



Ecotoxicity assessment of short- and medium-chain chlorinated paraffins used in polyvinyl-chloride products for construction industry



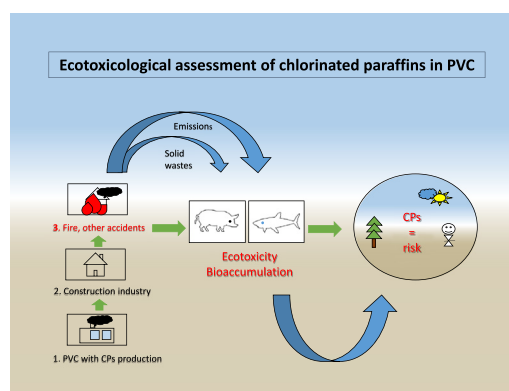
Klára Kobetičová*, Robert Černý

Department of Materials Engineering and Chemistry, Faculty of Civil Engineering, Czech Technical University in Prague, Thákurova 7, CZ-166 29 Prague, Czech Republic

HIGHLIGHTS

- SCCPs and MCCPs used in PVC production are toxic and bioaccumulative POPs.
- In this paper, ecotoxicity of SCCPs and MCCPs is assessed by two LCA methodologies.
- The results indicate potential ecological risks of MCCPs use in some PVC products.
- SCCPs in PVC should better be replaced by some inorganic materials than by MCCPs.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:

Received 31 January 2018

Received in revised form 20 April 2018

Accepted 24 May 2018

Available online 1 June 2018

Editor: Adrian Covaci

Keywords:

Short-chain chlorinated paraffins
Medium-chain chlorinated paraffins
Polyvinyl chloride
Construction
Ecotoxicity

ABSTRACT

Short chain chlorinated paraffins (SCCPs) have been commonly used as plasticizers and flame retardants in polyvinyl-chloride (PVC) products for the construction industry. During the last few years the production of SCCPs has been banned or reduced in Europe, Japan, USA, and Canada due to their toxic and bioaccumulative effects but they have been still produced and used under less controlled conditions worldwide. Middle chain chlorinated paraffins (MCCPs) were suggested as a suitable alternative to SCCPs for PVC production instead. In this paper, the ecotoxicity of SCCPs and MCCPs is studied using the methods of potentially affected fraction of species (PAF) and the most sensitive species (MSS). Characterization factors (CFs) are estimated for SCCPs by the PAF method (for MCCPs suitable ecotoxicological indexes are not available) and for MCCPs by the MSS method (for SCCPs PEC values are negligible). Results of the present study indicate that from an ecotoxicological point of view, MCCPs may present similar ecological risks as SCCPs. Therefore, it is recommended both SCCPs and MCCPs not to be used worldwide in PVC products for the construction industry. The most suitable alternative for SCCPs seems to be inorganic compounds but their environmental impacts have not been sufficiently excluded yet.

© 2018 Elsevier B.V. All rights reserved.

1. Introduction

Polyvinyl chloride (PVC) is the third most commonly used plastic on the Earth, right after polyethylene and polypropylene. It is produced by

the polymerization process from vinylchlorine and for the first time it was synthesized in 1935. More than one half of the world-produced PVC is used in the construction industry for pipes, window and door frames, floor and roof coverings. PVC generally contains various additives for the improvement of its properties, such as fillers, plasticizers, flame retardants, and stabilizers.

Short chain chlorinated paraffins (SCCPs) and middle chain chlorinated paraffins (MCCPs) belong to the most frequently used plasticizers

* Corresponding author.

E-mail addresses: klara.kobeticova@fsv.cvut.cz, (K. Kobetičová), cernyr@fsv.cvut.cz (R. Černý).

and flame retardants at the PVC production worldwide (Glüge et al., 2016). SCCPs are polychlorinated C10–C13-alkanes and MCCPs with C14–C17 have a chlorination degree varying from 30% to 70% (w/w) (EURAR, 2008). Similarly to other halogenated flame retardants, the efficacy of SCCPs and MCCPs consists in interfering with the key reaction of combustion where free hydrogen and hydroxyl radicals react with oxygen. They release halogen atoms into the gaseous phase before the material reaches the ignition temperature. Hydrogen being freed up from the burning material is then fixed with the halogen to form hydrogen-halogen. This process increases caking of the polymer, decreases the amount of volatile flammable products, and thus contributes to retarding of polymer burning (e.g., Petrová et al., 2015). Zhan et al. (2017) observed that SCCPs are evolved from PVC after heating to 100–200 °C; a one-hour thermal treatment caused a release of 1.9–10.7% of embedded SCCPs.

However, SCCPs and MCCPs belong to persistent organic pollutants and are classified as carcinogenic and persistent, bioaccumulative and toxic substances. SCCPs have higher acute and chronic toxicity than MCCPs but MCCPs are more bioaccumulative (ECB, 2008; Glüge et al., 2016; Xia et al., 2017a, 2017b) and more accumulative in the environment (ECB, 2008) due to their higher molecular size and relevant properties. SCCPs were also recommended for further evaluation because of their possible endocrine disruption role (Lassen et al., 2014).

