Modeling of Short Chain Chlorinated Paraffins in the Nordic Environment

Ingjerd Sunde Krogseth[1,2], Knut Breivik[2,3], Martin Schlabach[2], Frank Wania[4], Jon Arnot[4]

1: University of Life Sciences, NO-1432 Ås, Norway, 2: Norwegian Institute for Air Research, P.O. Box 100, NO-2027 Kjeller, Norway, 3: University of Oslo, Department of Chemistry, P.O. Box 1033, NO-0315 Oslo, Norway, 4: Department of Physical and Environmental Sciences, University of Toronto, Scarborough, Canada

Introduction

- The understanding of the environmental behaviour of short chain chlorinated paraffins (SCCPs, $C_xH_{2x+2-y}Cl_y$) remains fragmented.
- SCCPs are often treated as "one" compound, but consist of 46 formula groups (CxCly, 10≤x≤13, 1≤y≤x) and thousands of isomers, which raises the question of their relative risk.
- The main purpose of this new project is to evaluate the understanding of the link between emissions and human exposure of SCCPs in the Nordic environment.
- Here, an initial benchmarking study has been performed for all 46 formula groups relative to seven PCBs, with evaluation of persistence (P), bioaccumulation (B) and long-range atmospheric transport potential (L_A).

Method

- A mechanistic, dynamic and integrated environmental fate and bioaccumulation multimedia model (CoZMoMAN) (Breivik et al., 2010), parameterized for the western part of the Baltic Sea drainage basin, was applied (Fig. 1).
- Each formula group of SCCPs was represented by one isomer. Physical-chemical properties were gathered from the scientific literature or estimated if necessary (Table 1).
- A hypothetical emission scenario was applied, using 1 t/yr to air for 70 years, followed by zero emission for 10 years.
- P was calculated as the percentage left in the physical environment after 10 years without emissions.
- B was evaluated by recording the concentration in a 29 year old female following 70 years of constant emissions.

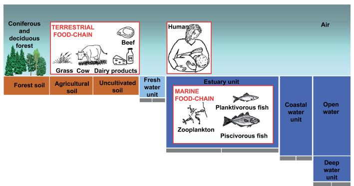

Figure 1: Illustration of the model CoZMoMAN.

- L_A was calculated as the characteristic travel distance (Bennett et al., 1998), i.e. the distance it takes for the air concentration to decrease to ≈37 % (1/e) of the initial concentration.

Results & discussion

- P of SCCPs are comparable to the least persistent of the PCBs (Fig. 2). P tends to increase with increasing degree of chlorination.
- SCCPs are comparable to PCBs with regard to L_A, but exhibit minor differences (Fig. 3). A more detailed analysis suggests that deposition rather than reaction limits L_A for most SCCPs.
- SCCPs appear to be less bioaccumulative than PCBs, but the results are highly sensitive to the input metabolism rate constants (Fig. 4). B tends to increase with increasing number of carbon- and chlorine atoms.

Further research

- Property data (Table 2, Fig. 4) remain uncertain. An uncertainty- and sensitivity analysis is therefore planned.
- In the next part of the project a realistic emission scenario will be applied, and results compared with measured environmental levels in the Nordic environment.

Acknowledgements

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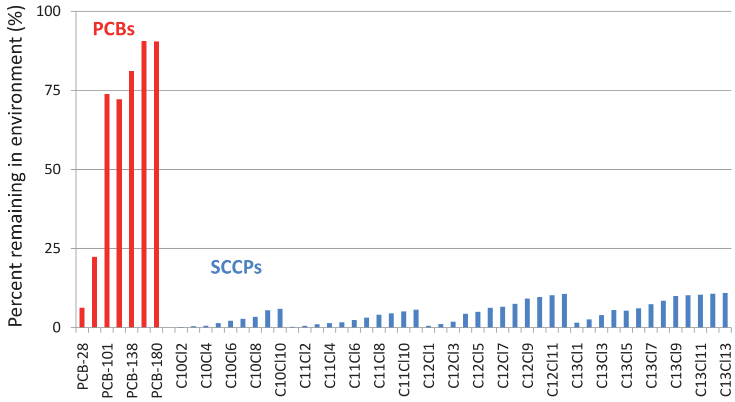

Figure 2: Persistence (% remaining in the physical environment after 10 years without emissions).

