Pentachloroanisole (PCA)

Government of Canada
July 2012

Table of Contents

List of Tables

Executive Summary

The Government of Canada has examined additional information to further characterise the environmental fate and behaviour of pentachloroanisole (PCA) in water, soil and sediment and its potential for long-range transport. The following approach was taken:

- re-examine the registrant-conducted radioactive pentachlorophenol (^{14}C-PCP) biotransformation studies reviewed during the re-evaluation of PCP by the U.S. EPA and the Government of Canada to determine whether PCA was observed and whether any characterisation could be made about its persistence;
- examine Government of Canada unpublished monitoring information of PCA in remote areas;
- examine studies available from the published literature to see if any additional information on the fate and behaviour of PCA could be used to further characterise its behaviour.

The following is a summary of the Government of Canada's findings:

PCA is not a registered substance and is not released directly into the environment. PCA is a transformation product of PCP. In North America, PCP is used primarily as a heavy-duty wood preservative to treat electrical utility poles and crossarms. It is also used on posts and industrial construction timbers. Historically, PCP was used extensively as a general biocide, fungicide, bactericide, herbicide, molluscicide, algaecide and insecticide by agriculture and other industries including textiles, paints, oil drilling and forestry. In Canada, all uses other than preserving utility poles and crossarms were withdrawn and expired in 1990. Another source of PCP is through the metabolism of HCB and other organochlorines in various organisms including fungi, caterpillars, fish, rats, birds, monkeys and humans.

PCA in the environment is produced through a common soil reaction, biomethylation of PCP. In general, the formation of PCA from PCP is not the major route of dissipation of PCP. The primary route of PCP dissipation is transformation to less chlorinated phenols, such as tetrachlorophenol and trichlorophenols, and the formation of bound residues. It has been determined previously that PCP is not persistent in soil, sediment and water since half-life estimates are below internationally recognised persistence criteria (UNECE, 2009).

PCA cannot be formed from abiotic transformation processes of PCP such as hydrolysis and photolysis. PCA is sparingly soluble in water and has a high Koc value indicating that it is likely to be immobile to slightly mobile in soils and partition to sediment in aquatic systems. The Henry's Law Constant indicates that PCA is expected to be volatile from moist soil and aquatic systems. The log Kow indicates a potential to bioaccumulate.

Soil biotransformation studies indicate that PCA is formed from PCP primarily under aerobic conditions. The primary route of transformation of PCA in both soil and sediment is demethylation back to PCP which is than transformed to less chlorinated phenols and bound residues. In studies where PCP was used as the starting material, neither the usual half-life

estimation methods nor a combined residue approach (total residues PCP + PCA) were found to be accurate methods for classifying the persistence of PCA. The overall half-life estimate using a combined residue approach was driven by the rapid PCP degradation rate since it was at much higher concentrations than PCA. The half-life estimates for PCA alone derived from studies conducted with PCP as a starting material were confounded by simultaneous formation and degradation and should be considered conservative upper-bound estimates. From these studies, conservative half-lives for PCA were estimated to be between 20-35 days and were well below the persistence criteria of 180 and 365 days for soil and sediment, respectively. These values indicate that PCA is not expected to persist in soil and sediment. See Table 1 for a summary of persistence information.

Bioremediation studies inoculated with fungi indicated that some species preferentially transform PCP to PCA. It is thought to be a detoxification mechanism allowing the fungus to tolerate and biodegrade otherwise toxic levels of PCP. Although these studies are not representative of typical soil conditions and should not be used to classify persistence, they showed that PCA was volatile when tested in liquid media and that understaturated air favours the partitioning of PCA from water to air. They also showed that despite forming a significant amount of PCA, both PCP and PCA were degraded relatively quickly in these test systems and that PCA was not volatile when tested with the same fungal species in soils.

In aquatic systems, PCA is expected to partition to sediment and air based on its physico-chemical properties. One study examining the fate of PCP and its transformation products after an oil spill showed that under field conditions, PCP is biomethylated to PCA and that both PCP and PCA partitioned to the sediments and dissipated over time. There was also evidence that PCP transformed to lower chlorinated phenols (tetrachlorophenols and trichlorophenols). Since PCP was present throughout this period, PCA was under a state of continuous formation which precluded the ability to derive an estimated half-life. In addition, the field study did not capture any losses due to volatility. This field study did, however, confirm that PCA is expected to partition to sediment when present in aquatic systems and confirms that persistence estimates in sediment would represent the behaviour in aquatic systems.

Various studies showing residues of PCA in various matrices are available in the published literature. Most of this information, however, originates from impacted environments where PCP is currently being used or was used historically. Since media from these studies are continuously exposed to PCP (and possibly to PCA via soil/sediment biomethylation of PCP), the value of this information in determining environmental persistence and/or evidence of long range transport is questionable.

Additional analysis of monitoring data has been provided which distinguishes between local and non-local sources of PCA. As an example, the Atlas et al. (1986) study is often referred to as evidence of the long range transport of PCA. However, high levels of an unstable and rapidly oxidised transformation product of PCP, TCHQ (tetrachlorohydroquinone) were also measured with PCA. The authors speculated that the appearance of TCHQ indicated that the source of PCP/PCA may actually be local, not remote.

There are six studies (Welch et al. 1991; Su et al. 2008; Hung et al. 2005; Rawn et al. 2001; Muir 2007 in Hoferkamp et al. 2010 and MacDonald et al. 2000) showing PCA residues in air, snow

and sediment in remote locations. In addition, the Government of Canada has collected additional unpublished information on residues in air in remote areas (Hung et al. unpublished archive data, Environment Canada).

Additional analysis of the published literature indicates there is evidence that oceans are a major continuous source of semi-volatile organochlorine substances (SOCs) including PCA in the environment. Schreitmuller and Ballschmiter (1995) indicated that the North Atlantic Ocean is undersaturated and the South Atlantic is close to a gas-water exchange equilibrium with PCA and three other SOCs. Particularly under conditions of a diminishing input of SOCs from continental sources, the air-surface water equilibrium will render the oceanic system to be a global nonpoint source of anthropogenic compounds in marine air. Similarly, Hoferkamp et al. (2010) indicated that with the exception of lindane and α-endosulfan (Weber et al., 2006) there is insufficient data to assess whether air concentrations are resulting in net deposition to Arctic Ocean and lake waters or whether these waters are actually outgassing the currently used pesticides (including PCA) monitored in the arctic. Other sources to the ocean could include long distance transport in ocean currents as has been postulated for β-HCH (Li et al., 2002). Glacier runoff could be an important source for some lakes and estuaries (Blais et al., 2001; Bizzotto et al., 2009).

Although PCA does not meet internationally recognised persistence criteria, the continuous release from current sources and the semi-volatile nature of PCA has made PCA ubiquitous and susceptible to long range transport.

The log K_{OW} and the bioconcentration factor (BCF) values for PCA reported by Oliver and Niimi (1985) for fish exceed the laboratory criteria cut-off values for the determination of bioconcentration. However, additional laboratory and field information also indicate that PCA is metabolised and depurated in various species including fish, earthworms and mammals.

There is not enough information provided in monitoring studies to calculate a true field bioaccumulation factor (BAF) since residues in biota are low and water concentrations are not often reported in the same studies. However, there are three references (Vorkamp et al. 2004; Bentzen et al. 2008 and Swachkhammer et al. 1988) and additional information provided by Environment Canada (Muir, unpublished) showing low levels residues in biota in remote locations. As noted by Vorkamp et al. (2004), the concentrations in top predatory marine mammals do not exceed the concentrations in marine fish, contradicting the typical pattern of bioaccumulation in the food chain. Compared with the results for chlorobenzenes and other chlorinated pesticides (aldrin, dieldrin, endrin, endosulfan, heptachlor, methoxychlor and mirex) the concentrations of PCA are considered to be low in biota.

Despite PCA being ubiquitous in air and found in multiple other media, PCA has not been detected in appreciable levels in field biota thereby contradicting the bioaccumulation potential predicted by the aquatic BCF value. Metabolism, depuration, biodegradability and bioavailability of PCA are likely significant factors in reducing the likelihood of bioaccumulation and biomagnification in aquatic systems.

Table 1: Summary of Persistence Information in soil, sediment and water

Persistence half-life criteria as defined in Annex D	Half-life estimates	Reference
Soil (6 months-aerobic)	>75% of both PCP and PCA disappeared in 30 days in five soils.	D'Angelo and Reddy (2000)
	Approximate half-life of 35 days for PCA.	Kuwatsuka and Igaresh (1975)
	Approximate half-life of 5 weeks for PCA.	Haimi et al. (1993)
	5.6% PCA converted to PCP in 24 days.	Murthy et al. (1979)
	weeks-months (estimated at 37.5 days and 61.8 days by the EPISuite model for fugacity modelling)	BioWin 4.0 (primary transformation) in U.S. EPA (2011)
Sediments and flooded soil (6 months)	Approximately 20 days.	Kuwatsuka and Igarashi (1975)
	42% PCA converted to PCP in 24 days.	Murthy et al., (1979)
Water (2 months)	-Indicates in aquatic systems, partitioning of PCA to sediment is expected. -Indicates persistence estimates in sediment would be representative of the behaviour in aquatic systems.	Pierce and Victor (1978) and U.S. EPA (2011)
	-physical-chemical properties indicate that volatilisation to air and partitioning to soil/sediment is expected.	U.S. EPA (2011)

Table 2: Summary of Bioaccumulation Information

Bioaccumulation criteria as defined in Annex D Stockholm Convention on POPs	Endpoint	Reference
Log Kow	5.45	Opperhuizen and Voors, 1987
Laboratory Bioaccumulation		
Oncorhynchus mykiss	BCF: 15 000 ± 4 950 (low concentration); 20 000 ± 13 200 (high concentration)	Oliver and Niimi, 1985

Poecilia reticulate	BCF could not be determined. PCA was rapidly eliminated with half-lives between 1 and 4 days.	Opperhuizen and Voors (1987)
Oncorhynchus mykiss	BCF was not determined. Half-lives of PCA were 6.3, 9.8, 23 and 6.3 days in blood, liver, fat and muscle, respectively.	Glickman et al., 1977
Earthworms	BAF: 5-40	Haimi et al, 1992; Haimi et al., 1993
Mice	Following injection of PCA into female mice, elimination of [^{14}C]PCA equivalents was rapid with half-lives ranging from 5-10 hours in all tissues except liver. Excretion of ^{14}C was primarily through the urine. There was no evidence of PCA in either the urine or feces. PCP was detected in the urine and feces at approximately 2 and 32% of the applied radioactivity, respectively. The majority of the ^{14}C was associated with the PCP conjugate. The authors concluded that PCA must be demthylated prior to conjugation and/or excretion	Vodicnik et al., 1980
Field residues in biota in remote areas		
Greenland (2004) Terrestrial animals Marine invertebrates Marine fish Seabirds Marine mammals	 n.d.- 0.20 ng/g lw n.d -0.74 ng/g lw n.d-2.3 ng/g lw n.d-0.36 ng/g lw n.d.-0.86 ng/g lw	Vorkamp et al., 2004
Alaska (2003) Polar bears, fat:	 n.d.*-27 ng/g ww, n.d.-42 ng/g lw	Bentzen et al, 2008
Remote lake, Northern Wisconsin (1988) Lake trout white fish, whole body:	 3.6 ng/g lw and 6.5 ng/g lw	Swachkhammer et al, 1988
Arctic: Ringed seals: Sea run Arctic char: Landlocked Arctic char: Burbot:	 n.d.-0.82 ng/g lw n.d.-0.10 ng/g lw n.d.-1.83 ng/g lw n.d.-3.85 ng/g lw	Muir, unpublished

n.d.: below the limit of detection

* <0.1 ng/g

Table 3 : Summary of information on long-range transport

Air		
Arctic (2000-2003)	4.9 pg/m^3	Su et al., 2008
Canadian and Russian Arctic	2.6-4.0 pg/m^3	Hung et al., 2005
Canadian Arctic (1993-1994)	2.3-3.1 pg/m^3	Macdonald et al, 2000
Canadian Arctic (1992-2008)	n.d.-4.2 pg/g m^3 (range of annual medians)	Hung et al., archive data, Environment Canada
Snow		
Melted snow: Particles: Brown snow	1230 pg/L 4.3 mg/g 1442 pg/L	Welch et al., 1991
Snow :	0.4-0.6 ng.m^2/yr	Muir 2007 in Hoferkamp et al., 2010
Sediment		
Northern Canadian Lakes Sediment (1992-1995)	0.33-4.52 ng/g dw (range of maximum values with lower concentrations in surface sediments)	Rawn et al., 2001

n.d.: below the limit of detection

Chapter 1: Background

1.1 Details of sources of PCP and PCA in the environment

There are several sources of PCP in the environment including the release of PCP when used in accordance with currently registered uses. Also, many sites contaminated from the historical use of PCP as an agricultural pesticide and from improper practices of wood treatment plants (e.g., spills from industrial holding ponds from wood treatment facilities prior to current guidelines) continue to be sources of PCP in the environment. Releases to the environment may also occur through revolatilisation from adsorbed residues of PCP/PCA.

It should be noted that PCP is also a transformation product of other organochlorines such as HCB and, PCNB (quintozene) (Murthy and Kaufman, 1978 and U.S. EPA RED for PCNB, 2006) and lindane (Engst et al. 1979). These organochlorine substances are global pollutants and have been detected in remote locations.

Pentrachloroanisole (PCA) is introduced into the environment through the methylation of pentachlorophenol (PCP) by soil or sediment micro-organisms. This occurs primarily in the aerobic environment. Biomethylation (PCP → PCA) is a ubiquitous reaction, but generally not the major route of PCP degradation (Valo and Salkinoja-Salonen, 1986). PCA is not produced from PCP through abiotic transformation processes such as hydrolysis and photolysis (soil, water and air). Figure 1.1 is a figure representing examples of sources of PCP/PCA in the environment.

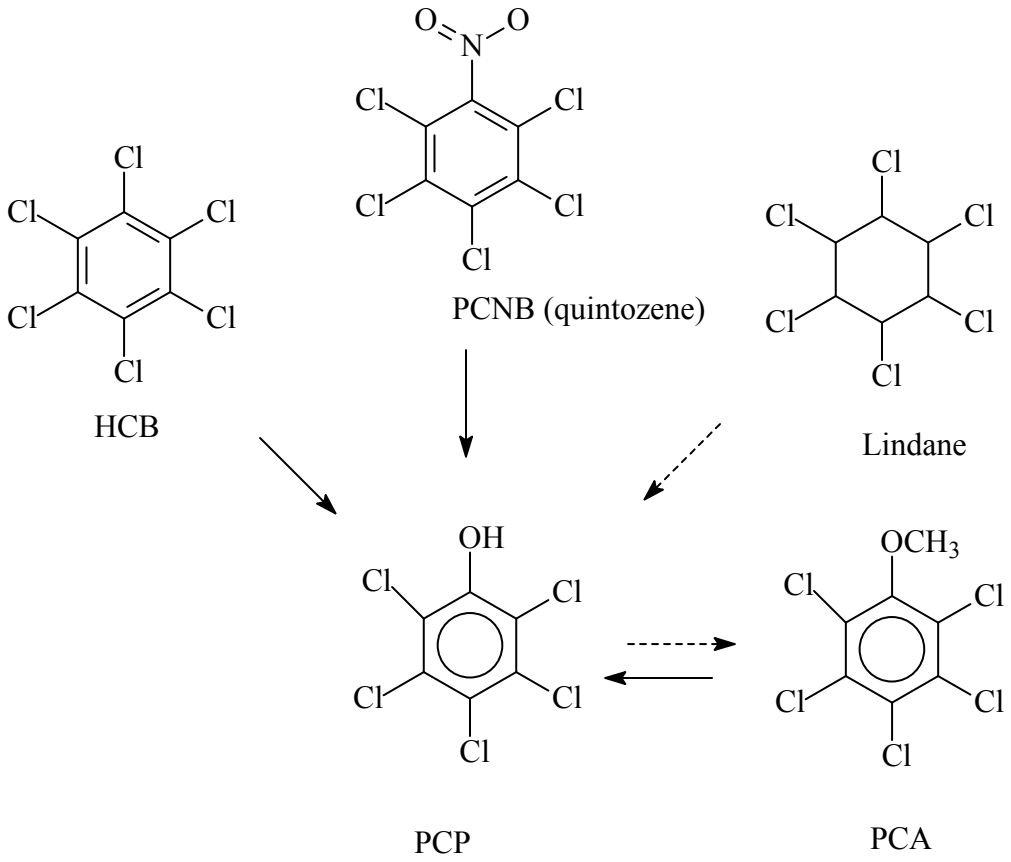


Figure 1: Examples of several sources of PCP in the environment.