The production and import of SCCPs has been prohibited in the EU (POPRC, 2016), Japan (WCC, 2014), and in the USA and Canada (van Mourik et al., 2016) but MCCPs are currently only listed as “priority substances” for risk assessment under the Council Regulation 793/93/EEC. All chlorinated paraffins are also listed as “priority substances” for the Water Framework Directive. On the international level, MCCPs along with SCCPs are controlled through the OSPAR Convention which protects the marine environment of the north-east Atlantic Ocean.

SCCPs are very stable and their release into the environment, which occurs not only during a fire of building structure but also at a common building usage and PVC processing and recycling (Zhan et al., 2017), will continue yet for a long time after their ban due to the large quantities of PVC produced before. In total, 2,200,000 t of SCCPs have been used between 1935 and 2015 (Glüge et al., 2016). The highest production volumes of SCCPs and MCCPs were reached after 2006, when China scaled up their production from 260,000 t/year in 2006 to 1,000,000 t/year in 2013 (Xu et al., 2014). Currently, SCCPs and MCCPs are still used as plasticizers and flame retardants or in other applications in Asia, Africa and the Americas (with the exception of USA and Canada) without any significant restriction and monitoring (Glüge et al., 2016; van Mourik et al., 2016). China, Russia, and India will thus probably remain the major producers and consumers of SCCPs and MCCPs also in the near future. Therefore, investigations on the ecotoxicity of SCCPs and MCCPs present an actual topic in environmental science and engineering.

Life cycle assessment (LCA) is a method to deal with the environmental impacts associated with products, substances, or service (ISO 14040; ISO 14044). Present LCA softwares include various methodologies for Life Cycle Impact Assessment (LCIA) and they are focusing on preferred impact categories. One of these impact categories is ecotoxicity. Environmental impacts can be assessed for freshwater environment (water or sediment), salt environment (water or sediment), or soil. The effect of comparing products, chemicals, or services in LCA is expressed by characterization factors (CFs) describing and quantifying the cause–effect chain of an emission of a substance to the environment.

In the presented study, two ecotoxicity modeling approaches are used. The first model is based on potentially affected fraction (PAF) of species (e.g., Goedkoop and Spriensma, 1999; Hauschild and Pennington, 2002; Pennington et al., 2004; Salieri et al., 2015) and uses endpoint or/and midpoint level. This concept has been used in the USEtox model (USEtox, 2017), that was developed under the umbrella of the United Nations Environment Program and the Society for Environmental Toxicology and Chemistry (Rosenbaum et al., 2008;

Hauschild et al., 2008). The PAF expresses the toxicity put on ecosystems due to the presence of a single chemical or a mixture of chemicals. In many studies based on PAF, the species sensitivity distribution (SSD) concept has been applied. This method uses the available toxicity data for different species with respect to a particular chemical to derive a joint sensitivity distribution, from which the fraction of potentially affected species is determined. Hazard concentration causing x -percentile effect (HC_x) is so derived. The most commonly used levels are HC_5 and HC_{50} . The first affecting 5% of species is considered as protective for the whole community (Smetanová et al., 2014). Characterization factors in the USEtox model are located at endpoint.

The second model is based on the most sensitive species (MSS) and its lowest ecotoxicological index value (lethal concentration, LC_x , or effective concentration, EC_x , where x means that this concentration affects $x\%$ of species, or no observed effect concentration, NOEC). This value is compared to modeled substance levels in an affected environment. Characterization factors in the MSS model reflect the damage on the ecosystem quality (species diversity changing) and are located somewhere along the cause–impact pathway, typically at the point after which the environmental mechanism is identical for each environmental flow assigned to that impact category (ISO 14040; ISO 14044).

The PAF- and MSS-based models are applied for the ecotoxicity assessment of SCCPs and MCCPs used in PVC products for the construction industry and the obtained results are discussed. The ecotoxicological data on SCCPs and MCCPs are used for the calculation of both acute and chronic points, based on the toxicity data for different trophic levels. Limitations of both types of models are discussed and possible improvements are proposed. Alternatives to SCCPs and MCCPs for PVC products are suggested as well.

2. Methods

2.1. Concept of potentially affected fraction (PAF) of species

The most widespread endpoint model USEtox (USEtox, 2017) estimates the characterization factor (CF) of a substance for the impact category of freshwater ecotoxicity as:

$$CF = EF \times FF \times XF \quad (1)$$

where EF ($PAF \cdot m^3 \cdot kg^{-1}$) is the effect factor that represents the ecotoxicity and which is expressed in terms of potentially affected fraction of species, FF (day) is the fate factor which expresses the residence time of a substance in a particular environmental compartment (freshwater), XF (dimensionless) is the exposure factor which is the fraction of a chemical dissolved in freshwater (Rosenbaum et al., 2008; Larsen and Hauschild, 2007a, 2007b).

