11	293.5
Winter [*]	0.27	NM	NM	NM	2.43	2.70	90	10	285.2
Spring [*]	0.40	3.09	0.23	0.06	3.38	3.78	89	11	287.4
Winter ^[5]	NG	NG	NG	NG	NG	NG	67	33	271.3
Summer ^[5]	NG	NG	NG	NG	NG	NG	94	6	299.2
Summer ^[4]	NG	NG	NG	NG	NG	NG	95	5	Unknown
Spring ^[3]	NG	NG	NG	NG	NG	NG	91	9	282.4

*This study

⌘Average temperature during sampling period

Table S3. Calculated passive uptake rates for SCCPs

Location	Absorption rate m ³ day ⁻¹	Notes	Reference
China, Japan, South Korea	4.2	Calculated from comparison of total mass collected on active sampler and total mass on passive sampler	[6]
Aspendale, Melbourne	3.2 ±0.9	Calculated from comparison of total mass collected on active sampler and total mass on passive sampler	This study

Table S4. Concentrations of SCCPs measured in a blank sample, ambient air sample and ambient air plus exhaust air sample during March 2010

Sample number	Sample type	SCCPs ng m ⁻³	Location
1	Blank	<0.06	30m away from 2&3
2	Ambient	15.7	Co-located
3	Ambient plus exhaust	10.5	Co-located
4	Ambient	11.1	50m away from 2&3

Table S5. Co-located paired SCCP samples

Sample	Month	year	Sample A ng m ⁻³	Sample B ng m ⁻³	Repeatability ^{II}
1	February	2013	16.3	21.6	28.0
2	May	2013	9.0	5.9	41.9
3	August	2013	1.0	2.7	89.6
4	September	2013	3.0	3.8	25.7
5	March	2010	15.7	11.1	34.3
Average			7.9	9.0	38.3
Blank [#]			0.5		

$$^{\text{II}} \text{ Repeatability} = \frac{\text{abs}(\text{Sample A} - \text{Sample B}) \times 100}{\text{mean}(\text{of A \& B})}$$

[#]based on an average blank level and a typical air volume.

Table S6. Concentrations of SCCPs measured in two ambient samples and one blank sample analysed at NMI and NILU

Sample On	Sample Off	Sample type	SCCPs NMI ng m ⁻³	Uncertainty ng m ⁻³	SCCPs NILU ng m ⁻³	Uncertainty ng m ⁻³
01/10/2010 18:18	08/10/2010 17:50	Blank	<0.86		0.14	
13/09/2010 12:47	24/09/2010 10:35	Ambient	6.3	±2.5	4.8	±1.9
24/09/2010 12:35	01/10/2010 17:12	Ambient	4.7	±1.9	12.7	±5.1

Table S7. Concentrations of short chain chlorinated paraffins observed at Aspendale during 2013

Date on	Date off	SCCPs ng m ⁻³
<i>Active samples</i>		
07/01/13	08/02/13	28.4
08/02/13	05/03/13	18.9
05/03/13	02/04/13	9.3
02/04/13	30/04/13	3.3
30/04/13	31/05/13	7.4
31/05/13	28/06/13	4.2
28/06/13	30/07/13	2.2
30/07/13	03/09/13	1.9
03/09/13	01/10/13	3.4
01/10/13	04/11/13	5.7
04/11/13	03/12/13	18.6
03/12/13	06/01/14	20.5
annual median		6.6
annual average		10.4
st deviation		8.8
maximum		28.4
minimum		1.8
<i>Passive samples</i>		
07/01/13	03/04/13	11.7
28/06/13	01/10/13	3.6
01/10/13	06/01/14	13.0
28/06/13	06/01/14	9.7

07/01/13	06/01/14	8.4
annual average		8.4

Table S8. Concentration of SCCPs measured indoors and outdoors of 10 dwellings

Dwelling	Date on	Date off	SCCPs ng m ⁻³ indoors	SCCPs ng m ⁻³ outdoors	Indoor : outdoor ratio	Occupied during sampling	Age years
1	31/12/08	07/01/09	21.0	45.7	0.46	No	49
2	02/01/09	09/01/09	25.9	35.1	0.74	No	65
3	08/01/09	15/01/09	25.9	56.4	0.46	Yes	16
4	12/01/09	19/01/09	28.2	30.1	0.94	Yes	4
5	20/01/09	27/01/09	23.4	70.2	0.33	No	7
6	21/01/09	28/01/09	43.4	82.0	0.53	No	75
7	29/01/09	05/02/09	60.6	81.6	0.74	No	76
8	30/01/09	06/02/09	32.1	28.2	1.14	Yes	31
9	09/02/09	16/02/09	17.3	35.2	0.49	Yes	75
10	10/02/09	17/02/09	21.7	28.4	0.76	Yes	12
Average			30.0	49.3	0.61		
Median			25.9	40.5	0.63		
Maximum			60.6	82.0			
Minimum			17.3	28.2			