Chapter 2: Fate and behaviour in the environment

2.1 Physical and chemical properties relevant to the environment

PCA is sparingly soluble in water (< 1 mg/L). The Koc estimate (KOCWIN v.2.0 in EPA 2011) of 2474 (MCI method) and 13800 (Kow method) indicate that PCA is likely to be immobile or have slight mobility when in soils as per the McCall et al. (1981) classification scheme. The high K_{OC} also indicate that in aquatic systems, PCA is likely to partition to sediment.

The estimated log Kow is 5.30, (derived from KOWWIN v1.68, U.S. EPA, 2011) and the experimentally determined K_{OW} is 5.45 (Opperhiuzen and Voors 1987) indicating PCA is very hydrophobic and has the potential to bioaccumulate.

The Henry's law constant for PCA is estimated as 1.94×10^{-3} atm-m^3/mole, using a group estimation method and 7.12×10^{-5} atm-m^3/mole, using a bond estimation method (HENRYWIN v.3.2, U.S. EPA, 2011), indicating the potential to volatilise from moist soils and water surfaces. The modelled vapour pressure of 0.0458 Pa, using the modified Grain method (MPBPVP v1.43, U.S. EPA, 2011) and the vapour pressure of 0.0933 Pa (Dobbs and Grant 1980) indicates the

potential for very high volatility. Combined, these values indicate that aerial transport is possible. See Table 2.1-1 for the summary of physical and chemical properties.

Table 2.1-1 Physical and chemical properties of PCA relevant to the environment

Properties	Value	Comments	Reference
Water solubility 25°C	<1 mg/L	Sparingly soluble	http://cameochemicals.noaa.gov/chemical/20850
Vapour pressure (25°C)	0.0458 Pa 0.0933 Pa	Very high volatility Very high volatility	Modified Grain Method Dobbs and Grant (1980)
Henry's law constant atm/m^3/mol	1.94x 10^{-3} atm-m^3/mole (Group method) (1/H = 12.7) 7.12 x 10^{-5} atm-m^3/mole (Bond method)	Potential to volatilize from water or moist soil. Rapidly lost from a water surface.	(HENRYWIN v3.2 in U.S. EPA 2011)
Dissociation constant (pK_a)	Not Applicable	-	-
Log Octanol/water partition coefficient (LogKow)	5.30 (modelled) 5.45 (laboratory)	Indicates the potential for Bioaccumulation	KOWWIN v1.68 in U.S. EPA 2011 Opperhuizen and Voors (1987)
K_{OC}	2474 L/kg 13800 L/kg	Slight mobility in soil* Immobile in soil*	MCI method, KOCWIN 2.0 K_{OW} method, KOCWIN 2.0 in U.S. EPA (2011)
UV/visible absorption spectrum	Not Available	-	-

* McCall et al. (1981) classification scheme.

QSAR Predictions and Estimates for Persistence:

QSAR estimates derived from EPI (Estimation Program Interface) Suite 4.1 (U.S. EPA 2011) for both PCP and PCA. The output summaries are presented in Appendix II.

The half-life estimation most relevant for persistence classification under UNECE LRTAP is the primary biodegradation (Biowin 4: transformation of a parent compound to an initial metabolite). A summary of the model outputs for the BioWin QSAR estimates are presented in Table 1.2-2. The results from the BioWin 4.0 output are shaded.

Table 1.2-2 EPI Suite 4.1 predictions of rapid aerobic and anaerobic biodegradation of PCA and PCP

Model	Endpoint		Comment
	PCP	PCA	
Probability of Rapid Biodegradation:			
Biowin 1 (linear model)	-0.1755	-0.1661	Does not biodegrade fast (probability)
Biowin 2 (non-linear model)	0.000	0.0002	Does not biodegrade fast (probability)
Expert Survey Biodegradation Results			
Biowin 3 (ultimate biodegradation*)	1.6340	1.4885	Recalcitrant (Months-longer) (estimate: 180 days)
Biowin 4 (primary biodegradation**)	2.6765	2.6937	Weeks-months (estimate: 37.5 days (U.S. EPA default); 61.75 days (alternative default)
MITI Biodegradation Probability			
Biowin 5 (MITI linear model)	0.0149	0.1046	Not readily degradable
Biowin 6 (MITI non-linear model)	0.0031	0.0049	Not readily degradable
Anearobic Biodegradation Probability:			
Biowin 7 (anaerobic biodegradation potential)	-1.0946	-1.0768	Does Not Biodegrade Fast
Ready Biodegradability Prediction:	**NO**	**NO**	

*Ultimate biodegradation is the transformation of a parent compound to carbon dioxide and water, mineral oxides of any other elements present in the test compound, and new cell material.
**Primary biodegradation is the transformation of a parent compound to an initial metabolite.
Shaded row indicates the output value that most closely matches the soil persistence classification.

Discussion:

The EPI Suite is a Windows-based suite of physical/chemical property and environmental fate estimation programs. It estimates physical/chemical properties and environmental fate and transport, and includes estimation programs for octanol-water partition coefficient (KOW), organic carbon-normalized partition coefficient for soil and sediment (KOC), atmospheric oxidation potential, Henry's Law constant, water solubility, melting point, boiling point, vapor pressure, octanol-air partition coefficient (KOA), sorption to aerosols, biodegradation, bioconcentration (BCF) and bioaccumulation factors (BAF), hydrolysis, removal of chemicals in sewage treatment plants, and multimedia modeling. EPI Suite is a screening-level tool and should not be used if acceptable measured values are available. A clear understanding of the estimation methods and their appropriate application is very important.

The Biowin model predicts similar numbers for both PCP and PCA. The Biowin output for PCP and PCA indicate that at the screening level, exposure estimates indicate that both chemicals would not undergo rapid aerobic or rapid anaerobic biodegradation. The half-life estimation most relevant for persistence classification is the primary biodegradation (Biowin 4: transformation of a parent compound to an initial metabolite) and the results indicate that the estimated half-life for both PCP and PCA is weeks-months. This classification is estimated at 37.5 days (alternate estimate of 61.8 days) by the EPISuite model for Fugacity modelling.

2.2 Abiotic transformation

2.2.1 Soil (hydrolysis and phototransformation)

PCA was not detected in any of the U.S. EPA-reviewed abiotic transformation studies conducted with PCP (U.S. EPA 2008). A summary of the abiotic radiolabelled studies are provided in Table 2.7-1. Since PCA is formed via biomethylation, it is not expected to be formed from PCP under abiotic conditions.

Based on its chemical structure it would not be expected to hydrolyze (Lyman et al 1982 in U.S. EPA 1992). No other information on the hydrolysis and phototransformation of PCA was found.

2.2.2 Air

The Henry's law constant for PCA is estimated as 1.94E-3 atm-m^3/mole, using a group estimation method and 7.12E-5 atm-m^3/mole, using a bond estimation method (HENRYWIN v.3.20 in U.S. EPA 2011). This value indicates that that PCA has the potential to volatilize from water or moist soil. Based on this value for Henry's law constant, the volatilization half-life from a model river (1 m deep, flowing 1 m/sec, wind velocity of 5 m/sec) is estimated to be 2.2 hours. The volatilization half-life from a model lake (1 m deep, flowing 0.05 m/sec, wind velocity of 0.5 m/sec) is estimated to be 6.9 days (Estimated by Group SAR Method in U.S. EPA 2011).

PCA can be photo-oxidised in the atmosphere through reactions with hydroxyl (OH) radicals. The calculated half-life for PCA based on this reaction is 9.8 days, with an atmospheric (OH) concentration of 1.56 E6 OH/cm^3 (AopWin v1.96 in U.S. EPA, 2011). No experimental data are available on atmospheric degradation.

The physical-chemical properties indicate that there is the potential for long-range transport. Field evidence addressing the potential for long-range transport is discussed under section 2.4.3.

2.3 Biotransformation

2.3.1 Soil biotransformation

2.3.1.1 Aerobic

In a radiolabeled aerobic biotransformation study reviewed by the U.S. EPA (U.S. EPA 2008), PCP degraded in aerobic sandy loam soil with an observed half-life of 7-14 days; the calculated first-order half-life was approximately two months. The major degradation products of PCP were 2,3,4,5-tetrachlorophenol, 2,3,6- and 2,4,6-trichlorophenol and CO_2. Bound residues accounted for up to 64% of the radioactivity. Additional analysis of the bound residues indicated that 76%, 21% and 3% of the bound residues were associated with the humin, fulvic and humic fractions, respectively. In a supplemental study in which aerobic soils were subsequently flooded and kept under anaerobic conditions, up to 10% of the bound residues were released as PCP. PCA was not one of the standards used to compare with the observed transformation products, however, all other major transformation products were identified and there were no significant amounts of unidentified radioactivity and overall recoveries were >91.3%. It is unlikely that PCA was a major transformation product in the studies submitted for registration. A summary of the results of the biotransformation study are found in Table 2.7-2.

Biomethylation of PCP to PCA is a common reaction in soil, but generally not the major route of PCP transformation (Valo and Salkinoja-Salonen 1986). Of the aerobic soil studies that were reviewed, PCA was generally detected at < 5% of the applied PCP and showed some evidence of further degradation. Some references available in the open literature, including EHC 71 (1987), Englehardt (1986), Kaufman (1978), U.S. EPA (2008) and the Risk Profile document for PCA submitted to the Task Force in May 2009 (Government of Canada 2009), cite the Murthy et al. (1979) study as evidence of PCA being formed as a major soil metabolite under aerobic conditions. However, a critical review of the study has shown that this was not the same conclusion reached by the original authors. The study authors concluded that the major degradative pathway of PCP is through reductive dechlorination and that the production of PCA was greater in aerobic than in anaerobic soils. It should be noted that closer examination of the data from the PCP-treated aerobic soil study showed that only 14.7% of the applied radioactivity treated was extractable, 51.5% of which was identified as PCA and 33.4% as PCP. This would result in a maximum concentration of PCA of 7.5% of the total applied radioactivity and not 51.5% as reported in some published literature summarising Murthy et al. (1979). The remaining radioactivity was attributed as follows: 44.6% to bound residues and 40.7% to unaccounted radioactivity. There is also some uncertainty in the results of this study since some samples were methylated prior to analysis thereby possibly converting some of the PCP to PCA. It is expected that the PCA concentrations reported represent a conservative estimate as PCA concentration may have been overestimated.

The authors of the Murthy et al. (1979) reference also speculated that some of the PCA residues may be incorporated into soil components as bound residues, however, this has not been confirmed by any of the studies included in this literature search. The Government of Canada did not find any published literature or registrant-conducted studies where bound residues were released and identified as PCA. In fact, a registrant-conducted study using radiolabeled PCP

showed that under anaerobic conditions, small amounts (<10%) of bound residues were released under anaerobic conditions as PCP, not PCA.

In a laboratory experiment conducted by Haimi et al. (1993), chloroanisoles (2,3,4,6-tetrachloroanisole; containing approximately 10% PCA) were added to soil with and without earthworms in test vessels. The concentrations of 2,3,4,6-tetrachloroanisole and pentachloroanisole in earthworms and soil decreased in soil with an approximately half-life of 5 weeks in both the soils with and without earthworms. There was evidence of demethylation of PCA to pentachlorophenol and tetrachloroanisole to tetrachlorophenol. The overall rate of disappearance was attributed to degradation, metabolism to unidentified compounds and to the formation of non-extractable compounds. The authors noted that the high rate of metabolism and/or degradation of the chloroanisoles were corroborated by the high respiration activity found with the high concentrations of chloroanisoles.

D'Angelo and Reddy (2000) performed a laboratory study on PCP loss in 10 different wetland soils with no previous exposure to PCP to examine strategies to enhance biotransformation, which included testing various test concentrations and manipulations of electron acceptors and donors under anaerobic conditions. Only the results of the aerobic transformation study are reported here. Seven of the aerobic soils showed production of PCA during the first week of incubation. In the presence of O_2, most soils produced PCA within 1 d after PCP treatment. Subsequently, PCP and PCA were lost from many soils without the appearance of chlorinated intermediates, indicating either mineralization to CO_2 or chemical binding or attachment. The authors reported that PCP transformation proceeded by two different pathways (methylation and dechlorination). Aerobic PCP transformation in soil initially produced small amounts of PCA in seven of the ten soils tested at maximum rates between 0.9 and 3.4 µmol/kg/d. Five of the seven soils exhibited losses of PCA. These five soils transformed PCP and PCA with maximum rates between 32 and 77 µmol/kg/d and first order rate constants were between 0.139 and 0.338 day^{-1}. Greater than 75% (75%-100%) of both chemicals (PCP and PCA) disappeared in 30 d from five soils. In the other two soils that produced PCA, no loss of either PCP or PCA was observed over the 30 day observation period. The two remaining soils showed no PCA production and no loss of PCP. Measured soil properties were not correlated to aerobic transformation rates. Transformation was attributed to biological activity since sterile control soil samples, autoclaved with $HgCl_2$+, showed no changes in PCP concentration during the study. See graph A and E in the Figure below.

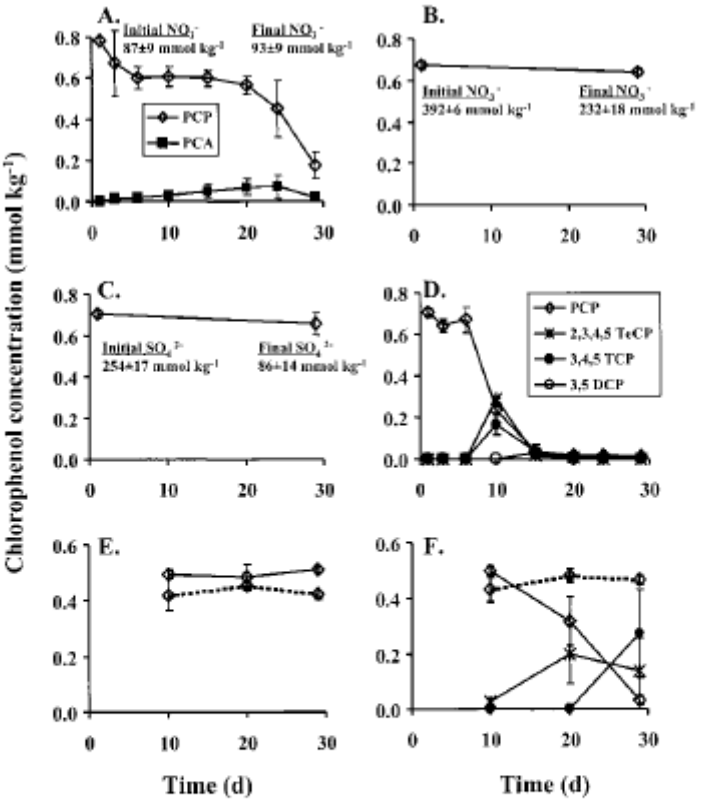


Fig. 2. Microbial transformation of pentachlorophenol (PCP) in Houghton Lake constructed marsh soil (HLPI) under four electron acceptor reducing conditions, and in aerobic and methanogenic sterile controls: (A) O_2; (B) NO_3^-; (C) SO_4^{2-}; (D) CO_2; (E) O_2 + 2% $HgCl_2$; and (F) CO_2 + 2% $HgCl_2$. Dotted lines in (E) and (F) represent autoclave + $HgCl_2$ treatments. Initial and final NO_3^- and SO_4^{2-} refer to concentrations at the beginning and end of the experiment. Each value represents the mean of three replications ± one standard deviation.