2.1.1. Effect factor

The effect factor can be generally defined as

$$EF = 0.5 / HC_{50_{EC/LC50}} \quad (2)$$

where $HC_{50_{EC/LC50}}$ is the concentration at which 50% of included species is exposed above their chronic EC_{50} or LC_{50} level. In this study, the EF of SCCPs was estimated using ecotoxicity values from previously published studies on freshwater organisms representing the three trophic levels recommended by the USEtox model (algae, crustacean, fish) (Larsen and Hauschild, 2007b). The ecotoxicity data for PAF derivation were collected from IUCLID Chemical Data Sheets and complemented with published data (Table 1). Only acute or chronic LC/EC_{50} values for the endpoints of growth, biomass, mortality, and immobilization from tests were used. In the case of multiple EC_{50} values per one species (*D. magna*, see Table 1), the geometric mean was used. Acute LC_{50} values were divided by 2 (Rosenbaum et al., 2008). Chronic NOEC data were

Table 1
Ecotoxicological data (EC₅₀, LC₅₀) of SCCPs for CF calculation based on USEtox.

Species	SCCPs	Endpoint	Concentration (mg·l ⁻¹)	Source
<i>Freshwater environment</i>				
<i>Fish</i>				
<i>O. mykiss</i>	C10–12, 58% CI	60 d-LC ₅₀	0.34 mg·l ⁻¹	Madeley and Maddock, 1983
<i>Invertebrates</i>				
<i>D. magna</i>	C10–13, 62% CI	48 h-EC ₅₀	0.14 mg·l ⁻¹	Koh and Thiemann, 2001
<i>D. magna</i>	C10–12, 58% CI	48 h-EC ₅₀	0.53 mg·l ⁻¹	Thompson and Madeley, 1983a
<i>D. magna</i>	C10–13, 62% CI	48 h-EC ₅₀	0.075 mg·l ⁻¹	Koh and Thiemann, 2001
<i>D. magna</i>	C10–12, 58% CI	72 h-EC ₅₀	0.024 mg·l ⁻¹	Thompson and Madeley, 1983a
<i>D. magna</i>	C10–12, 58% CI	96 h-EC ₅₀	0.018 mg·l ⁻¹	Thompson and Madeley, 1983a
<i>D. magna</i>	C10–12, 58% CI	120 h-EC ₅₀	0.014 mg·l ⁻¹	Thompson and Madeley, 1983a
<i>Algae</i>				
<i>Selenastrum capricornutum</i>	C10–12, 58% CI	96 h-EC ₅₀	3.7 mg·l ⁻¹	Thompson and Madeley, 1983a,b
<i>S. capricornutum</i>	C10–12, 58% CI	7 d-EC ₅₀	1.6 mg·l ⁻¹	Thompson and Madeley, 1983a,b
<i>S. capricornutum</i>	C10–12, 58% CI	10 d-EC ₅₀	1.3 mg·l ⁻¹	Thompson and Madeley, 1983b

not used because of the scarcity of data and major uncertainties related to NOEC derivation (e.g., Smetanová et al., 2014).

Table 1 contains results for SCCPs only. The data for the effective concentrations (expressed as EC₅₀ or LC₅₀ values) of MCCPs were not found in the literature. Therefore, PAF and CF values could not be calculated for MCCPs.

2.1.2. Exposure factor

The exposure factor is defined as

$$X_{F_{\text{freshwater}}} = \frac{1}{1 + (K_p \times \text{SUSP} + K_{oc} \times \text{DOC} + \text{BCF} \times \text{BIOMASS})/1,000,000} \quad (3)$$

where K_p is the partition coefficient between water and suspended solid (l·kg⁻¹), SUSP is the suspended matter concentration in freshwater, K_{oc} is the partition coefficient between dissolved organic carbon and water, DOC is the dissolved organic carbon concentration in freshwater, BCF is a bioconcentration factor in fish (l·kg⁻¹) and BIOMASS is a biota concentration in water.

Most of the parameters included in the exposure factor calculation (K_p, SUSP, DOS, BIOMASS) are local and most appropriate for case studies. Nevertheless, USEtox contains constant values for these parameters, except for K_p. They are given in Table 2. As the K_p value for SCCPs was not available, the value of 1 was used instead of K_p to avoid affecting the result; SCCPs are persistent in water but they can be absorbed into a sediment.

2.1.3. Fate factor

The fate factor links the quantity released into the environment to the concentration or mass occurred in a given compartment (Rosenbaum et al., 2008; Hauschild et al., 2008). This analysis is mandatory based on substance information, such as molecular weight, K_{ow} (octanol/water partition coefficient), K_{oc}, vapor pressure, solubility in water, and degradation rate in the concrete environmental compartments. The nested model adopted by USEtox has been usually applied in recent scientific studies (e.g., Salieri et al., 2015; Plouffe et al., 2016). Rate constants between compartments were used in the

Table 2
USEtox data for the calculation of the exposure factor of SCCPs.

SUSP	15 mg·l ⁻¹
DOC	5 mg·l ⁻¹
BIOMASS	1 mg·l ⁻¹
K _{oc}	1.26·K _{ow}
BCF (fish)	0.05·K _{ow}

mathematical matrix for the calculation of FF freshwater value based on the USEtox model (Rosenbaum et al., 2007). The basic physico-chemical properties and partition coefficients of SCCPs for the calculation of FF are listed in Table 3.