Table S9. Concentrations of SCCPs in background, rural and urban sites from previous studies

Site	Min ng m ⁻³	Max ng m ⁻³	Mean ng m ⁻³	SD ng m ⁻³	No. obs	Sampling type	Reference	
Background								
Egbert, Canada, 1990	0.065	0.924	0.543		120	Hi-vol filter+PUF	[10]	
Alert, Canada, 1992	<0.001	0.0085				Hi-vol filter+PUF	[11]	
Alert, Canada, 1994 –1995	0.0011	0.0072				Not given	[12]	
Svalbard, Norway, 1999	0.009	0.057	0.019	0.008	5	Hi-vol filter+PUF	[7]	
Fildes Peninsula, Antarctica, 2013	0.0096	0.0208	0.0149	4.1	24	Hi-vol filter+PUF	[13]	
Bear Island, Norway, 2000	1.8	10.6	6.0	3.4	7	Hi-vol filter+PUF	[8]	
Range — background	<0.001	0.924						
Rural								
Lancaster, U.K., 1997	0.0054	1.085	0.320	0.320	26	Hi-vol filter+PUF	[4]	
Lancaster, U.K. 1997/98			0.099			Not given	[14]	
Lancaster, U.K., 2003	<0.18	3.40	1.10	1.00	20	Hi-vol filter+PUF	[3]	
Various sites, U.K., 2003*	0.15	2.24	0.60	0.56	20 sites	Passive PUF	[3]	
Sites CNU5 and CNU18, China, 2008#	8	60	43.7		18 sites	18 sites	Passive PUF	[6]
Site JAU2 and JAU11, Japan, 2008#	0.35	0.94	0.70		12 sites	12 sites	Passive PUF	[6]
Sites SKR1 and SKR5, South# Korea, 2008#	0.79	1.08	0.87		7 sites	7 sites	Passive PUF	[6]
Range — rural	0.005	60						
Urban/industrial								
Various sites, U.K., 2003*	0.55	6.37	2.03	1.93	20 sites	Passive PUF	[3]	

Site	Min ng m ⁻³	Max ng m ⁻³	Mean ng m ⁻³	SD ng m ⁻³	No. obs	Sampling type	Reference
Various sites, China, 2008 [#]	13.5	517	143	106	18 sites	Passive PUF	[6]
Various sites, Japan, 2008 [#]	0.3	14.8	2.9	3.4	12 sites	Passive PUF	[6]
Various sites, South Korea, 2008 [#]	0.6	9.4	2.5	2.4	7 sites	Passive PUF	[6]
Melbourne, Australia, 2008 - 2013	1.9	82.0	24.3	24.1	27	Hi-vol filter+PUF	This study
Pearl River Delta, China, summer, 2009/2010	2.01	106	29.5	28.4	14 sites	Passive PUF	[15]
Pearl River Delta, China, winter, 2009/2010	0.95	26.5	5.2	3.8	14 sites	Passive PUF	[15]
Beijing, China, Winter, 2011	1.9	33	7.7	6.7	14	Hi-vol filter+PUF	[5]
Beijing, China, Summer, 2011	112	332	200	57	23	Hi-vol filter+PUF	[5]
Melbourne, Australia, 2008–2013	1.9	82.8	24.4	24.1	27	Hi-vol filter+PUF	This study
<hr/>							
Range — urban/industrial	0.6	517					
<hr/>							
Indoor air							
Lancaster, UK, workshop, 2003* Lab, office house	0.2	11.9	3.6	5.5	4	Passive PUF	[3]
Stockholm, Sweden, 2006/07	2	147	49	35	44	Low-vol filter+PUF	[16]
Melbourne, Australia, 2009	17	61	30	13	10	Hi-vol filter+PUF	This study
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Range	0.2	61					

*Calculated from reference [3], assuming a sampling rate of 17 m³ day⁻¹.^[3]

[#]calculated from Figs 2 and 3.^[6]

N: number of samples or sites

Table S10. Soil and air concentrations of SCCPs, ratios and references

Values are either mean \pm two standard deviations or mean (range) or when indicated by the superscript §, the median