Figure 2.3-1: Experimental results demonstrating that transformation of PCP is due to microbial transformation (D'Angelo and Reddy 2000).

In a study conducted by Kuwatsuka and Igarashi (1975), the transformation of PCP in relationship to soil properties was studied under upland and flooded conditions using 10 different soils collected from rice fields, upland fields and one sample of a subsoil from the forest. The authors reported that transformation of PCP in soils was faster under flooded conditions than upland conditions. The transformation under flooded conditions was more rapid in soils collected from rice fields than in those from adjacent upland fields. The reverse was true under upland conditions. The transformation rate was highly correlated with organic matter content in the soil. The rate was slightly correlated with the clay mineral composition, free ion content, phosphate absorption coefficient and C.E.C., but hardly at all with texture, clay content, degree of saturation, soil pH and available phosphorus content. The transformation products detected included tetrachlorophenol (maximum of 3% of the applied PCP at day 5), trichlorophenol (maximum of 2.5% of the applied PCP at day 5), PCA (maximum of 1% of the applied PCP at day 5 with a decline to 0.5% at 35 days) and various other transformation products detected in trace amounts. Although not reported by the study authors, an observed half-life of

approximately 30 days for PCA can be estimated from the graphs provided in the study. This is considered a conservative half-life estimate since PCP was present in the test system over the course of the study and would have behaved as a continuous source of PCA. The authors indicated that PCA formation and subsequent degradation back to PCP was reported previously by Kuwatsuka and Igarashi (1971, 1972 and 1973), however, these studies are only available in Japanese and were therefore not reviewed by the Government of Canada.

Chung and Aust (1995) conducted a degradation study of PCP in soil in a closed system with radiolabelled material with a species of white rot fungi that preferentially produces PCA to detoxify PCP. Although significant amounts of PCA were produced, no volatile organic compounds, including PCP or PCA were detected in the volatile traps. Degradation half-lives were reported in the study, but are not reported here as these are not relevant for persistence classification since the study was conducted with an isolated white rot fungus instead of mixed soil microflora as required under standard protocols.

In another closed system experiment, Klowskowski et al. (1981) conducted a study examining the transformation of PCP in a closed soil-plant-system system. In this test system, PCP was found to be non-persistent in both outdoor and laboratory test systems. All volatile products captured in the laboratory test were determined to be carbon dioxide; no other volatile products, including organic volatile products (e.g., PCA), were detected.

Degradation Pathway in Aerobic Soils:

Kaufman (1978) summarised the degradation pathway of PCP via several pathways including methylation. Kaufman indicated that methylation yields the PCA and other phenolic products in the soil. These products, however, are ultimately dealkylated and returned to the chlorinated phenol degradation pathways. Reductive dechlorination appears to be the most significant PCP degradation pathway in soil. These pathways ultimately lead to ring cleavage and complete degradation of the PCP moiety. Numerous mono-, di-, tri- and tetrachlorinated phenols have been reported as soil degradation products of PCP. An additional observation by Kaufman (1978) that should be noted is that PCP metabolism by isolated soil microorganisms appears to occur by oxidative mechanisms, whereas reductive dechlorination is more prominent in soil. Thus, some discrepancies appear to exist between the degradative pathways observed in soil and those observed in isolated microbial cultures. The degradation studies conducted with isolated cultures are therefore discussed in a separate section (Section 2.3.3).

Uncertainties regarding potential losses due to dissipation:

In the Haimi et al. (1993), D'Angelo and Reddy (2000) and Kuwatsuka and Igarashi (1975) papers, it is unclear whether vessels were securely sealed over the course of the study. Based on the volatility of PCA observed in several laboratory studies, additional information was considered to assess whether half-lives could be characterised as representative of transformation/degradation or dissipation/volatilisation.

Analysis of the information available in the published literature indicates that PCA was only found in the volatile fraction of laboratory studies conducted under very specific test systems (liquid culture medium) with specific test species that preferentially convert PCP to PCA (e.g.,

some species of white rot fungi) (e.g., Badkoubi et al. 1996; Walter et al. 2004). The experimental results showing the volatility of PCP and PCA were not repeated when similar studies were conducted in soil using radiolabeled material in closed test systems (Walter et al. 2005; Chung and Aust 1995). See Section 2.3.3 for additional details on these two studies. The lack of volatility observe in the laboratory studies conducted with soil is likely due to the strong sorption to soil as predicted by the high estimated K_{OC} values.

Additional supporting information such as the following also support that laboratory half-lives predicted for soil are likely to be a result of transformation and not volatilisation and/or dissipation:

-PCA was volatile in laboratory studies conducted with liquid medium. PCA was not volatile in studies conducted with soil;
-in the three soil degradation studies (Haimi et al. 1993, D'Angelo and Reddy 2000 and Kuwatsuka and Igarashi 1975), a pattern of formation and decline of PCA is observed over the course of the studies;
-increased CO_2 production was observed in studies when soils were treated with tetrachloroanisole and pentachloroanisole when compared to control soils indicating that degradation was occuring (Haimi et al. 1993);
-when PCP was tested in soil under controlled laboratory conditions with radiolabelled test material, good radioactive recovery and volatile traps, PCA was not volatile (Chung and Aust 1995);
-PCA is demethylated to PCP under aerobic conditions (Haimi et al. 1993 and Murthy et al. 1979);
-the major degradative pathway for PCP is reductive dechlorination to lower chlorinated phenols and binding to soil (Murthy et al. 1979; Valo and Salkinoja-Salonen 1986);
-PCP is not considered persistent as per criteria outlined in POPs protocols;
-all five reviewers of the PCP dossier concluded that PCP does not meet persistence criteria in soil (UNECE 2009);
-In several biodegradation studies conducted with PCP, PCA appears as a minor transformation product (<10%). Any half-life calculation using combined residues (PCP+PCA) results in similar half-life predictions for PCP alone. As PCP was found not to meet persistence criteria, a combined residue half-life would also result in PCP/PCA not meeting the persistence criteria.

In general, reported half-lives for soil are most likely a result of biodegradation based on evidence of a degradation pathway, the presence of successor transformation products (PCP-TeCA-TCA, CO_2). The absence of PCA in volatile traps and good radioactive recoveries indicate that volatilisation was not a significant route of disappearance in the laboratory soil half-life calculations.

2.3.1.2 Anaerobic

In a flooded sandy loam soil, radiolabeled PCP degraded with a half-life of 1-2 months (calculated first-order half-life of 34 days) (U.S. EPA 2008 and U.S. EPA 2008). Various isomers of tetrachlorophenol and trichlorophenols were formed as major transformation products. Volatiles were negligible (1.4% of the applied radioactivity) and nonextractable residues were 7.8% of the applied radioactivity. PCA was not one of the standards used to compare with the observed transformation products, however, all the major transformation products were identified. There were no significant amounts of unidentified radioactivity and overall recoveries were only slightly outside the acceptable range 78.2-135%. It is unlikely that PCA was a major transformation product in the studies submitted for registration. A summary of the results of the biotransformation study are found in Table 2.7-2.

Murthy et al. (1979) observed small amounts of PCA in test soils treated with radiolabeled PCP exposed to anaerobic conditions. The authors concluded that the principal degradation pathway of PCP in anaerobic soil would seem to be by progressive dechlorination to tetra- and tri-chlorophenols, with lesser formation of pentachloroanisole. In addition, Murthy et al. (1979) conducted a supplemental study with soils treated with PCA incubated under both aerobic and anaerobic conditions to assess degradation. The study authors reported that 42% of the applied PCA was transformed to PCP in 24 days. In the anaerobic portion of the study, 98.8% of the radioactivity was recovered in the soil indicating that any losses due to volatilisation were insignificant. Since recovery was good and the successor transformation product (PCP) was identified, the half-life estimate can be attributed to degradation, not dissipation or volatilisation. It should be noted, however, that the analytical sample work-up uses a methylation step prior to analysis thereby possibly converting some of the PCP to PCA. It is expected that the PCA concentrations reported represent a conservative estimate as any additional PCA produced during the sample analysis would contribute to a slight overestimation of PCA concentrations.

D'Angelo and Reddy (2000) did not observe any PCP transformation to PCA under anaerobic soil conditions in 10 different soils under various anaerobic conditions.

Weiss et al. (1982) found that, one year after application of PCP to flooded soil in the laboratory, most of the radioactivity was found as bound residues. The authors identified conversion products which indicate at least four different reaction mechanisms: reductive dechlorination; methylation; conjugation; incorporation into insoluble macromolecules. Only 0.09% of the applied radioactivity was measured as PCA. Other lesser chlorinated anisoles were also found (tetra- and tri-chloroanisoles).

Kuwatsuka and Igarashi (1975) found that PCP was rapidly degraded in soil under flooded conditions. Transformation products included tetrachlorophenol (maximumof 4% of the applied PCP at day 5), trichlorophenol (maximum of 2% of the applied PCP), PCA (maximum of 2% of the applied PCP at day 10 and declined to 1% of the applied PCP at 30 days) and various other transformation products detected in trace amounts. Based on the graphs provided in this study, an observed half-life of approximately 20 days for PCA can be estimated. This is considered a conservative half-life estimate since PCP was present in the test system over the course of the study and would have behaved as a continuous source of PCA.

The principal degradation pathway of PCP in anaerobic soil is progressive dechlorination to tetra- and tri-chlorophenols. The formation of pentachloroanisole appears to be a minor pathway. When present in anaerobic soil, PCA converts to PCP and follows the PCP degradation pathway.

2.3.2 Aquatic biotransformation

2.3.2.1 Aerobic

In a study submitted by a registrant and reviewed by the U.S. EPA (U.S. EPA 2008), radiolabeled PCP degraded in aerobic flooded sandy loam soil with an observed half-life of 14 days; the calculated first-order half-life was 4.9 days. The major degradation products of PCP were 3,4-dichlorophenol, various isomers of tetrachlorophenol and trichlorophenol. Bound residues and volatiles accounted for up to 41% and 0.9% of the radioactivity, respectively. PCA was not one of the standards used to compare with the observed transformation products, however, all the major transformation products were identified, there were no significant amounts of unidentified radioactivity and overall recoveries were good (88-117%). It is unlikely that PCA was a major transformation product in the studies submitted for registration. A summary of the results of the biotransformation study are found in Table 2.7-2.

2.3.2.2 Anaerobic

No laboratory studies examining the behaviour in PCA in sediment were found. The information derived from the anaerobic soil studies will be used as surrogate information.

2.3.2.3 Aquatic Field Study

Pierce and Victor (1978) studied the fate of PCP and its transformation products in an aquatic system after an accidental release in 1974 of wood-treating wastes containing PCP in fuel oil and a second spill in 1976. The authors reported that PCP and its transformation products, TeCP and PCA measured in water and in fish for over six months following the spill. Fish were observed to accumulate PCP and PCP transformation products (PCA and TeCP) rapidly from the water. The concentrations in fish decreased as the concentration in the water decreased, but required six to ten months to reach background levels. Interpretation of the data is complicated by the chronic influx of PCP from the contaminated watershed areas and the possible periodic release of small amount of PCP-containing waste from the industrial holding pond.

The average values as reported by Pierce and Victor were plotted and are presented in Figures 2.3-1 to 2.3-10.

At all sites, PCP underwent simultaneous degradation and partitioning from the water column to the sediment as is shown by the simultaneous decrease in the water concentrations of PCP and the increase in the sediment concentrations of PCP and its transformation products. TeCP and PCA.

Concentrations of PCA in the water column remained low during the observation period. Initial low concentrations of PCA increased gradually in the sediment over the four-month period. At

these sites, significant amounts of PCP were still available as a source of PCA. The continuous formation of PCA from PCP precluded an assessment of the degradation/persistence of PCA. However, due to the presence of TeCA (tetrachloroanisoles) and tetrachlorophenol, as reported by the authors, it is possible that some transformation of PCA was occurring.

Decreased concentrations of PCP, PCA and TeCP were observed at Site A, however, this site was located in a stream and there is too much uncertainty regarding the fate of the sediment to make any conclusion regarding dissipation half-lives (e.g., sediments may have been washed downstream or buried over time).

The low solubility of PCA in water (<1 mg/kg) and the high estimated K_{OC} value (2474 and 13800 L/kg) indicate that PCA is likely to partition to sediment in aquatic systems. Given the absence of PCA in the technical product, it is likely that in this aquatic system, PCA was formed through the biomethylation of PCP in the sediment. Once in the sediment, it is likely that simultaneous formation of PCA from PCP and demethylation of PCA back to PCP was occurring as predicted by the laboratory transformation studies. Since significant amounts of PCP were available as a source of PCA over the monitoring period, the continuous formation of PCA from PCP precluded a half-life calculation of PCA. However, the increase in concentration of the tetrachlorophenols indicates that PCP was also undergoing dechlorination to lower chlorinated phenols predicted by the laboratory studies to be the main degradation pathway of PCP.

As this was a field study, it was not possible to capture all potential losses including the loss due to volatilisation. The physical and chemical properties of PCA indicate that volatilisation is a potential source of loss from water. The fate dynamics between PCP and PCA in sediment, water and air in the aquatic environment preclude assessing a true degradation half-life from field or monitoring data. However, qualitative information such as the partitioning behaviour of PCA in aquatic systems (i.e., movement from water to sediment) and the degradation of PCP to lower chlorinated phenols is consistent with the biotransformation and mobility observed in the laboratory studies.