2.2. Concept of the most sensitive species (MSS)

The concept of the most sensitive species is based on a calculation of the predicted no effect concentration (PNEC) using the effective concentration value from the chronic test on the most sensitive species. This concept was used, e.g., in EDIP 97 and EDIP 2003 (Potting and Hauschild, 2004) or Institute of Environmental Sciences (CML) of Leiden University (Guinée et al., 2002). The CFs for SCCPs have never been calculated by any of the mentioned models. Therefore, estimations based on the CML methodology (Hauschild and Potting, 2004) were used in the present study. The CF for individual freshwater compartment was estimated according the following formula (Guinée et al., 2002):

$$CF = \frac{\frac{PEC}{PNEC} (CPs)}{\frac{PEC}{PNEC} (\text{reference substance})} \quad (4)$$

where PEC (predicted environmental concentration) is based on the modeled substance concentration/mass level expressed as emissions into the concrete environmental compartment per year. The NOEC/EC_{10–50} value is used for PNEC calculation, when the selected value is divided by the uncertainty factor of 1–1000 (EC, 2003). PNEC is expressed

Table 3
Physico-chemical properties of SCCPs and partition coefficients for the calculation of the fate factor.

SCCPs properties	Unit	Source
Molecular weight	176.4–630.2 g·mol ⁻¹	Příbylová et al., 2006
K _{ow}	~100,000	ECB, 2008
K _{oc}	1,995,226 l·kg ⁻¹	Příbylová et al., 2006
K _{doc}	~8000 l·kg ⁻¹	USEtox
BCF (fish)	7816 l·kg ⁻¹	ECHA, 2018
Water solubility (25 °C)	0.15–0.47 g·l ⁻¹	ECB, 2008
Vapor pressure (40 °C)	0.021 Pa	Příbylová et al., 2006
Biodegradability	1630 days	ECB, 2008
Half-time in air	0.81–10.5 days	POPRC, 2015
Half-time in sediment	~1 year	POPRC, 2016
Degradation rate in air	3.97 × 10 ⁻⁶ s ⁻¹	Muir et al., 2000
Degradation rate in water	1.37 × 10 ⁻⁷ s ⁻¹	Muir et al., 2000
Degradation rate in sediment	2.10 × 10 ⁻⁷ s ⁻¹	BIOWIN 3 model in EPISuite recommended in USEtox
Degradation rate in soil	4.46 × 10 ⁻⁸ s ⁻¹	Muir et al., 2000

as reciprocal value (1/PNEC) for CPs as well for reference substance (Guinée et al., 2002; Kočí, 2009):

$$CF = \frac{PEC \times PNEC \text{ (CPs)}}{PEC \times PNEC \text{ (reference substance)}} \quad (5)$$

In accordance with some recommendations for ecotoxicological analyses of persistent organic pollutants (e.g., Guinée et al., 2002; ČSN EN ISO 14040), pesticide 1,4-DCB was selected as the reference substance in the present study. The data for the calculation of CFs using the MSS concept are given in Table 4.

3. Results

3.1. PAF method

USEtox database contains various factors or PAF values for several thousands of compounds (mostly organic non-ionic substances). However, the environmental factors for any chlorinated paraffins (CP) are not included. All CPs have the same mode of action. Therefore, if less than five values were available (all species except freshwater crustacean *D. magna*), the PAF values were estimated according to Aldenberg and Luttik (2002) where the authors used different substances with the same toxic mode of action (we used toxicity values of CPs with varied properties). Acute EC₅₀ values were transformed to chronic values using the acute to chronic factor of 2 (USEtox, 2017).

The HC₅₀, EF, XF, FF, and CF values for the freshwater environment are presented in Table 5. HC₅₀ values were estimated on trophic level, not species level due to the lack of model species (Larsen and Hauschild, 2007a, 2007b). The calculations performed using the data in Table 1 showed 1 toxic value for fish, 7 toxic values for crustacean, 3 toxic values for algae. XF value was estimated using the values given in Tables 2, 3, based on the USEtox model, version 2.02 (USEtox, 2017). SCCPs have a relatively wide range of Kow values (Table 3); Kow = 100,000 was used for the estimation of XF in this study. FF was calculated using the USEtox model and data in Table 3.

3.2. MSS method

The CFs (Table 6) were calculated using the formulas given in the USES-LCA methodology (Guinée et al., 2002); the PEC and PNEC values were taken from the literature (Table 4). In the calculations, the values corresponding to flame retardants application (EURAR, 2008) or the lowest values were used when a possibility of selection occurred. The CF for freshwater environment was estimated in the range of 30×10^{-9} kg 1,4-DCB-eq·kg⁻¹ to 300×10^{-9} kg 1,4-DCB-eq·kg⁻¹ and the CF for soil in the range of 0.07×10^{-6} kg 1,4-DCB-eq·kg⁻¹ to 1.75×10^{-6} kg 1,4-DCB-eq·kg⁻¹. SCCPs emissions into the environment were negligible in the case of PVC, in contrast to other SCCPs applications (EURAR, 2008). For this reason, the CF could not be calculated (effectively, it could be considered close to zero).