Location	Soil ng g ⁻¹	Air ng m ⁻³	Soil/Air ratio m ³ g ⁻¹	Reference
Pearl River Delta ^[6]	12.1 \pm 4.4 (2008)	18.2 \pm 9.1 (2008)	1.0 \pm 0.3	Wang, Y. et al. (2013)

Table S11. Physical properties of SCCPs

SCCP	Molecular weight	HL Pa m ³ mol ⁻¹	V _p 25°C Pa	K _{ow}	Sw μg l ⁻¹	Boil pt °C
1,10 dichlorodecane	211				257	275
1,10 dichlorododecane	239	499	5.0×10 ⁻¹			168
1,12 Dichlorododecane	239	648	6.8×10 ⁻²		22.4	
Trichlorododecane	273			5.85		
1,2,9,10 Tetrachlorodecane	280	17.7	2.8×10 ⁻²	5.93	328	
Tetrachlorodecane	280			6.04-6.20	141	
1,2,10,11 Tetrachloroundecane	294	6.3	1.0×10 ⁻²		575	
1,2,11,12 Tetrachlorododecane	308		3.5×10 ⁻³			
Pentachlorodecane (a+b)	314	4.9				
Pentachlorodecane (c+d)	314	2.6				
Pentachloroundecane (a+b)	328	1.46			546	
Pentachloroundecane (c+d+e)	328	0.68			962	
Pentachlorododecane (a+b)	342		5.4×10 ⁻³		449	
Pentachlorododecane (c+d)	342		4.0×10 ⁻³		657	
Pentachlorododecane	342	1.37	1.6×10 ⁻³ –1.9×10 ⁻³			
Hexachlorodecane	349		1.1×10 ⁻³ –2.2×10 ⁻³			
Hexachloroundecane	363		2.4×10 ⁻⁴ –4.9×10 ⁻⁴			
Hexachlorododecane	377		1.1×10 ⁻³ –2.2×10 ⁻³			
Hexachlorododecane	377	1.37	1.4×10 ⁻³ –5.2×10 ⁻³			

K_{ow} of SCCPs ranges from 5.16 to 8.12^[17] (Drouillard 1996 MSc thesis, Env Canada)

Vapour Pressure SCCPs: 2.8×10⁻⁷ – 0.066 Pa (Drouillard 1996 MSc thesis, Env Canada)

Water solubility: 0.49 – 1260 $\mu\text{g l}^{-1}$ (Drouillard 1996 MSc thesis, Env Canada)

Vapour Pressure SCCPs: 2.8×10^{-7} – 0.028 Pa^[18] (Env Canada)

Henry's Law Constant: 0.68 – 17.7 Pa m³ mol⁻¹ [18].

Water solubility: 6.4 – 2370 $\mu\text{g l}^{-1}$ [18].

K_{ow}: 4.39 – 8.69.

Table S12. Locations of sites employed for soil moisture

Soil moisture site	Latitude	Longitude
1	37.75	144.80
2	37.95	145.05
3	37.95	144.65
4	37.65	145.10
5	38.15	145.15
6	38.00	145.25

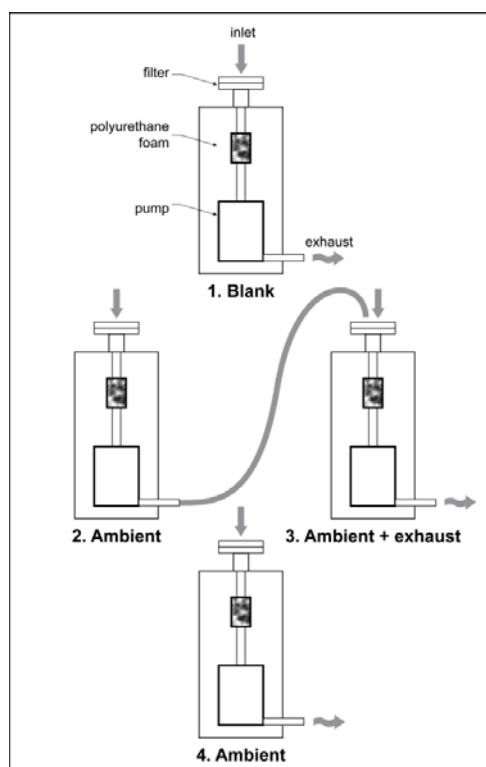


Fig. S1. The arrangement of samplers used in the exhaust study to identify and quantify any potential contamination.