Figure 2.3-1: Fate of Pentachlorophenol in the water column of an aquatic ecosystem following a spill in 1976 at Site A. (Pierce and Victor, 1978)

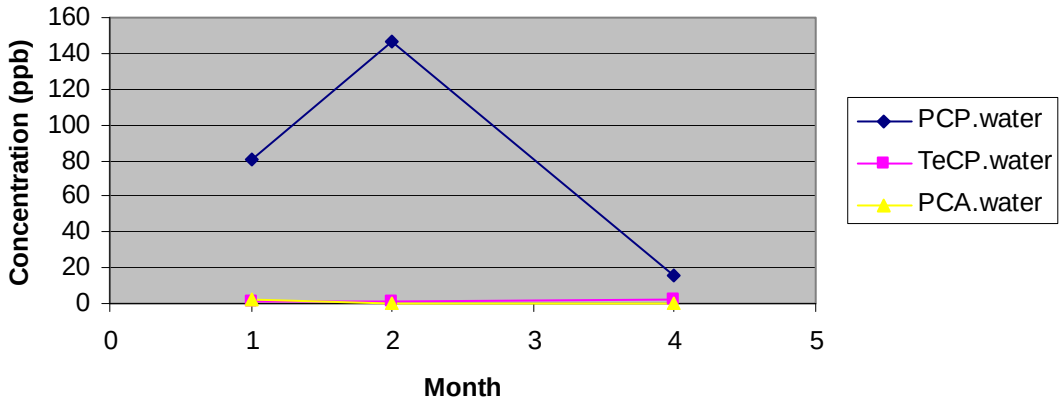


Figure 2.3-2: Fate of PCA and TeCP in the water column of an aquatic ecosytem following a PCP spill in 1976 at Site A(Pierce and Victor, 1978)

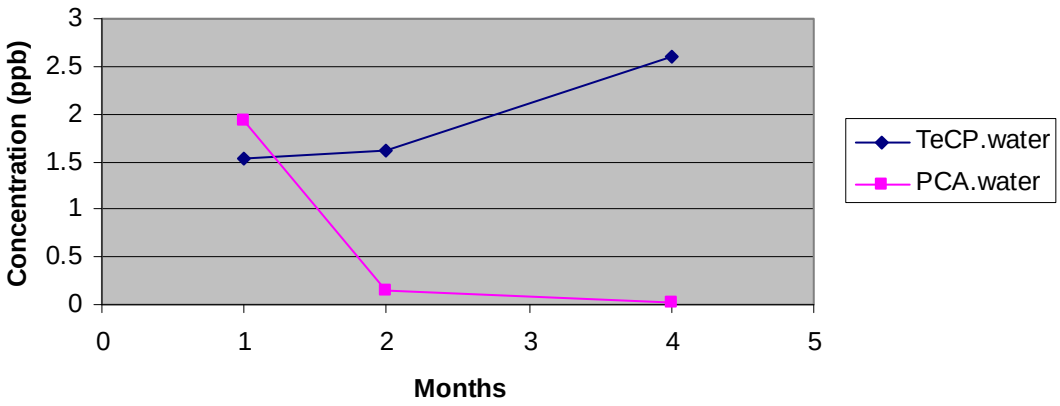


Figure 2.3-3: Fate of Pentachlorophenol in the sediment of an aquatic ecosystem following a spill in 1976 at Site A. (Pierce and Victor, 1978)

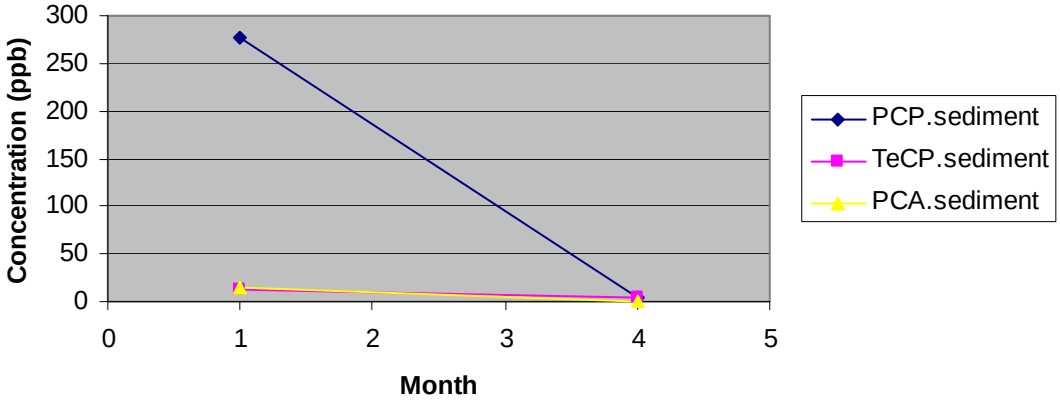


Figure 2.3-4: Fate of Pentachloroanisole (PCA) and 2,3,5,6-Tetrachlorophenol in the sediment of an aquatic ecosystem following a spill in 1976 at Site A. (Pierce and Victor, 1978)

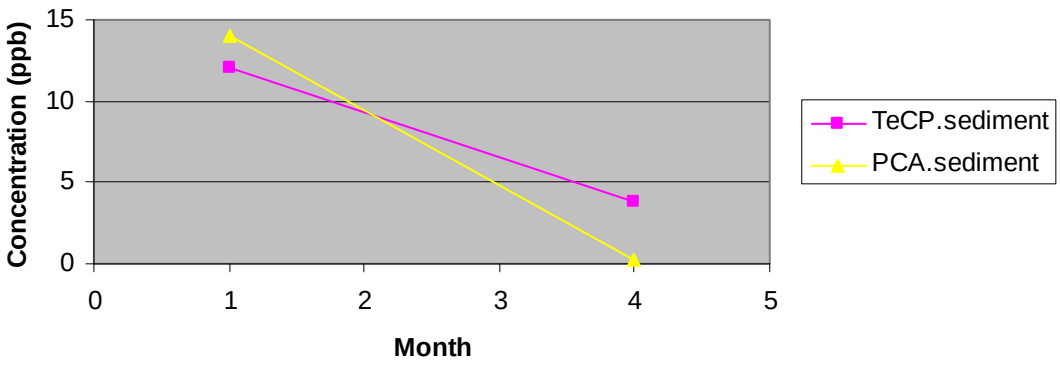


Figure 2.3-5: Fate of Pentachlorophenol in the water column of an aquatic ecosystem following a spill in 1976 at site B. (Pierce and Victor, 1978)

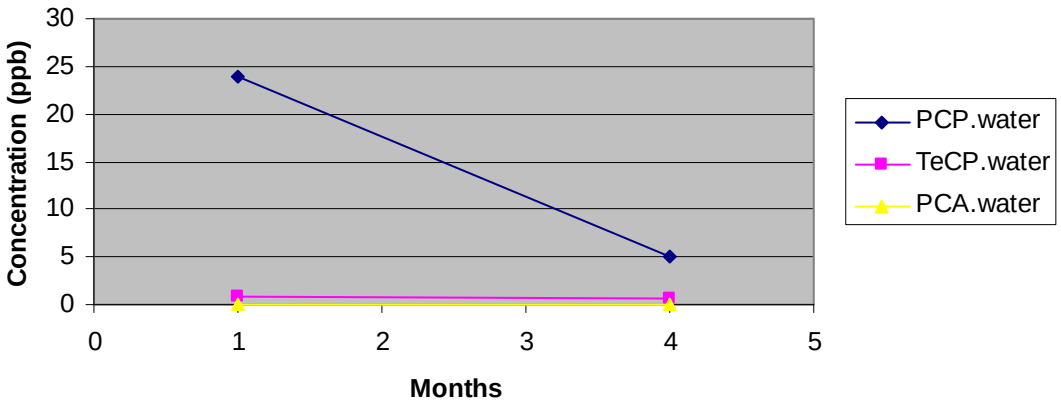


Figure 2.3-6: Fate of PCA and TeCP in the sediment of an aquatic ecosytem following a PCP spill in 1976 at Site B. (Pierce and Victor, 1978)

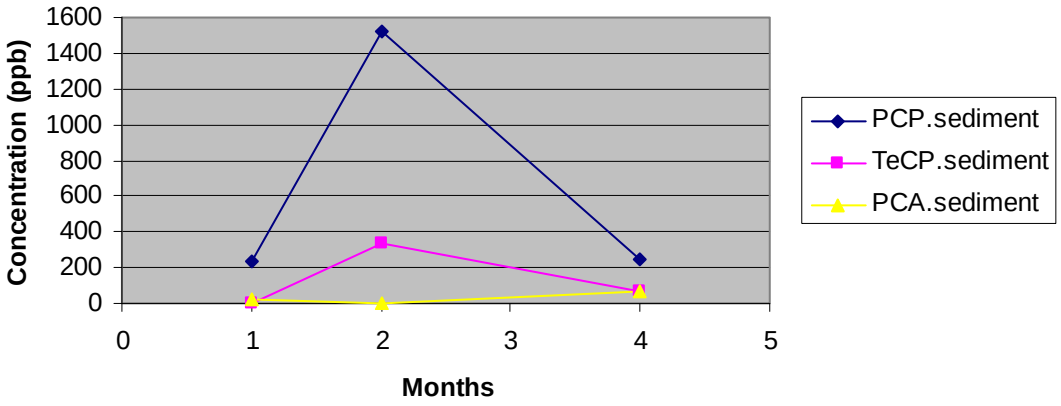


Figure 2.3-7: Fate of PCP, PCA and TeCP in the water column of an aquatic ecosytem following a PCP spill in 1976 at Site C. (Pierce and Victor, 1978)

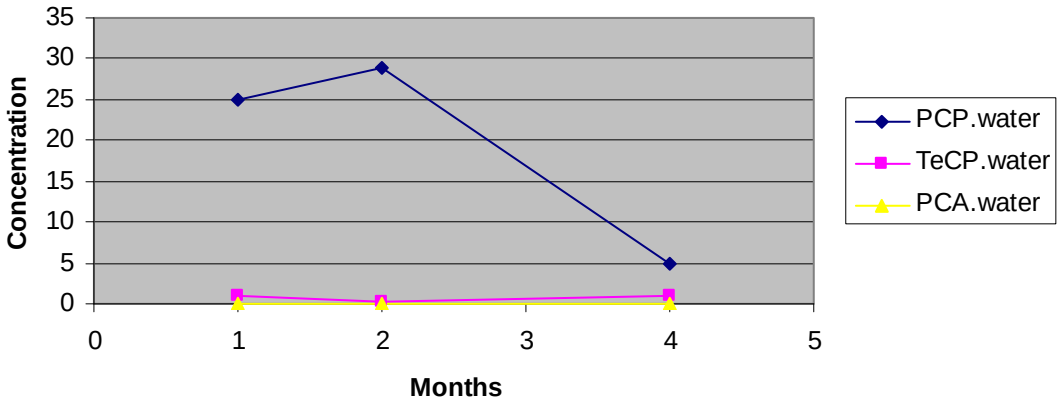


Figure 2.3-8: Fate of PCP, PCA and TeCP in the water column of an aquatic ecosytem following a PCP spill in 1976 at Site C. (Pierce and Victor, 1978)

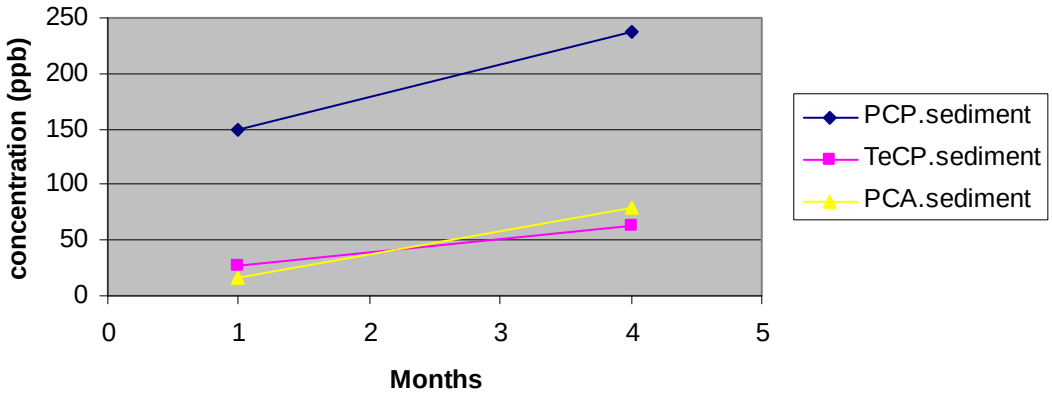


Figure 2.3-9: Fate of PCP, PCA and TeCP in the water column of an aquatic ecosytem following a PCP spill in 1976 at Site D. (Pierce and Victor, 1978)

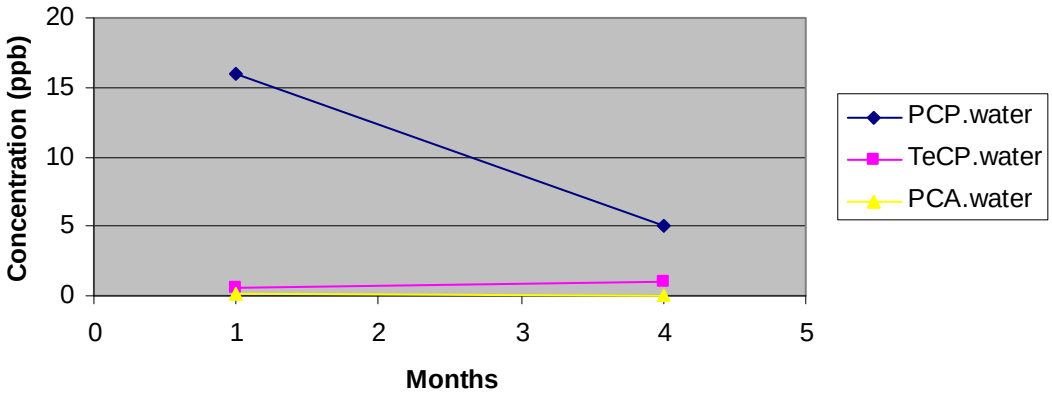
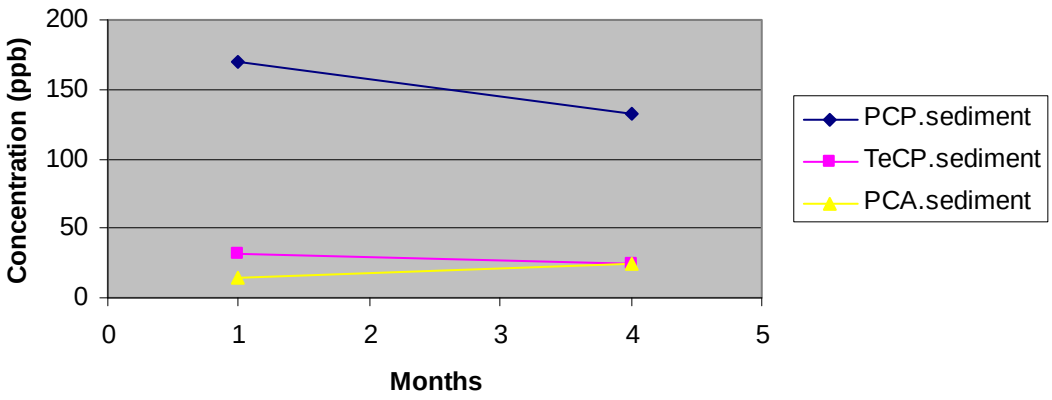


Figure 2.3-10: Fate of PCP, PCA and TeCP in the sediment of an aquatic ecosytem following a PCP spill in 1976 at Site D. (Pierce and Victor, 1978)



2.3.3 Fungal and Bacterial Biodegradation

Pentachloroanisole formation from PCP metabolism is well established in fungi (Cserjesi and Johnson 1971; Lamar and Dietrich 1990; Okeke et al. 1997; Tuomela et al. 1999 and Chung and Aust 1995). PCP methylation to PCA can be mediated by common aerobic fungi such as *Trichoderma virgatum, Phanerochaete chrysosporium*, *Phanerochaete Sordida, Lentinula edodes* (Walter et al. 2004; Lamar et al. 1990; Okeke et al. 1997; Cserjesi and Johnson, 1971). Some white-rot fungi are effective at o-methylating chlorinated phenols (Walter et al. 2004). There are two strains of white rot fungi (*Phanerochaete* spp.), *P. chrysoporium* and *P. sordida,* which have been studied extensively for bioremediation purposes. In the presence of *P. chrysoporium and P. sordida*, pentachlorophenol is rapidly methylated to PCA which is further mineralised. Other white-rot fungi such as *Trametes versicolor* do not convert PCP to PCA

(Walter et al. 2004; Walter et al. 2005). In the organisms that preferentially convert PCP to PCA, conversion appears to be a detoxification step that allows metabolism of otherwise toxic levels of PCP. Unlike PCP, PCA is not an inhibitor of oxidative phosphorylation and is therefore less toxic to wood-rotting fungi and other microbes (Chung and Aust 1995; Sukuki 1983b).

Many discrepancies were noted in the results obtained from various fungal studies depending on the experimental design and the species tested. Some discrepancies existed between the degradative pathways observed in media inoculated with a mixed microflora and those inoculated with isolated microbial cultures; the amount of volatile organics reported in studies conducted with liquid culture versus soil and field-scale bioremediation tests (e.g., Walter et al. 2004; Walter et al. 2005); the amount of volatile organic compounds when volatile traps were placed inside or outside the test vessels (Larmar et al. 1990; Badkoubi et al. 1996). As an example, Lamar et al. (1990) found that despite an apparently superior ability to mineralise PCP in liquid culture, *P. sordida* 13 did not deplete PCP from a sterile soil as rapidly or to as great an extent as did *P. chrysosporium*. However, rates and extents of PCP depletion by the two fungi in a contaminated field soil were similar. Also, the loss of PCP via mineralisation in soils inoculated with *P.chrysosporium* was negligible (i.e., <2%). Since loss via mineralisation is not a major transformation process of PCP depletion in soils inoculated with white-rot fungi, a superior ability to mineralise PCP in liquid culture does not appear to be useful for screening fungi for remediating PCP-contaminated soil.