Table 5

The average log HC₅₀, effect factor (EF), exposure factor (XF), fate factor (FF), and characterization factor (CF) for SCCPs in freshwater environment.

Average log HC ₅₀ (based on mg·l ⁻¹)	EF (PAF·m ³ ·kg ⁻¹)	XF (–)	FF ^a (day)	CF ^a (PAF·m ³ ·day·kg ⁻¹)
–0.539	1730	0.227	9.64–10.10	3790–3950

^a SCCPs consist of a mixture of compounds with various properties. Therefore, FF and CF were calculated for the lowest and the highest values of characteristic properties (molecular weight, water solubility).

4. Discussion

Generally, SCCPs have a high ecotoxicity and bioaccumulation potential (see Tables 1 and 3) in aquatic environment but lower toxicity in soils where ecotoxicity values are hundreds to thousands mg/kg of dry soil (Bezchlebová et al., 2007; Sverdrup et al., 2006). MCCPs have lower acute toxic potential thanks to their higher molecular size but even higher bioaccumulation rate than SCCPs. For these reasons, the danger of CPs lies in their long-lasting chronic exposition and bioaccumulation in human or other mammals milk (e.g., Kalantzi and Alcock, 2012; Xia et al., 2017a, 2017b; Huang et al., 2017). The results of recent studies also showed that SCCPs can be released into the human indoor environment (e.g., Coelhan and Hilger, 2014; Huang et al., 2017) and it is necessary to subject the use of these substances to a new, more detailed discussion.

The used ecotoxicological data (EC/LC₅₀) are relevant for each application, mainly in Europe and North America because they CPs were tested on model organisms representing these areas (the local model organisms should better be used for the ecotoxicity evaluation in arctic, subtropical, or tropic areas). Thus, the HC₅₀ and EF were estimated for freshwater environment (see Table 5). In addition, the data entering into XF and FF estimation have usually a more local background than the effect factors (see Eq. (3)), most of the CP values originate from Europe, North America, Taiwan, Africa, China, and Australia (Glüge et al., 2016).

The CF values determined in this paper (based on USETOX model, see Table 5) were relatively high (3790–3950 PAF·m³·day·kg⁻¹). It indicated a high impact on the environment. Unfortunately, the calculated data could not be compared with the results obtained by other investigators because relevant studies focusing on CPs do not exist. Therefore, other POPs, such as PCBs, DDD, chlordane were used for the comparison. The database of CFs based on USETOX model showed that they were in the range of thousands to ten thousands of PAF·m³·day·kg⁻¹ (Rosenbaum et al., 2008), which was in accordance with the CF values obtained in this paper. The LC₅₀ or EC₅₀ values of MCCPs for the calculation of CFs based on USETOX model were not available. However, one can suppose that these potential values would be in the same range.

In the case of CML method, the CF was calculated only for MCCPs. The predicted environmental concentration (PEC) was negligible for SCCPs used in PVC; no risk was thus assumed for this application of SCCPs. As also in this case any data published by others were not found, POPs as 2,3,7,8-TCDD or Aldrin (Guinée et al., 2002) were used for a comparison. CFs for these substances were either of the same

Table 4
Data for the calculation of characterization factors using the MSS concept.

		Freshwater (µg·l ⁻¹)	Source	Soil (mg·kg ⁻¹)	Source
SCCPs	PEC	Negligible	(EURAR, 2008)	Negligible	(EURAR, 2008)
	PNEC	0.5	(ECB, 2008)	1.8	(ECB, 2008)
MCCPs	PEC	0.15–1.59	(Annex XV Restriction Report, 2008)	0.52–13.9	(Annex XV Restriction Report, 2008)
	PNEC	1.0	(ECB, 2008)	10.6	(ECB, 2008)
1,4-DCB	PEC	0.1	(EC, 2004)	0.073 (use)	(EC, 2004)
	PNEC	20	(EC, 2004)	0.097 (use)	(EC, 2004)

Table 6
Characterization factors of SCCPs and MCCPs for PVC applications.

	Freshwater ($\text{kg}\cdot\text{l}^{-1}$)	Soil ($\text{kg}\cdot\text{kg}^{-1}$)
SCCPs	–	–
MCCPs	$(30\text{--}300) \times 10^{-9}$	$(0.07\text{--}1.75) \times 10^{-6}$

order of magnitude or several orders lower/higher than the values obtained for MCCPs. However, it is necessary to note that the PEC or PNEC values of MCCPs and 1,4-DCB as a reference substance used in the present study may not be the same as the data entering CML analyses (Guinée et al., 2002) and that the value characterizing the whole impact is a sum of CFs and the amount of substance emissions into the specific environment.

PEC/PNEC ratios for MCCPs in PVC were found higher than 1 in some cases. Thus, the risk potential from their levels in the environment was not negligible. The risks (PEC/PNEC ratios > 1) associated with MCCPs were observed in various uses of PVC as plastisol coating, extrusion, or open conversion (Annex XV Restriction Report, 2008). Therefore, it can be concluded that both SCCPs and MCCPs remain actual human and environmental hazard substances worldwide.