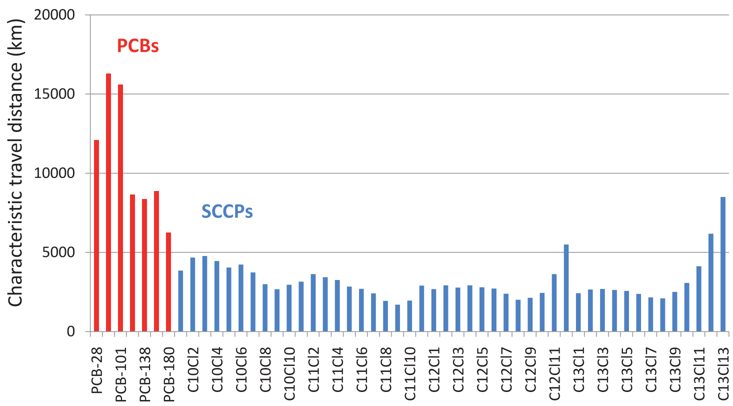

Figure 3: Long-range transport potential (in km).

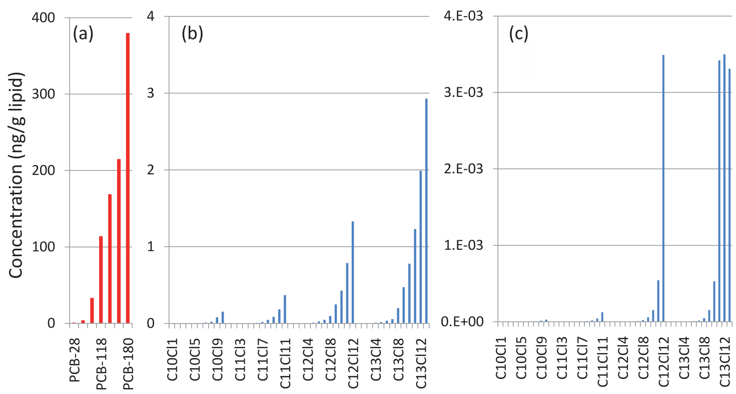

Figure 4: Concentration in a 29-year old female following 70 years of constant emissions (a) PCBs, (b) SCCPs based on estimated metabolism rate constants and (c) SCCPs based on experimental metabolism rate constants.

Table 1: Property data for SCCPs.

Property	Range of values	Reference
Log K_{ow}	4.6 – 7.4	Hilger et al., 2011; KOWWIN (Epiwin 4.1, Experimental Value Adjusted method)
Log K_{aw}	-6.7 – -0.8	Drouillard et al., 1998; KOWWIN (Epiwin 4.1, Experimental Value Adjusted method)
Heat of phase transfer (ΔU, J/mol)	ΔU_{ow} = -20 000 ΔU_{aw} = 60 000	Assumed values
Activation energy (J/mol)	Atmosphere: 10 000 Other compartments: 30 000	Assumed values
Atmospheric reaction rate (cm^3/molecules×sec)	$1.0 \cdot 10^{-12} – 1.3 \cdot 10^{-11}$	AOPWIN (Epiwin 4.1)
Environmental half-life (h)	Water/forest canopy: $2.2 \cdot 10^3 – 3.3 \cdot 10^3$ Soil: $4.5 \cdot 10^3 – 6.6 \cdot 10^3$ Sediment: $2.0 \cdot 10^4 – 3.0 \cdot 10^4$	Sediment: Derived from ECB, 2008; Water = 1/9 × sediment, soil = 2 × water
Metabolism rate constant (h^{-1})	Grass: $2.1 \cdot 10^{-4} – 3.1 \cdot 10^{-4}$ Fish: $2.2 \cdot 10^{-4} – 3.3 \cdot 10^{-1}$* or $4.5 \cdot 10^{-5} – 2.4 \cdot 10^{-3}$** Mammals: $1.1 \cdot 10^{-3} – 6.6 \cdot 10^{-1}$* or $3.1 \cdot 10^{-4} – 1.7 \cdot 10^{-2}$**	Grass: Derived from half-life in forest canopy; Fish: *Derived from Fisk et al., 2000; **BCFBAF (Epiwin 4.1); Mammals: 5 x rate constant in fish (Arnot et al., 2010)
Feces/blood partition coefficient	$2.0 \cdot 10^{-8}$	Moser and McLachlan, 2002; Czub and McLachlan, 2004

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