As such, these studies should be interpreted with caution and their relevance to the actual environmental field should be considered. See Table 2.7-3.

Liquid Culture:

Studies showing the production of PCA as a major volatile product using liquid media inoculated with *P. chyrsosporium* include Walter et al (2004), Badkoubi et al. (1996), Okeke et al. (1994) and Lamar and Dietrich (1990).

In a study to determine growth substrate selection for white-rot fungi, Walter et al. (2004), conducted an additional experiment using liquid medium under laboratory conditions. The authors reported an unusually high amount of volatile in the traps (26-95% of the applied PCP; almost all PCP with traces of PCA). In the *P.chrysosporium* culture, 75% of the volatilised residues were attributed to PCA. The authors speculated that the large volatile fraction measured in the liquid culture may have been an artefact of the experimental design since the high volatile release seen in the liquid cultures was not observed in the soil microcosms (in the soil microcosms, volatile fractions were reported in the range of 1-2% of the applied).

Similar observations were also made by Badkoubi et al. (1996) examining *P. chrysosporium* in liquid culture. After 12 days, 82% of the PCP was volatilised as PCA. If the fungus is oxygen-limited for lignin peroxidise production, it will convert most of the PCP to the volatile PCA, the only volatile compound detected in the presence of *P. chrysosporium* in this experiment. When sufficient oxygen was available, the extent of mineralisation was much greater, up to 32%. Higher mineralisation was observed when the volatile transformation products had a chance to equilibrate between the solution and the headspace. Immediate removal of the volatile transformation products reduced PCP mineralisation. Therefore, the PCA remaining in the

solution and PCP will be mineralised and produce more $^{14}CO_2$ over time compared with the case when all PCA is depleted from the liquid and sorbed on the polyurethane volatile trap.

Soil:

Chung and Aust (1995) found that both PCP and PCA are readily mineralised in the soil by *P.chrysosporium* in soil. The rate of degradation increases with increasing concentration of PCA from 50 to 1600 ppm. At 100 ppm in soil, PCP was depleted in 18 days while 40% of the initial 100 ppm PCP was found as PCA. At 800 ppm, about 44% of the PCP remained after 18 days, but only about 10% of it appeared as PCA, and about 9% of the original 800 ppm PCP was mineralised. The rate of mineralisation of PCA increased with increasing concentration of PCA. Essentially no radioactivity (<0.05%) was found in the volatile organic traps and the aqueous fraction during the mineralisation of either PCP or PCA. It would therefore appear that the rate of methylation is rate-limiting at high levels of PCP, but significant rates of PCA degradation still occur. The authors concluded that *P. chrysosporium* can degrade PCP efficiently and produce no harmful intermediates during the degradation of PCP in soil and that both PCP and PCA are readily mineralised in soil.

In Lamar et al. (1990), the depletion of PCP by *P. chrysosporium* and *P. sordida* occurred in two-stages. In the first stage, the rapid deletion of PCP coincided with an accumulation of PCP. At the end of the first stage, 64% and 71% of the PCP was converted to PCA in *P. chrysosoporium* and *P. sordida* cultures, respectively. In the second stage, levels of PCP and PCA were reduced by 9.6 and 18%, respectively in soil inoculated with *P. chrysosporium* and by 3 and 23%, respectively in soil inoculated with *P. sordida*.

Other organisms:

The production of PCA from PCP has been observed in other isolated species of soil microflora. Rott et al. (1979) found PCA was produced in very small yields (<0.005%) in 5 of 10 bacterial strains tested. Haggblom et al. (1988) found that all strains of *Rhodoccoccus mycobacterium* tested initiated degradation of chlorophenols by para-hydroxylation, producing chlorinated-hydroquinones that were further degraded. Strains also o-methylated the chlorinated phenols, guaiacols, syringols and hydroquinone. This reaction occurred in parallel to the degradation reaction, but was slower. Okeke et al. (1993;1994;1997) found that transformation of PCP to PCA is an important route of PCP depletion during the early stages of PCP biotransformation by *L. edodes* (shiitake mushroom).

Conclusion:

Although the above mentioned studies provide some information on the degradation pathways and transformation products, they may not be appropriate for determining the relative production of PCA from PCP, nor persistence as described by domestic and international PBT policies given the specific conditions (growing conditions, species) under which the studies are conducted.

2.4 Mobility

2.4.1 Adsorption / desorption

The estimated soil adsorption coefficient (KOCWIN v2.0 in U.S. EPA 2001) is 2474 L/kg (MCI method) and 13800 L/kg (Kow method) (Appendix II). The Koc estimate of 2474 and 13800 indicate that PCA is likely to be immobile or have slight mobility when in soils as per the McCall et al. (1981) classification scheme. The high K_{OC} also indicate that in aquatic systems, PCA is likely to partition to sediment.

2.4.2 Leaching

After an extensive literature search no additional information on leaching of PCA was found.

2.4.3 Potential for Long-Range Transport

The Henry's law constant of PCA indicates that PCA will likely volatize rapidly from water. Based on this Henry's law constant, the volatilization half-life from a model river (1 m deep, flowing 1 m/sec, wind velocity of 5 m/sec) is estimated to be 2.2 hours. The volatilization half-life from a model lake (1 m deep, flowing 0.05 m/sec, wind velocity of 0.5 m/sec) is estimated as 6.9 days. Also, volatilisation of PCA has been observed in several laboratory studies using liquid medium (Badkoubi et al. 1996, Walter et al. 2004, Lamar et al. 1990).

Additional analysis of the information available in the published literature indicates that PCA was only found in the volatile fraction of laboratory studies conducted under very specific test systems (liquid culture medium) with specific test species that preferentially convert PCP to PCA (e.g., some species of white rot fungi) (e.g., Badkoubi et al. 1996; Walter et al. 2004). The experimental results showing the volatility of PCP and PCA were not repeated when similar studies were conducted in soil (Walter et al. 2005; Chung and Aust 1995).

A QSAR estimate of the phototransformation half-life of PCA in air is estimated to be 9.8 days (U.S. EPA 2011). No other information on half-lives of PCA in air was available.

Based on the QSAR estimate for the half-life in air and the detection in air and snow in the arctic, there is evidence indicating the PCA is persistent in air and can be transported to remote locations. Additional unpublished information provided by EC show the presence of PCA in arctic biota. Table 2.4.3-1 summarises the levels of PCA detected and reported in the open literature.

Various studies showing residues of PCA in various abiotic matrices are available in the published literature, however, most of this information originates from impacted environments where PCP is currently being used or was used historically. Since media from these studies are continuously exposed to PCP (and possibly to PCA via soil/sediment biomethylation of PCP), the usefulness of this information in determining environmental persistence and/or evidence of long range transport is questionable. Additional analysis has been provided which allows for distinguishing between local and non-local sources of PCA.

As an example, the Atlas et al. (1986) study was referred to in the Addendum for PCP (BiPRO GmbH, 2010) as evidence of the long range transport of PCA. However, high levels of an unstable and rapidly oxidised transformation product of PCP, TCHQ (tetrachlorohydroquinone) were also measured with PCA. The authors speculated that the appearance of TCHQ indicated that the source of PCP/PCA may actually be local, not remote. In another study, Schreitmuller and Ballschmiter (1995) conclude that the general source of PCA and other semi-volatile organic compounds such as HCH and tetrachlorodimethoxybenzene in pristine marine air is from the oceanic system. Due to the air-surface water equilibrium, as anthropogenic inputs of PCP into air decreases, the authors predict that the oceans will become the nonpoint source of these substances.

There are six studies (Welch et al. 1991; Su et al. 2008; Hung et al. 2005; Rawn et al. 2001; Muir 2007 in Hoferkamp et al. 2010 and MacDonald et al. 2000) showing residues in air, snow and sediment in remote locations. These are indicated by the shaded rows in Table 2.4.3-1.

In addition, Environment Canada has provided the PMRA with additional unpublished information on residues in air in remote areas (Hung et al. unpublished archive data, Environment Canada). New information on the concentrations in ambient air at the Arctic research station in Alert, Canada are summarised in Table 2.4.3-2.

Considerations:

The monitoring of PCA in arctic air is information indicating that PCP/PCA residues in sediment, snow and biota in remote areas may be due to long range transport. However, whether PCA in these remote matrices is due to the continuous environmental loading from the long range transport of PCP/PCA from current uses of PCP, revolatilisation of PCP/PCA residues from historically contaminated sites and/or the degradation of local organochlorine substances such as PCP, HCB and PCNB cannot be determined. There is also additional supporting evidence that historical organochlorine contamination in oceans is a major continuous source of semi-volatile organochlorine substances (SOCs) including PCA in the environment. Schreitmuller and Ballschmiter (1995) indicated that the North Atlantic Ocean is undersaturated and the South Atlantic is close to a gas-water exchange equilibrium with PCA and three other SOCs. Particularly under conditions of a diminishing input of SOCs from continental sources, the air-surface water equilibrium will render the oceanic system to be a global nonpoint source of anthropogenic compounds in marine air. Similarly, Hoferkamp et al. (2010) indicated that with the exception of lindane and α-endosulfan (Weber et al., 2006) there is insufficient data to assess whether air concentrations are resulting in net deposition to Arctic Ocean and lake waters or whether these waters are actually outgassing the currently used pesticides (including PCA) monitored in the arctic. Other sources to the ocean could include long distance transport in ocean currents as has been postulated for β-HCH (Li et al., 2002). Glacier runoff could be an important source for some lakes and estuaries (Blais et al., 2001; Bizzotto et al., 2009).

Given there is several current sources of PCA in the environment, it is constantly being both formed and degraded and it is a semi-volatile chemical, low levels of PCA appear to be ubiquitous. These factors confound the use of monitoring data alone to determine the intrinsic persistence and long-range transport of PCA. The laboratory studies conducted under controlled

conditions using degradation kinetics appropriate for transformation products (i.e., either by accounting for both formation and decline or by using PCA as the starting material) would be the preferable method to characterise the fate and persistence of PCA.

Table 2.4.3-1 Residues of PCA detected in various matrices as reported in the open literature as originally reported in BiPRO GmbH (2010) with corrections in red text.

Compartment	Year	Location	Concentration	Comment	Reference
Sediment	1998-1999	Mississippi River, USA	~~≤2700 ng/kg~~ ≤ 7.4 ng/g	PCP was not detected at any site, however, PCA was detected in almost every sample. The authors stated that PCP is probably present in sediments and converted to PCA. Concentrations were 2-4 times higher in the spring than in summer at every site (1989 and 1990). The main source of PCA in the spring is the Ohio River (highly contaminated industrial river).	Rostad et al. 1999
Brown Snow	1988	Canadian Arctic	melted snow: 1230 pg/L particles: 4.3 mg/g Brown snow: 1442 pg/L	Long-range-transport via fine particulates. Origin of brown snow: Asia.	Welch et al. 1991
Water	1998	Yangtze River,China	0.6 ng/L	Sampled from an area with history of intensive use of polychlorinated organic compounds in agriculture and industry (including PCP as an agricultural pesticide)	Jiang et al. 2000
Sediment	1998	Yangtze River, China	~~≤4800 ng/kg~~ <1 ng/g	Values were taken from a graph and were difficult to read. The actual value reported for PCA was < 1 ng/g (not ≤4800 ng/kg as reported in the UNECE Document)	Jiang et al. 2000
Soil	1989	Finland	~~≤1g/kg~~ 0.01-1 µg/g (mg/kg)	Soil taken from a contaminated site. Sawmill had been closed for 30 years.	Haimi et al. 1993
Air	1985	South Pacific Ocean	PCA:9.0 pg/m^3 TCHQ-DE: 6.2 pg/m^3	Residues of TCHQ indicate that the source of PCP/PCA is local. TCHQ is unstable and is rapidly oxidized. TCHQ-DE is a transformation product of PCA.	Atlas et al. 1986
Air	1985	New Zealand	PCA:2.0 pg/m^3 TCHQ-DE: 13.4 pg/m^3		Atlas et al. 1986
Air	2000-2003	Arctic	Mean: 4.9 pg/m^3	Air concentrations showed strong seasonal/spatial variations. At ALT, air concentrations were lower in summer than in winder. At PTB,	Su et al. 2008

Compartment	Year	Location	Concentration	Comment	Reference
				concentrations were higher in summer than in winter. Three episodes of elevated PCA concentrations were observed in June-August 2002 at PTB. Back-trajectories indicate that the air masses largely originated from the Eurasian portion of the arctic Ocean or the Russian Arctic. At KNG and LFL, no patterns were observed. Mean and median concentrations were comparable at ALT, KNG, LFL and PTB. PCA air concentrations were low at VKK in July-September 2002.	
Air		Canadian and Russian Arctic	2.6 – 4.0 pg/m^3	Greater than 17% of all samples exceeded "breakthrough" (amt of chemical on front PUF/amt on back PUF) > 0.333.	Hung et al. 2005
Sediment	N/A	Alexandrian Harbour, Egypt	"Near or below detection limits"	Potentially impacted by wastewater disposal (sewage and industrial) and agricultural run-off.	Barakat et al. 2002
Air	2004-2005	Durban, South Africa	"detected in all samples" max: 20±13 pg/m^3 at one site (Nizam)	The elevated levels of PCA at Nizam were twice that measured at other sites. The authors indicated that this may suggest a local source, but uncertainties in measurements must be recognised.	Batterman et al. 2008
Sediment	2000	Yellow Sea	Sediment: ND-0.04 ng/g dw Biota: ND-0.95ng/g dw	Borders with China, North and South Korea. Highly impacted body of water. Industrial wasterwater containing major pollutants from port cities, and non-point source contaminants of agricultural origin, oil discharge/exploration	Oh et al. 2005
Sediment	1992-1995	Seven Yukon Lakes	Max values in lakes range from 0.33-4.52 ng/g dw with lower concentrations in surface sediment	Concentrations of the OC compounds [HCH-lindane, CHL-chlordane, CBz-chlorinated benzenes (including TCP, TeCP and PCP) and PCA] were similar to concentrations reported for other Arctic lake sediments previously studied, and show little evidence of major local inputs.	Rawn et al. 2001
Snow	2005	Devon Ice-Cap, Canada	Flux = 0.4-0.6 ng.m^2/yr	No details given.	Muir ~~and Zheng~~ 2007 in Hoferkamp

Compartment	Year	Location	Concentration	Comment	Reference
					et al. 2010
Air	1993-1994	Can. Arctic	2.3-3.1 pg/m^3 <0.01(LOD) – 20.5 pg/m^3 Average weekly atmospheric concentrations Particle: 0.01-0.02 pg/m^3 Gas: 1.80-4.12 pg/m^3	Concentrations in Alert, Dunai and Tagish	Macdonald et al. 2000

-shaded rows indicate measured values are likely a result of long-range transport.
-N/A- Not Available

Table 2.4.3-2 Environment Canada Unpublished: PCA in ambient air at Alert, Canadian Arctic. Concentration of pentachloranisole in ambient air at Alert between 1992-2008 (pg/m^3), (Hung et al. archive data, Environment Canada)

Year	Number of Samples	Number of Detects	% Detects	Mean	SD	Median	Range
1992	39	28	72	3.0	2.3	2.7	<MDL-8.8
1993	49	36	73	2.1	1.5	1.9	<MDL-5.6
1994	52	50	96	3.1	1.4	3.0	<MDL-6.0
1995	49	46	94	2.6	1.5	2.3	<MDL-7.6
1996	51	47	92	2.8	2.3	2.2	<MDL-16
1997	50	44	88	1.3	0.7	1.1	<MDL-2.9
1998	49	47	96	3.7	2.3	3.5	<MDL-12
1999	52	49	94	4.3	2.3	4.4	<MDL-8.9
2000	52	50	96	3.4	2.1	3.0	<MDL-10
2001	52	52	100	6.0	5.2	4.2	0.8-20
2002	52	27	52	13	13.7	11	<MDL-55
2003	51	40	78	1.1	0.7	1.0	<MDL-3.0
2004	53	40	75	53	323	1.1	<MDL-2356
2005	52	4	8	2	5.0	0.6	<MDL-24
2006	52	25	48	1.0	2.0	0.6	<MDL-13
2007	27	0	0	<MDL	<MDL	<MDL	<MDL
2008	27	4	15	0.5	0.4	0.6	<MDL-1.7
1992-2008	809	589	73	6.5	6.5	1.7	<MDL-2356

Notes: MDL=0.6 pg/g m^3 (Su et al. 2008)

2.5 Bioaccumulation

Aquatic Organisms:

Laboratory Studies:

In a bioaccumulation study conducted by Oliver and Niimi (1985), rainbow trout (*Oncorhynchus mykiss)* were exposed to PCA (and 17 other compounds simultaneously) at average water concentrations of 0.9 ± 0.3 and 10 ± 6.2 ng/L for 96 days. BCFs in the low concentration tank appeared to reach a steady state on day 35. BCFs in the high concentration tank were more variable, but a steady state appeared to have been reached on day 50. Concentrations of PCA in the water were variable over time. Variation was 33% in the low concentration tank (0.9 ± 0.3 ng/L) and was ca. 66% in the high concentration tank (10 ± 6.2 ng/L). However, even if the water concentrations were variable, average BCFs would still be well above 5000 (15,000 ± 4,950 and 20,000 ± 13,200 in the low and high concentration tanks, respectively). This study meets or exceeds the fish BCF study guideline as outlined in the U.S. EPA Fish BCF study OPPTS 850.1730. No depuration phase was conducted, but this does not affect the quality of the study.