The application of SCCPs as semivolatile persistent organic pollutants with ecotoxicological effects and high bioaccumulative potential will probably decrease in the future; the ban on its use imposed by EU, Japan, USA, and Canada may be followed by some other countries. MCCPs which began to replace SCCPs in PVC applications during the last years will probably be a temporary solution only. The possible SCCPs and MCCPs alternatives for the future use in PVC might become LCCPs, phthalates, tri-alkyl phosphates, aryl phosphates, or inorganic compounds (e.g., Petrová et al., 2015; Annex XV Restriction Report, 2008). However, some of those substances are also toxic (e.g., phthalates) and the efforts to ban them worldwide were already initiated. Little information is available on the LCCPs degradation to MCCPs or SCCPs, which limits the relevance of their future use. As phosphor will probably become a scarce resource in the future (e.g., Ma et al., 2015; Adar et al., 2016), a replacement of SCCPs and MCCPs by phosphates may be a questionable solution. Therefore, inorganic compounds can be currently considered as the best alternatives to SCCPs and MCCPs although it should be noted that the environmental impacts of their applications in PVC products for construction industry were not analyzed yet.

5. Conclusions

The ecotoxicity of SCCPs and MCCPs used in PVC products for the construction industry was assessed in the paper. The obtained results showed that the characterization factor (CF) in the PAF method was for SCCPs in the freshwater environment 3790–3950 $\text{PAF}\cdot\text{m}^3\cdot\text{day}\cdot\text{kg}^{-1}$. This CF could not be determined for MCCPs because of the lack of effective ecotoxicological values. In the MSS method the CF values for SCCPs could not be calculated because PEC values were negligible. The CF for freshwater environment was estimated in the range of 30×10^{-9} kg 1,4-DCB- $\text{eq}\cdot\text{kg}^{-1}$ to 300×10^{-9} kg 1,4-DCB- $\text{eq}\cdot\text{kg}^{-1}$ and the CF for soil in the range of 0.07×10^{-6} kg 1,4-DCB- $\text{eq}\cdot\text{kg}^{-1}$ to 1.75×10^{-6} kg 1,4-DCB- $\text{eq}\cdot\text{kg}^{-1}$. The PEC/PNEC ratios for MCCPs in PVC were found higher than 1 in some cases, which indicated a risk potential.

Based on the findings gathered in this paper, it can be suggested that MCCPs should be given similar attention as SCCPs; from an ecotoxicological point of view MCCPs may present similar risks, perhaps even higher. Therefore, not only SCCPs but also MCCPs should be banned worldwide in PVC products for the construction industry. The most suitable alternative seems to be inorganic compounds but their environmental impacts are yet to be analyzed.

Acknowledgment

This research has been supported by the Czech Science Foundation, under project No P105/12/G059.