A 7-d static bioaccumulation study conducted on guppies (*Poecilia reticulate)* by Opperhuizen and Voors (1987) was not considered appropriate for the determination of bioaccumulation factors for classification purposes because the test system was not at equilibrium and recovery rates were extremely low (22.5% for PCA) due to a continuous decrease in aqueous concentrations. However, additional information on the behaviour of PCA in fish can be obtained from the study. The authors concluded that chloroanisoles were eliminated rapidly from the fish. Half-lives for the tetra- and the pentachloroanisoles were between one and four days. Since a rapid decrease of the total amount of test compounds in the aquarium was found for all congeners, the calculation of bioconcentration factors was not possible. Only estimates of the concentration ratio between fish and water are made. Based on the observed high loss of the test compounds from the system and the formation of metabolites, the authors suggested that the total clearance is dominated by transformations of the chloroanisoles. Clearance rates of chlorinated anisoles in fish are much higher than expected from their estimated hydrophobicity. The authors speculated that this may be explained by metabolic hydrolysis of the ether bonds into corresponding hydroxyl groups. Due to these high elimination rates, bioconcentration factors are relatively low, compared to those of chlorobenzenes and other hydrophobic chemicals.

In a bioaccumulation study conducted Glickman et al. (1977), rainbow trout were exposed to ^{14}C-PCA at concentrations of 0.024 mg/L. Fish were sampled at 1, 2, 4, 8 and 12 hours in the uptake study and, after transfer to clean water they were sampled at 0, 4, 8, 15, 24, 48, 72, 96, 120, 144 and seven days. Half-lives of PCA in tissues of rainbow trout were 6.3, 9.8, 23 and 6.3 days in blood, liver, fat and muscle, respectively. Corresponding extrapolated half-lives of PCP were 6.2, 9.8, 23 and 6.9 hours. PCP–exposed trout showed no methylation of PCP to PCA in any of the tissues studied. However, the bile of the PCA-exposed trout contained PCP glucuronide as well as PCA, indicating demethylation of PCA *in vivo* by the rainbow trout.

Aquatic Field Bioaccumulation:

Pierce and Victor (1978) studied the fate of PCP and its transformation products in an aquatic system after exposure from an accidental release of wood-treating wastes containing PCP in fuel oil in 1974 and a second spill in 1976. The authors reported that PCP and its transformation products, TeCP and PCA persisted in water and in fish for over six months following the spill. Interpretation of the data is complicated by the chronic influx of PCP from the contaminated watershed areas and the possible periodic release of small amount of PCP-containing waste from the industrial holding pond.

Fish were observed to accumulate PCP and PCP transformation products (PCA and TeCP) rapidly from the water. The concentrations in fish decreased as the concentration in the water decreased, but required six to ten months to reach background levels.

Terrestrial organisms:

BAFs of PCA and TeCA in earthworms exposed to soil from a contaminated site were reported as 5-40 (Haimi et al. 1992, Haimi et al. 1993). In a laboratory experiment, the concentrations of 2,3,4,6-tetrachloroanisole and pentachloroanisole were high in earthworms one week after introduction. Concentrations in earthworms and soil decreased to a low level at a considerable rate (in approximately 5 weeks). Similar degradation rates were observed in the control soils without earthworms and the soils with earthworms. In the earthworms, the concentration of 2,3,4,6-TCA and PCA increased until week 15, after which they decreased.

Vodicnik et al. (1980) determined that following injection of PCA into female mice that elimination of [^{14}C]PCA equivalents was rapid with half-lives ranging from 5-10 hours in all tissues except the liver. Excretion of ^{14}C was primarily through the urine. However, there was no evidence of parent PCA in either urine or feces. PCP was detected in the urine and feces at approximately 2 and 32% of applied radioactivity, respectively. The majority of the ^{14}C was associated with the PCP conjugate. The authors concluded that PCA must be demethylated prior to conjugation and/or excretion.

Other references include Ikeda and Sapienza (1995) and Ikeda et al. (1994). These have not been reviewed, but are provided here as additional references.

The above information on bioaccumulation is summarised in Table 2.6-1.

Field Residues in Biota

Information on residues in biota has been reported previously in the PCP addendum (BiPRO GmbH, 2010). The majority of the studies reporting residues in various biota are from highly impacted environments and are thus a result of local contamination of PCP/PCA. There are three references (Vorkamp et al. 2004; Bentzen et al. 2008 and Swachkhammer et al. 1988) showing low levels residues in biota at or below detection limits in remote locations indicating that PCA is ubiquitous. In should be noted that Vorkamp et al. (2004) also indicated that the concentrations in top predatory marine mammals did not exceed the concentrations in marine fish, contradicting the typical pattern of bioaccumulation in the food chain. Of the various tissues

analysed, the highest concentrations were found in the muscle, ranging from 0.08 ng/g lw (lipid weight) to 1.1 ng/g lw in beluga. Summarising the results for OCS, HCBD and PCA, it can be noted that all compounds occur in biota from Greenland, indicating the ubiquitous presence of these compounds in the environment. Compared with the results for chlorobenzenes and chlorinated pesticides, the concentrations are considered to be low. The references from remote areas are indicated by the shaded rows in Table 2.6-2.

New unpublished information has also been collected by the Government of Canada on residues in biota in remote arctic areas (email: Environment Canada to Health-Canada 23-05-2011). The concentrations in biota in remote areas are summarised in Table 2.6-3. From 2000-2010, the range of concentrations in polar bears, ringed seal, arctic char, landlocked char, lake trout and burbot are reported to be <0.1-42 ng/g lipid, <LOD-0.82 ng/g lipid , <LOD-0.095 ng/g lipid, <LOD-1.83 ng/g lipid, <LOD-0.35 ng/g lipid and <LOD – 3.85 ng/g lipid, respectively.

Additional Considerations

PCP is a major metabolism product of HCB in a variety of different animals including fungi, caterpillars, fish, rats, birds, monkeys and humans (Sanborn et al. 1977; Frankovic et al. 1995; Kasokat et al. 1989; Metcalf et al. 1973; Mehendale et al. 1975; Koss et al. 1976; Szokolay et al. 1980; Mehendale and Matthews 1973 in Courtney 1979; Lui and Sweeny 1975 in Courtney 1979; Renner 1981; Gomez-Catalane et al. 1987; To-Figueras et al. 1997; Engst et al. 1975; van Ommen et al. 1985; van Ommen et al. 1986; Muller et al. 1978; Deberts et al. 1981).
The pathway of metabolism of HCB in mammals was reviewed by Debets and Strik (1979) and by Renner (1988) as reported in EHC 195, 1997. HCB is metabolised into less chlorinated benzenes, chlorinated phenols, and other minor metabolites via three distinct pathways: i) oxidation giving rise to phenolic metabolites including PCP, tetrachlorohydroquinone and tetrachlorobenzoquinone; ii) glutathione conjugation leading to pentachlorothiophenol, pentachlorothioanixoles and other sulphur-containing metabolites; and iii) a minor pathway that yields lower chlorinated benzenes.

PCP is also a metabolic transformation product of PCNB (quintozene) in various mammals including rats and monkeys (EHC 41 1980; Muller et al. 1978; Kogel et al. 1979, Renner 1981). In the environment, the U.S. EPA (2008b) has also reported that PCP was detected as a metabolite of PCNB in several registrant-submitted environmental fate studies and in the published literature, Murthy and Kaufman (1978) reported PCP in anaerobic soils; Begum et al. (1979) reported PCP in onion plants and Torres et al. (1996) reported PCA in formation by a soil micromycetes.

There is also literature information on the formation of PCP from lindane. Kujawa et al. (1977) reports PCP as a transformation product of lindane in rats. In the summary report by Engst et al. (1979), the following references are cited as showing PCP was found as a transformation product of lindane: Balba and Saba (1974) reports PCP produced from lindane in plants, Engst et al., 1978a and Gopalaswamy and Aryar (1976) in mammals.

The EHC124 (1991) review of lindane, also cites several studies identifying chlorophenols, including PCP, as transformation products of lindane in animals (Grover & Sims 1965; Chadwick & Freal 1972a,b; Freal & Chadwick 1973; Kurihara & Nakajima 1974; Chadwick et

al. 1975; Engst et al. 1976; Kujawa et al. 1977; Stein et al. 1977; Tanaka et al. 1977; Engst et al. 1978b; Tanaka et al. 1979; Aiyar 1980; Fitzloff et al. 1982).

The presence of PCP or PCA in remote areas may be due in part to the metabolism of organochlorine substances already present in remote areas.

Conclusion:

The BCF values for PCA reported by Oliver and Niimi (1985) for fish exceed the laboratory criteria cut-off values for bioconcentration. However, additional laboratory and field information also indicate that PCA is metabolised and depurated in various species including fish, earthworms and mammals.

Although there is field evidence of PCA residues in various abiotic and biotic matrices from both impacted environments and environments with no obvious local source of PCP/PCA, there is not enough information provided in most of these studies to calculate a true field bioaccumulation factor (BAF) since residues in biota are low and water concentrations are not often reported in the same studies.

There are three references (Vorkamp et al. 2004; Bentzen et al. 2008 and Swachkhammer et al. 1988) and additional information provided by EC showing low levels residues in biota in remote locations. However, as noted by Vorkamp et al. (2004), the concentrations in top predatory marine mammals did not exceed the concentrations in marine fish, contradicting the typical pattern of bioaccumulation in the food chain. Compared with the results for chlorobenzenes and chlorinated pesticides, the concentrations (of PCA) are considered to be low.

Despite PCA being ubiquitous in air and found in multiple other media, PCA has not been detected in appreciable levels in biota in the field thereby contradicting the bioaccumulation potential predicted the aquatic BCF value. Metabolism, depuration, biodegradability and bioavailability of PCA are likely significant factors in reducing the likelihood of bioaccumulation and biomagnification in aquatic systems.

Table 2.6-1. Summary of Laboratory BCF and BAFs in Biota

Organism	Exposure Duration (days)	Exposure Concentration (ng/L)	BCF[1]	Depuration	Comments	Reference
Laboratory (fish)						
Oncorhyn-chus mykiss	35	0.9 ± 0.3	16000 ± 3500	Not reported.	Acceptable BCF study.	Oliver and Niimi 1985
	50	0.9 ± 0.3	14000± 2900			
	75	0.9 ± 0.3	12000± 2400			
	96	0.9 ± 0.3	17000± 7100			
	35	10 ± 6.2	11000± 3100			
	50	10 ± 6.2	20000± 2500			
	75	10 ± 6.2	15000± 2600			
	96	10 ± 6.2	24000± 5400			
Oncorhyn-chus mykiss	N/A	N/A	N/A	$T_{1/2}$: 6.3, 9.8, 23 and 6.3	Experimental. Radiolabeled.	Glickman et al. 1977

Organism	Exposure Duration (days)	Exposure Concentration (ng/L)	BCF[1]	Depuration	Comments	Reference
				days in blood, liver, fat and muscle, respectively.	Demethylation of PCA to PCP.	
Poecilia reticulata (Guppy)	7	40	~~9120*~~	Half-life:1-4 days Log Kd, oct: 5.45, log Kc: 3.96, K_1 (mL/g*d): 1710 K_2(d-1): 0.32	Not at equilibrium. 22.8% recovery. Continuous decrease in aqueous concentrations as contamination of the water was stopped before the fish were added. BCFs could not be calculated.	Opperhuizen and Voors 1987
Laboratory (mammals)						
Mice				Elimination half-lives of 5-10 hours in all tissues, except liver. The live half-life was 19.3 hours.	Excretion primarily through the urine as PCP-conjugate. PCA must be demethylated prior to excretion. Determined via ^{14}C and no attempt to differentiate between PCA and transformation products	Vodicnik et al. 1980
Field						
Earthworms	1-20 weeks	0.06-1.0 µg/g dw (1.24 – 20.8 µg/g OC)	5-40	Half-life of 5 weeks in soil and in earthworms.	BCFs estimated by IEP (2008). Earthworm reproduction was not affected.	Haimi et al. 1992, Haimi et al. 1993

Table 2.6-2. Summary of Field Concentrations of PCA in Biota as originally reported in BiPRO GmbH (2010) with corrections in red text.

Organism	Year/Location	Tissue	Concentration	Comment	Reference
Caribou	2004/Greenland	Muscle	≤ 0.2 ng/g ~~200~~ lipid wt (lw)	-Residues above the LOD in 6/10 samples of marine invertebrates and fish. **-The concentrations in**	Vorkamp et al. 2004
		Blubber, kidney	Detectable residues		
Atlantic Cod		Muscle, liver	2.3 ng/g ~~2300~~ lw (median)		
Capelin, Cod		~~Muscle,~~ Liver	2.3 ng/g ~~2300~~ lw (median)		

Organism	Year/Location	Tissue	Concentration	Comment	Reference
Snow crab		Muscle Liver	0.66 ng/g ~~660~~ lw 0.45 ng/g ~~450~~ lw	**marine mammals did not exceed the concentrations in marine fish, contradicting the typical pattern of bioaccumulation in the food chain.** -Summarising the results for OCS, HCBD and PCA, it can be noted that all compounds occur in biota from Greenland, indicating the ubiquitous presence of these compounds in the environment. Compared with the results for chlorobenzenes and chlorinated pesticides, the concentrations are considered to be low.	
Altlantic salmon		muscle	<0.01 ng/g ww		
Redfish		muscle	<0.01 ng/g ww		
King Eider, thick billed murre		Liver	0.36 ng/g lw ~~360,~~ 0.22 ng/g ~~220~~ lw Of the seabird samples analysed, the only median concentrations above the detection limit were found in king eider and thick-billed murre liver.		
Harp Seal Narwhal Beluga		Muscle	<0.08 ng/g ~~80~~ lw 0.54 ng/g ~~540~~ lw 1.1 ng/g ~~1100~~ lw		
Marine Invertebrates			Residues above the LOD in 6/10 samples of marine invertebrates and fish.		
Fish	1980-84, Rivers USA	Whole Body	100000 ww in 30% of 112 stations		Schmitt et al. 1990
Cassave	2006, Tanzania	Roots Leaves	600 2100 fresh wt.		Marco et al. 2006
Lake trout White fish	1988, Siskiwit Lake USA	Whole body	~~360~~ 3.6 ng/g lw ~~650~~ 6.5 ng/g lw		Swackhammer et al. 1988
Mussels	Finland	Whole body	~~25000~~ < 1 - 274 ng/g lw		Herve et al. 1988
Mango	Tanzania 2002	Leaves	<0.5 to 3900 fw		Marco and Kishimba 2007
Oysters/Mussels	USA costal waters	Whole body	<0.25-8.99 ng/g dw		Wade et al. 1998
Bass Carp	2004, USA, Mobile River Basin	Whole Body	0.06-0.38 ng/g ww 0.72-3.18 ng/g ww		Hinck et al. 2008
Carp Catfish	2003, Colorado River and tributaries	Whole body	>0.1 ng/g in 46 of 48 samples, carp had >10 ng/g		Hinck et al. 2007
Pseudo-sciaena crocea	2000, Yellow Sea	Muscle Liver	ND-0.95 ng/g dw ND-0.02 ng/g dw ND-0.27 ng/g dw		Oh et al. 2005

Organism	Year/Location	Tissue	Concentration	Comment	Reference
Collichthys niveatus			ND-0.04 ng/g dw		
Polar Bears	2003, Beaufort Sea Coast, Alaska	Fat	<0.1-27 ng/g ww <0.1-42 ng/g lw		Bentzen et al. 2008
Fish	Salton Sea, Calif.	Muscle	0.15-0.20 ng/g fw		Riedel et al. 2002

Most information is from highly impacted areas. Shaded rows are from remote locations.

Table 2.6-3. Summary of concentration of pentachloranisole in seals and fish from Arctic (ng/g lipid) (Muir, unpublished data)

Location	Number of Samples	Number of Detects	% Detects	Concentration (ng/g lipid)			
				Mean	SD	Median	Range
Polar bears (Alaska; Bentzen et al 2008)							
	57	?		11	10		<0.1-42
Ringed seal (2000-2009)							
Arctic Bay	19	5	26	0.21	0.15	0.16	<MDL-0.48
Arviat	49	24	49	0.29	0.27	0.14	<MDL-0.82
Gjoa Haven	22	10	45	0.25	0.11	0.24	<MDL-0.48
Grise Fiord	15	0	0	<MDL			
Holman	51	30	59	0.07	0.10	0.011	<MDL-0.40
Inukjuaq	10	4	40	0.03	0.012	0.03	<MDL-0.05
Kangiksuluaaq	3	0	0	<MDL			
Pangnirtung	10	10	100	<MDL			
Resolute	55	26	47	0.09	0.1	0.07	<MDL-0.32
Sachs Harbour	37	26	70	0.005	0.021	0.001	<MDL-0.11
Overall	271	135	50	0.11	0.174	0.03	<MDL-0.82
Sea run Arctic char (2004-2009)							
AR	10	0	0	<MDL			
Cambridge Bay	20	0	0	<MDL			
KA	10	0	0	<MDL			
KK	8	8	100	0.04	0.024	0.05	0.04-0.10
Nain	21	3	14	0.04	0.0057	0.04	<MDL-0.05
PondfInlet	10	0	0	<MDL			
PU	10	0	0	<MDL			
VR	5	0	0	<MDL			
Overall	94	11	12	0.05	0.02	0.05	<MDL-0.095
Landlocked char (2000-2009)							
Amituk lake	25	18	72	0.01	0.009	0.02	<MDL-0.03
Char Lake	32	9	28	0.50	0.60	0.57	<MDL-1.83
Lake Hazen	50	13	26	0.07	0.004	0.005	<MDL-0.017
Resolute Lake	45	45	100	0.14	0.07	0.12	0.04-0.38
Overall	152	85	56	0.13	0.24	0.07	<MDL-1.83
Lake trout (2002-2009)							

Location	Number of Samples	Number of Detects	% Detects	Concentration (ng/g lipid)			
				Mean	SD	Median	Range
Great Bear Lake	10	10	100	0.04	0.026	0.04	0.02-0.08
Great Slave Lake	52	32	62	0.08	0.087	0.04	<MDL-0.35
Overall	62	42	68	0.07	0.079	0.04	<MDL-0.35
Burbot (2002-2009)							
Great Slave Lake	41	31	76	1.23	1.16	0.78	<MDL-3.85
Overall	41	31	76	1.23	1.16	0.78	<MDL-3.85

Table 2.3-1 Registrant abiotic transformation studies conducted with radiolabeled PCP.

Fate Study	Transformation products identified	Major	PCA	PMRA#	U.S. EPA MRID
Hydrolysis pH 4,5 pH 9 pH 7	Volatilisation of PCP was observed None (PCP was stable) None (PCP was stable)	none	Was not detected and is not expected to be produced.	1339469	42481101
Photolysis at pH 5, 7 and 9 (radiolabeled study, recovery >96%)	Tetrachlorohydroquinone, tetrachlorocatechol. Tetrachlorosorcinol and dichloromaleic acid and/or anhydride	dichloromaleic acid and/or anhydride (exceeding 10% and accumulating at study termination-68-100% at study termination)	Was not detected and is not expected to be produced.	1169849 or 1147042 (same study)	42855401
Photolysis in air	2,3,5,6-TeCP and 3 additional polar photodegradates.		Was not detected and is not expected to be produced.	1149165	43214601-unacceptable
Photolysis in Soil	-3 minor products (<10% and were not identified) -up to 2.25% were bound residues -0.032% were volatile T.P.s		Was not detected and is not expected to be produced.	1339490	41969201
Leaching from Utility Poles				1149166	43205001

Table 2.3-2: Biotransformation studies conducted with radiolabeled PCP according to internationally recognised guidelines.

Biotransformation Study	Soil transformation products	Volatile transformation products	Bound residues	Comment	Reference PMRA# and/or EPA MRID
Aerobic Soil (1 yr, guideline study)	TeCP (2.4%), TCP (4.5%), both degraded by study termination. -no PCA standard, but good recovery (91.3%).	Volatile-27.3% CO_2 (26%), TCP (<1%)	- 64%: 76%-humin 21%-fulvic 3%-humin	Observed half-life of 7-14 days; the calculated first-order half-life was approximately two months; the majority of radioactivity (64%) was bound residues. No chloroanisoles were detected (TeCA, DCA, para- and meta-chloroanisoles). No PCA standard was used for degradate identification.	1169852; 1146988 Summary reported in U.S. EPA RED 2008, but this study is not listed in references
Anearobic Flooded Soil (aerobic, followed by flooding)	TeCP (d), TCP (s), 2-chloro-hydroquinone (i) and mucochloric acid (i) (up to 14% total)	Aerobic: 4.47% [CO_2: 4.06%, PCP: 0.26%, unidentified: 0.15%] Anaerobic: 1.85% [CO_2: 0.54%, PCP: 0.80%, unidentified: 0.51%]	Up to 44.8% (19 days) and then decreased to 38% (60 days) 52%-humin 38%-humic 11%-fulvic	<10% of bound residues were released under anaerobic conditions (measured as PCP) Mean mass balance was 96.5%	PMRA: 1339503 MRID: 41995201
Aerobic Aquatic Biotransformation	TeCP (10%), TCP(83%) (d), dichlorophenol (37%) (i)	<1%	40.9% (study termination)	Mass balance: 88.1-117%	PMRA: 1339564 MRID: 42288601
Anearobic aquatic sediment	TeCP(10%)(d) and TCP(78%)(i)	2.1%	7.8%	Mass balance: 78.2-135%	PMRA: 1339535 MRID: 42436801

(i) increasing in concentration by study termination
(d) decreasing in concentration by study termination
(s) stable

Table 2.3-3: Literature studies containing information on the degradation of PCA.

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
Aerobic Soil (LRTAP criteria: $t_{1/2}$: > 6 months)					
Laboratory Aerobic soil	PCP	Aerobic PCP transformation initially produced small amounts of PCA. PCA was detected in 7 of the 8 soils tested. ->75% of both PCP and PCA disappeared in 30 days in five soils. -No evidence of loss of PCP or PCA in 2 of the soils where PCA was produced.	Small amounts of PCA. Authors indicated that PCA was either mineralised to CO_2 or bound to soil.	Closed system. However, headspace gases were only analysed for CH_4, CO_2 and O_2.	D'Angelo and Reddy 2000
Moist aerobic soils (24 d)	PCP	None	The principal reaction involved reductive dehalogenation (production of progressively simpler chlorophenols, TeCP, TCP and DCP). The degradation of PCP and PCA are reductive in anaerobic soils, and oxidative in aerobic soils. Higher levels of bound residues were observed in aerobic soils than anaerobic.	Limited amount of study details were reported. Extraction efficiencies were extremely poor for the aerobic soils treated with PCP (14.7%) and a significant amount of radioactivity was lost. Organic volatile compounds and CO_2 were not collected.	Murthy et al. 1979
Laboratory aerobic soil		**5.6% of PCA was converted to PCP in 24 days.**		Based on further investigation by Murthy et al., 1979 that was not published but is referred to by Kaufman 1978.	Reported in Kaufman 1978 and Murthy et al. 1979

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
Field Study soil	TCA and PCA	**Half-life of 5 weeks in soil and in earthworms.**	Evidence of demethylation to tetrachlorophenol and pentachlorophenol. Rate of disappearance was also attributed to degradation, metabolised to other compounds not measured or were in non-extractable form.	Closed system. Respiration (CO_2 evolution) was measured weekly. The rate of metabolism and/or degradation of chloroanisoles was high in the aerobic and humus – rich soil (and earthworms) used in our studies. This was corroborated by high respiration activity found with high concentrations of chloroanisoles.	Haimi et al. 1993
Field study upland soil	PCP	Rapid degradation of PCP. PCA reached a maximum of 1% of the applied PCP at day and was 0.5% by day 35. **Observed PCA half-life of approximately 30 days in upland (aerobic) conditions.**	Transformation products included TeCP (max. 4%), TCP (max 2%) and PCA (max 1%). Others were detected in trace amounts.	Test system was covered with aluminum foil. The half-lives for PCA were not reported by the study authors, but can be read from the graphs provided.	Kuwatsuka et al. 1975
Anaerobic Soil (LRTAP sediment criteria: $t_{1/2}$: > 6 months)					
Laboratory Anaerobic soil	PCP and PCA	N/A	Trichlorophenol, tetrachlorophenol, with lesser formation of pentachloroanisole (5.1%) The principal degradation pathway of PCP in anaerobic soil would seem to be by progressive dehydrodehalogentation to tetra- and tri-chlorophenols, with	Volatile organic compounds were trapped for the anaerobic portion of the study. Only 0.4-0.5% of the radioactivity was allotted to volatile organic compounds.	Murthy et al. 1979

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
			lesser formation of pentachloroanisole. Conversion of PCA to PCP.		
Anaerobic soil	PCP and PCA	**42% of PCA was degraded to PCP in 24 days.**		Very good recovery of radioactivity. 98.8% of the radioactivity was recovered in the soil. Volatile organic compounds were also captured and only accounted for 0.4-0.5% of the total radioactivity.	Murthy et al. 1979 and reported in Kaufman 1978
Field study (flooded)	PCP	Rapid degradation of PCP. **Observed half-lives for PCA were approximately 25 days in flooded conditions.**	Transformation products included TeCP (max. 4%), TCP (max 2%) and PCA (max 2% at day 10 and was 1% by day 35). Others were detected in trace amounts.	The test system was covered with aluminum foil. The half-lives for PCA were not reported by the study authors, but can be read from the graphs provided.	Kuwatsuka et al. 1975
Paddy Soil (rice fields)	PCP	PCP degraded within a few weeks of application. No conclusions regarding PCA can be drawn from this study.	TeCP, TCP, DCP and 3-chlorophenol. Reductive dechlorination was found to occur in paddy soil.	The analytical methods precluded the differentiation between the chlorophenols from the anisoles since the samples were treated with dimethyl sulphate (methylated). The authors allotted all of the residues chlorophenols (not chloroanisoles).	Ide et al. 1972

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
				This study is included in Table because it was quoted previously as evidence of the production of PCA.	
Flooded rice soil	PCP	No half-lives for PCA can be drawn from this study. Other lesser chlorinated anisoles were also found (tetra- and tri-chloroanisoles).	Most of the radioactive residues were associated with bound residues. PCA (0.09%), tetrachloroanisoles, trichloroanisoles	The author states that not only PCP, but its lower chlorinated products may also be methylated in soil, although it must be conceded that tetra- and tri-chloroanisoles could originate as well from PCA by dechlorination. Since the toxic effects of phenols are mainly caused by the hydroxyl group, the methylation may be regarded as an inactivation process. Limited uptake of residues from soil by rice plants.	Weiss 1982
Aquatic Field Studies (LRTAP water criteria: $t_{1/2}$: > 2 months)					
Contaminated Site-Spill		Low levels of PCA were observed. Partitioning of PCA to sediment. **Observed half-life of approximately 1.5 months in the sediment at site A.** **Half-lives at site B, C and D**	Tetrachlorophenols Pentachloroanisole Tetrachloroanisoles (small amounts and difficult to analyse)	Any losses of PCA due to volatilisation were not captured. Evidence of the accumulation of PCP and TeCP and PCA. The	Pierce and Victor, 1977

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
		could not be assessed due to continuous formation from PCP.		concentration in fish decreased as the concentration in the water decreased, but required 6-10 months to reach background concentrations.	
Fungal Degradation-Bioremediation Studies					
	Trichoderma virgatum	Only 10-20% of the original PCP was detected as PCA. **Approximate (observed) DT50 for PCA is about 33days.**	The formation of PCA is only the first step in the metabolism or a parallel reaction to degradation. PCA is not the only metabolic product since 80-90% of the original PCP was recovered neither as the free phenol for the PCA when incubated longer than 10 days.	PCA is less toxic to fungi. PCA was reported to be approximately 1000 less toxic than PCP. Less soluble than PCP (10x). PCA could not be detected by conventional reagents on TLC.	Cserjesi and Johnson 1971
	9 New Zealand native white-rot fungi (*Trametes versicolor, Junghuhnia vincta, Phanaerochaete cordylines,* unknown*)* were compared with *P.Chrysoporium*	In liquid culture, very little to no PCA was captured in the volatile fraction of *T. versicolor* isolates, **whereas 75% of the volatile fraction of *P. chrysosporium* consisted of PCA.**		In comparison with *P. chrysoporium, T. versicolor* produced very little PCA. The very large volatile fraction measured in the liquid culture experiments, may be an artefact of the experimental design. The PUF volatile trap in within	Walter et al. 2004

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
				the culture bottle. It is possible that mass-transfer between solid phase PCP, the solution phase, vapour phase, and the trapped volatiles has occurred. Whatever the cause of the high volatile release in liquid culture it was not observed in the soil microcosms. It is probably that soil and added organic matter retain PCP sufficiently to significantly reduce volatilization.	
Field Study	*T. versicolor* in soil/PCP	Field-Scale bioremediation.		PCA is not likely an intermediate transformation product of *T. versicolor*	Walter et al. 2005
	T. versicolor	Soil		Only trace amounts of anisoles such as PCA and TeCA were formed.	Tuomela et al., 1999
	P. chrysosporium in liquid culture	In 12 days, 82% of the PCP was volatilised as PCA. If the fungus is oxygen-limited for lignin peroxidise production, it will convert most of the PCP to the volatile PCA, the only			Badkoubi et al. 1996