References

- Adar, E., Karatop, B., Ince, M., Bilgill, M.S., 2016. Comparison of methods for sustainable energy management with sewage sludge in Turkey based on SWOT-T-FAHO analysis. *Renew. Sust. Energ. Rev.* 62, 429–440.
- Aldenberg, T., Luttik, R., 2002. Extrapolation factors for tiny toxicity data sets from species sensitivity distributions with known standard deviation. In: Posthuma, L., Suter, G.W., Traas, T.P. (Eds.), *Species Sensitivity Distributions in Ecotoxicology*. Lewis Publishers, Boca Raton (FL), pp. 103–118.
- Annex XV Restriction Report, 2008. Substance Name: Medium Chain Chlorinated Paraffins (MCCPs) (United Kingdom).
- Bezchlebová, J., Černohlávková, J., Kobetičová, K., Lána, J., Sochová, I., Hofman, J., 2007. Effects of short-chain chlorinated paraffins on soil organisms. *Ecotoxicol. Environ. Saf.* 67, 206–211.
- Coelhan, M., Hilger, B., 2014. Chlorinated paraffins in indoor dust samples: a review. *Curr. Org. Chem.* 18, 2209–2217.
- EC (European Commission), 2003. Technical Guidance Document on Risk Assessment. Part II. https://echa.europa.eu/documents/10162/16960216/tgdpart2_2ed_en.pdf.
- EC (European Commission), 2004. European Union Risk Assessment Report – 1,4-Dichlorobenzene (France).
- ECB, 2008. European Union Risk Assessment Report: Alkanes, C10–13, Chloro. Updated version 2008. 1st Priority List. vol. 81. European Chemicals Bureau, Joint Research Centre, European Commission, EUR 23396 EN. http://esis.jrc.ec.europa.eu/doc/risk_assessment/ADDENDUM/scpp_add_010.pdf.
- ECHA (European Chemicals Agency), 2018. <https://echa.europa.eu/cs/registration-dossier/-/registered-dossier/11315/2/3> (downloaded on 28.5.2018).
- EURAR, 2008. European Union Risk Assessment Report – Alkanes C10–13, Chloro (Luxembourg).
- Glüge, J., Wang, Z., Bogdal, Ch., Scheringer, M., Hungerbühler, K., 2016. Global production, use, and emission volumes of short-chain chlorinated paraffins – a minimum scenario. *Sci. Total Environ.* 573, 1132–1146.
- Goedkoop, M., Spriensma, R.T., 1999. The Eco-indicator 99: A Damage Oriented Method for Life Cycle Impact Assessment Methodology. PRe Consultants, Amersfoort.
- Guinée, J.B., Gorrié, M., Heijungs, R., Huppes, G., Kleijn, R., de Koning, A., van Oers, L., Wegener Sleeswijk, A., Suh, S., Udo de Haes, H.A., de Bruijn, H., van Duin, R., Huijbregts, M.A.J., 2002. Handbook on Life Cycle Assessment. Operational Guide to the ISO Standards. I: LCA in Perspective. IIa: Guide. IIb: Operational Annex. III: Scientific Background. Kluwer Academic Publishers, Dordrecht (ISBN 1-4020-0228-9, 692 pp.).
- Hauschild, M.Z., Pennington, D., 2002. Indicators for ecotoxicity in life cycle impact assessment. In: de Haes, H.A., Finnveden, U., Goedkoop, G., Hauschild, M., Hertwich, E., Hofstetter, P., Klopffer, W., Krewitt, W., Lindeijer, E., Jolliet, O., Mueller-Wenk, R., Olsen, S., Pennington, D., Potting, J., Steen, B. (Eds.), *Life Cycle Impact Assessment: Striving Towards Test Practice*. SETAC Press, Pensacola (Chapter 6, ISBN: 1-880611-54-6).
- Hauschild, M.Z., Potting, J., 2004. Spatial differentiation in life cycle impact assessment – the EDIP2003 methodology. Guidelines from the Danish Environmental Protection Agency, Copenhagen. 2004.
- Hauschild, M.Z., Huijbregts, M.A.J., Jolliet, O., Macleod, M., Margni, M.D., van de Meent, D., Rosenbaum, R.K., Mckone, T.E., 2008. Building a model based on scientific consensus for life cycle impact assessment of chemicals: the search for harmony and parsimony. *Environ. Sci. Technol.* 42, 7032–7037.
- Huang, H., Gao, L., Xia, D., Gao, L., Wang, R., Su, G., Liu, W., Liu, G., Zheng, M., 2017. Characterization of short- and medium-chain chlorinated paraffins in outdoor/indoor PM10/PM2.5/PM1.0 in Beijing, China. *Environ. Pollut.* 225, 674–680.
- ISO 14040 Environmental Management – Life Cycle Assessment – Principles and Framework, 2006
- ISO 14044 Environmental Management – Life Cycle Assessment – Requirements and Guidelines, 2006
- Kalantzi, O.I., Alcock, R.A., 2012. Short chain chlorinated paraffins in biota – levels and effects. Conference: 12th International Conference on Environmental Science and Technology (CEST) Location: Rhodes, Greece Date: SEP 08–10, 2011 Global Nest J. 14, pp. 66–71
- Kočí, V., 2009. Posuzování životního cyklu. Life Cycle Assessment - LCA, Vodní zdroje Ekomonitor spol. s.r.o. Chrudim, Czech Republic.
- Koh, I.O., Thiemann, W.H.P., 2001. Study of photochemical oxidation of standard chlorinated paraffins and identification of degradation products. *J. Photochem. Photobiol. A Chem.* 139, 205–215.
- Larsen, H.P., Hauschild, M., 2007a. Evaluation of ecotoxicity effect indicators for use in LCIA. *Int. J. LCA* 1, 24–33.
- Larsen, H.P., Hauschild, M., 2007b. GM-Troph a low data demand ecotoxicity effect indicator for use in LCIA. *Int. J. LCA* 12, 79–91.
- Lassen, C., Sørensen, G., Crookes, M., Christensen, F., Jeppesen, Ch.N., Warming, M., Mikkelsen, S.H., Nielsen, J.M., 2014. Survey of Short-chain and Medium-chain Chlorinated Paraffins. The Danish Environmental Protection Agency Strandgade 29 1401 Copenhagen K Denmark. www.mst.dk/english 1 COWI A/S, Denmark 2 Danish Technological Institute, Denmark 3 Building Research Establishment (BRE), U.K. (2014. ISBN: 978-87-93283-19-0).
- Ma, S.J., Hu, S., Chen, D., Zhu, B., 2015. A case study of a phosphorus chemical firms application of resource efficiency and ecoefficiency in industrial metabolism under circular economy. *J. Clean. Prod.* 87, 839–849.

- Madeley, J.R., Maddock, B.G., 1983. Toxicity of a chlorinated paraffin over 60 days. Chlorinated paraffin - 58% chlorination of short chain length n-paraffins. ICI Confidential Report BL/B/2291.
- van Mourik, L.M., Gaus, C., Leonards, P.E.G., de Boer, J., 2016. Chlorinated paraffins in the environment: a review on their production, fate, levels and trends between 2010 and 2015. *Chemosphere* 155, 415–428.
- Muir, D., Stern, G., Tomy, G., 2000. Chlorinated paraffins. *The Handbook of Environmental Chemistry*. 3, pp. 203–236.
- Pennington, D.W., Potting, J., Finnveden, G., Lindeijer, E., Jolliet, O., Rydberg, T., Rebitzer, G., 2004. Life cycle assessment part 2: current impact assessment practice. *Environ. Int.* 30, 721–739.
- Petrová, Š., Soudek, P., Vaněk, T., 2015. Flame retardants, their use and environmental impact. *Chem. Lett.* 109, 679–686.
- Plouffe, G., Bulle, G., Deschene, L., 2016. Characterisation factors for zinc terrestrial ecotoxicity including speciation. *Int. J. Life Cycle Assess.* 21, 523–535.
- POPRC, 2015. Short-chained Chlorinated Paraffins: Risk Profile Document UNEP/POPS/POPRC.11/10/Add.2. United Nations Environmental Programme Stockholm Convention on Persistent Organic Pollutants, Geneva.
- POPRC, 2016. Short-chain Chlorinated Paraffins (SCCPs) - Draft Risk Management Evaluation. Tech. Rep. Prepared by the intersessional working group on Short-Chain Chlorinated Paraffins Persistent Organic Pollutants Review Committee URL: <http://chm.pops.int/TheConvention/POPsReviewCommittee/Meetings/POPRC11/POPRC11Followup/tabid/4723/Default.aspx>.
- Potting, J., Hauschild, M., 2004. Background for Spatial Differentiation in Life Cycle Impact Assessment – The EDIP 2003 Methodology. Danish Environmental Protection Agency, Copenhagen.
- Přibyllová, P., Klánová, J., Holoubek, I., 2006. Screening of short- and medium-chain chlorinated paraffins in selected riverine sediments and sludge from the Czech Republic. *Environ. Pollut.* 144, 248–254.
- Rosenbaum, R.K., Margni, M., Jolliet, O., 2007. A flexible matrix algebra framework for the multimedia multipathway modeling of emission to impacts. *Environ. Int.* 33, 624–634.
- Rosenbaum, R.K., Bachmann, T.M., Gold, L.S., Huijbregts, M.A.J., Jolliet, O., Juraske, R., Koehler, A., Larsen, H.F., Macleod, M., Margni, M., Mckone, T.E., Payet, J., Schuhmacher, M., Meent, van de D., Hauschild, M.Z., 2008. USEtox – the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment. *Int. J. Life Cycle Assess.* 13, 532–546.
- Salieri, B., Righi, S., Pasteris, A., Olsen, S.I., 2015. Freshwater ecotoxicity characterisation factor for metal oxide nanoparticles: a titanium study on titanium dioxide nanoparticle. *Sci. Total Environ.* 505, 494–502.
- Smetanová, S., Bláha, L., Liess, M., Schafer, R.B., Beketov, M.A., 2014. Do predictions from species sensitivity distributions match with field data? *Environ. Pollut.* 189, 126–133.
- Sverdrup, L.E., Hartnik, T., Mariussen, E., Jensen, J., 2006. Toxicity of three halogenated flame retardants to nitrifying bacteria, red clover (*Trifolium pratense*) and a soil invertebrate (*Enchytraeus crypticus*). *Chemosphere* 64 (1), 96–103.
- Thompson, R.S., Madeley, J.R., 1983a. Toxicity of a chlorinated paraffin to *Daphnia magna*. ICI Confidential report BL/B/2358.
- Thompson, R.S., Madeley, J.R., 1983b. The acute and chronic toxicity of a chlorinated paraffin to the mysid shrimp (*Mysidopsis bahia*). ICI Confidential report BL/B/2373.
- USEtox, 2017. USEtox, version 2.02. <http://www.usetox.org/model/download/usetox2.02>.
- WCC, 2014. World Chlorine Council. International Chlorinated Alkanes Industry Association (ICAIA) newsletter. World Chlorine Council http://www.eurochlor.org/media/88258/20140908_icaia_newsletter_03_final.pdf.
- Xia, D., Gao, L.R., Zheng, M.H., Li, J.G., Zhang, L., Wu, Y.N., Gao, L., Tian, G.C., Huang, H.T., Liu, W.B., Su, G.J., Liu, G.R., 2017a. Health risks posed to infants in rural China by exposure to short- and medium-chain chlorinated paraffins in breast milk. *Environ. Int.* 103 (1–7). <https://doi.org/10.1016/j.envint.2017.03.013>.
- Xia, D., Gao, L.R., Zheng, M.H., Li, J.G., Zhang, L., Wu, Y.N., Tian, G.C., Huang, H.T., Gao, L., 2017b. Human exposure to short- and medium-chain chlorinated paraffins via mothers milk in Chinese urban population. *Environ. Sci. Technol.* 51, 608–615.
- Xu, C., Xu, J., Zhang, J., 2014. Emission inventory prediction of short chain chlorinated paraffins (SCCPs) in China (in Chinese). *Acta Sci. Nat. Univ. Pekin.* 50, 369–378.
- Zhan, F., Zhang, H., Wang, J., Xu, J., Yuan, H., Gao, Y., Su, F., Chen, J., 2017. Release and gas-particle partitioning behaviors of short-chain chlorinated paraffins (SCCPs) during the thermal treatment of polyvinyl chloride flooring. *Environ. Sci. Technol.* 51, 9005–9012.