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
		volatile compound detected in the presence of *P. chrysosporium* in this experiment. When sufficient oxygen was available, the extent of mineralisation was much greater, up to 32%. Higher mineralisation was observed when the volatile transformation products had a chance to equilibrate between the solution and the headspace. Immediate removal of the volatile transformation products reduced PCP mineralisation. Therefore, the PCA remaining in the solution and PCP will be mineralised and product more $^{14}CO_2$ over time compared with the case when all PCA is depleted from the liquid and sorbed on the polyurethane volatile trap.			
Non-sterile soil (18 days)	*Phanerochaete chyrsosporium*	At 100 ppm of PCP: 40% of PCP was mineralised to PCA. 0% PCP was detected. Beyond 18 days, there was still a linear rate of	PCA (as an intermediate), mineralization. **Essentially no radioactivity (<0.05%) was found in either the volatile**	*P. chyrsosporium* is able to mineralise high concentration of PCP and PCA. Both PCP and PCA are	Chung and Aust 1995

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
		mineralisation, suggesting that PCA was being mineralised during this time. 800 ppm: both PCP and PCA were detected at 18 d. The rate of mineralisation of PCA increased with increasing concentration (not linear).	**organic trap suggesting that PCP, PCA, or other intermediates were not volatile.**	readily mineralised in soil.	
Sterilised and non-sterilised soil	*Lentinula edodes* (Shitake mushroom)/PCP	**After 10 weeks, monocultures of *L. edodes* had eliminated both PCP and the chloroanisoles (including PCA). PCA, however, was still detected in soils with mixed microflora.**	PCA, TeCA, TeCP were detected, but concentrations were not reported.		Okeke et al. 1997
soil	*Lentinus edodes* (Shitake mushroom)/PCP	PCA was detected as a transformation product of PCP.	PCA was detected but concentrations were not reported.		Okeke et al. 1993
	P. chrysosporium and *Lentinus edodes* (Shitake mushroom)/PCP		PCA, TeCA, TeCP were detected but concentrations were not reported.		Okeke et al. 1994
	7 strains of *Phanerochaete* spp. *P. chrysorhiza,*	PCA accumulated initially and was degraded during a second stage beginning after 9 days of incubation. **PCA**		*Phanerochaete* spp. were sensitive to PCP. Growth was prevented at 5 ppm. However, *P. sordida* and	Lamar et al. 1990

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
	P. laevis, P. suguinea, P.filamentosa, P. sordida, Inonotus circinatus, P. chrysosporium In liquid culture and in soil	**was reduced by 18% in soil inoculated with *P.chyrosoporium* and by 23% in soil inoculated with *P. sordida* over 56 days.** **PCA was mineralised by both *P. sordida* and *P. chrysosporium* in liquid culture.**		*P. chrysosporium* were able to tolerate higher concentrations of PCP (25 ppm), albeit at greatly decreased mycelial extensions rates. Although PCA appears to be slightly more persistent in this study. Up to 13.8% of the total radioactivity in the liquid cultures was captured as volatiles.	
	P. chrysosporium and P. Sordida In field study	88%-91% decrease of PCP in 6.5 weeks. PCP and PCA were mineralised by *P. Chrysosporium* and *P. sordida*. PCA rapidly increased during the first 15 days after inoculation. After day 15, the amount of PCA in the soil inoculated with *P. chrysosporium* did not change significantly. In the soil incubated with *P. sordida*, PCA was 8% at day	In a field contaminated with 250 to 400 ppm PCP, 8-13% of the PCP was transformed to PCA	PCP was present in the soils at concentrations between 100-400 ppm over the course of the 45 day study. It is not possible to estimate a degradation rate for PCA given that there was continuous formation and decline over the course of the study. However, since the concentration did not change significantly after day 15, the rate of formation and degradation	Lamar and Dietrich 1990

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
		22.		were close to the same.	
Bacterial Degradation					
Microbial Degradation	Various species	PCA was produced in very small yields in 5 of the 10 strains. <0.005% to 0.02%.	Tetrachloroanisoles were formed by two pathways (dechlorination of pentachloroanisole or by methylation of tetrachlorophenoles)	The results show that sodium pentachlorophenolate can be transformed by a number of ubiquitous bacterial strains to different compounds. Since pentachlorophenol acetate is the major metabolite, it seems appropriate to give greater consideration to this compound than hitherto during further metabolism studies of pentachlorophenol in environmental samples.	Rott et al. 1979
	Rhodococcus, Mycobacterium		All strains initiated degradation of the chlorophenols by para-hydroxylation, producing chlorinated-hydroquinones, which were then further degraded. Parallel to degradation, strains also O-methylated nearly all chlorinated phenols, guaiacols, syringols and hydroquinones. O-methylation was a slow reaction compared with degradation. The preferred substrates of the O-methylting enzymes were those with the		Haggblom et al. 1988

Study Description	Test Substance	Half-Life or description of persistence (trend)*	Successor transformation Products	Comments	References
			hydroxyl group flanked by two chlorine substituents.		
	Mycobacterium sp. In a mineral salt water medium		*Mycobacterium* sp. metabolized PCP mostly through the methylation and at the same time part of PCP was hydroxylated at ortho and para positions to the hydroxyl group followed by successive methylation. Maximum rate of the methylation was observed between pH 6.5 and 7.0. The hydroxylation, however, was dominant below pH 6.0. The addition of nutrients into the incubation medium resulted in enhancement of the methylation and exclusive formation of PCA as a sole metabolite. Toxicity of PCA for *Mycobacterium* sp. and for germinating rice seeds was significantly low compared with PCP.		Suzuki 1983b

*For those studies conducted where PCP and PCA was tracked, observed half-lives for PCA should be considered conservative, but cannot be considered a true half-life since formation and degradation would be occurring simultaneously. In the cases where formation and degradation is occurring simultaneously, the true half-lives are expected to be shorter.

Chapter 3: Effects on non-target species

Information on the toxicity of PCA has been discussed previously by the UNECE Task Force. PCA is considered to have met toxicity criteria.

PCP is toxic to microorganisms as PCP is an inhibitor of oxidative phosphorylation (Crosby 1981).

The toxic effect of phenols are mainly caused by the hydroxyl group, the methylation may be regarded as an inactivitation process (Weiss et al. 1982). Several authors have examined the relative toxicity between PCA and PCP and is summarised in the Table 3.2-1.

3.1 Effects on terrestrial organisms

Several authors have concluded that the methylation of PCP results in detoxification of the molecule by deactivating the hydroxyl molecule (Table 3.1-2). For several species of fungi, methylation allows for otherwise toxic levels of PCP to be metabolised. As an example, Chung and Aust (1995) and Aust and Stahl (1998) reported that the biodegradation of pentachloroanisole in both liquid and soil is relatively facile (see Figure 3.1-1 from study authors). In Chung and Aust (1995), the authors reported that the rate of degradation increases with increasing concentration of PCA from 50 to 16000 ppm. PCA, unlike PCP, is relatively nontoxic to the fungus. Thus, methylation of PCP results in detoxification, allowing metabolism. Bioremediation of otherwise toxic levels of PCP should therefore be possible. The graph provided in Figure 3.1-1 shows the increased rate in mineralisation with increasing concentration of PCA.

There is limited information on the toxicity or the metabolism of PCA in birds or invertebrates. The principal route of PCA metabolism in mice (Vodnick et al. 1980) and fish (Glickman et al. 1977) is demethylation to PCP. It is unlikely that PCA is more toxic than PCP.

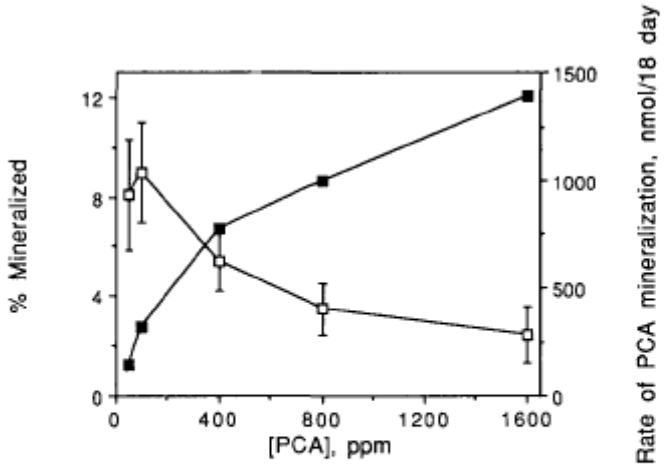


Fig. 3. Effect of PCA concentration on its rate of mineralization by *P. chrysosporium*. Various concentrations of PCA in nonsterile soil were incubated with *P. chrysosporium* and assayed for the percentage of the PCA mineralized (□) and the rate of PCA mineralization for 18 d (■). Values for the percent mineralized are the means ± standard deviations for triplicate cultures.

Figure 3.1-1 Effect of PCA concentration on the rate of mineralisation by P. chrysosporium.

3.2 Effects on aquatic organisms

Limited information is available to judge the toxicity of PCA to aquatic organisms. On an acute basis, PCA appears to be very highly toxic to aquatic invertebrates and highly toxic to fish. One referenced study suggests that PCA is approximately 1000x less toxic to fish than PCP, however, this was a non-standard toxicity test and details of the study were not available for review.

No information is available on the chronic toxicity of PCA. The principal route of PCA metabolism in mice (Vodnick et al. 1980) and fish (Glickman et al. 1977) is demethylation to PCP. It is unlikely that PCA is more toxic than PCP.

Conclusion:

The toxicity information provided for PCA reported by Task Force and the additional information provided above indicate PCA meets the criterion for toxicity.

Table 3.2-1 Effects of PCA on organisms

Organism	Exposure	Endpoint value	Degree of toxicity	Reference
Terrestrial Organisms				
Mice	N/A	318±22 (m)	-	Renner et al. 1986

		331±22 (f) mg/kg		
Rat		≥ 500 mg/kg	-	Dieke et al. 1947
Earthworms		≥500 µg/g	*Only acutely toxic at high concentrations.*	Salminen and Haimi 1991 in Haimi 1993
Aquatic Organisms				
Daphnia magna	Acute (48 h)	48-h EC50: 27.2 µg/L	*Very highly toxic*	Brooke 1991
Cladocera	Acute (time not specified)	LC50: 27 µg/L	*Very highly toxic*	Sanchez-Bayo 2006
Hydra attenuate	Acute (96 h)	MAC: 10 µg/L	*Slightly to moderately toxic*	Mayura et al. 1991
Pimephales promelas	Acute (96 h)	LC50: 650 µg/L	*Highly toxic*	Brooke 1991
		LC50: >1.2 mg/L		

Table 3.2-2 Studies examining the relative toxicity of PCA and PCP

Organism	Exposure	Relative Toxicity (PCA and PCP)	Comment	Reference
Terrestrial organisms				
Fungi *Phanerochaete chyrsosporium*	50-1600 ppm	Less toxic than PCP. The biodegradation of pentachloroanisole in both liquid and soil is relatively facile (Chung and Aust, 1995). The rate of degradation increases with increasing concentration of PCA from 50 to 16000 ppm. Methylation of PCP also result in detoxification, allowing metabolism of otherwise toxic levels of PCP.	As PCP was converted to PCA, the rate of mineralisation increased.	Aust and Stahl 1998

Fungus *Trichoderma virgatum Penicillium Cephaloascus fragrans*	20, 80, 320 and 1000 mg/L for 3 and 7 days	Using malt agar or wood media, PCA was much less toxic to test fungi than PCP.		Cserjesi and Johnson 1972
Mycobacterium sp. and germinating rice seeds		PCA was far less toxic to both *Mycobacterium* sp. and germinating rice seeds than PCP. In the case of *Mycobacterium* sp., the methylation of PCP may be regarded as an inactivation process.		Sukuki 1983b
Aquatic Organisms				
Fish Juvenile Coho salmon *Oncorhynchus kisutch*	2 mg/L PCP and 4 mg/L PCA	Toxicity was measured by mean survival time. The toxicity of PCA to fish was estimated to be 1000 times less than that of PCP.	No other study details were provided.	Cserjesi and Johnson 1972

3.3 Effects on biological methods of sewage treatment

Not reviewed and outside the scope of this document.

Chapter 4: List of abbreviations

bw	body weight
d	day(s)
EPI	Estimation Program Interface
Kow	octanol water partition coefficient
Koa	octanol air partition coefficient
Kd	adsorption quotient
Koc	adsorption quotient normalized to organic carbon
LC50	lethal concentration 50%
LD50	lethal dose 50%
LOAEL	lowest-observed-adverse-effect-level
<LOD	below the level of detection
<LOQ	below the level of quantification

lw	lipid weight	
MDL	method detection limitND	not detected (below the level of detection)
NOAEL	no-observed-adverse-effect-level	
PCA	pentachloroanisole	
PCP	pentachlorophenol	
ppm	parts per million	
TeCP	Tetrachlorophenol	
mg/L	milligrams per litre	
mg/kg	milligrams per kilogram	
μg	micrograms	
ng/g	nanograms per gram	

References

[Atlas et al. 1986] Atlas, E., K. Sullivan, and G.S. Giam, Widespread occurrence of poyhalogenated aromatic ethers in the marine environment. Atmos. Environ. 20:1217‐1220 (1986).

[Aust and Stahl 1998] Aust, S.D. and J.D. Stahl. 1998. Chapter 3: Biodegradation of Dioxin and Dioxin-like Compounds by White-Rot Fungi. In Biodegradation of Dioxins and Furans, edited by Rolf-Michael Wittich. Springer-Verlag and R.G. Landes Company. P.61-73.

[Badkoubi et al. 1996] Badkoubi, A., D.K. Stevens and I.P. Murarka; Quantification of pentachlorophenol transformation product distribution in the presence of Phanerochaete chrysosporium; Arch. Environ.Contam. Toxicol. 30:1‐8 (1996).

[Barakat et al. 2002] Barakat, A.O., M. Kim, Y. Qian and T.L.Wade. 2002. Organochlorine pesticides and PCB residues in sediments of Alexandria Harbour, Egypt. Mar. Pollut. Bull. 44:1421‐1434.

[Batterman et al. 2008] Batterman, S.A., S.M. Chernyak, Y. Gounden, M. Matooane, R.N. Naidoo. 2008. Organochlorine pesticides in ambient airin Durban, South Africa. Sci. Total Environ. 397:119‐130.

[Bentzen et al. 2008] Bentzen, T.W., D.C.G. Muir, S.C. Amstrup and T.M. O'Hara. 2008. Organochlorine concentrations in blood and adipose tissue of Southern Beaufort Sea polar bears. Sci. Tot. Environ. 406:352‐367.

[Begum et al. 1979] Begum, S., I. Scheunert, A. Hague, W. Klein, and F. Korte. 1979. Conversion of[14C] pentachloronitrobenzene in Onions. Pestic. Biochem. Physiol. 11:189‐200.

[Betts et al. 1955] Betts, J.J., James, S.P., and Thorpe, W.V. (1955) The metabolism of pentachloronitrobenzene and 2,3,4,6-tetra-chloronitrobenzene and the formation of mercapturic acids in the rabbit. Biochem. J., 61: 611-617.

[BiPRO GmbH 2010] BiPRO GmbH, 2010. Addendum for PCP provided to the UNECE Task Force on POPs. March 18, 2010. 41pp.

[Bizotto et al., 2009] Bizzotto EC, Villa S, Vaj C, Vighi M. Comparison of glacial and non-glacial-fed streams to evaluate the loading of persistent organic pollutants through seasonal snow/ice melt. Chemosphere 2009;74(7):924–30.

[Blais et al., 2001] Blais JM, Schindler DW, Muir DCG, Sharp M, Donald D, Lafreniere M, et al. Melting glaciers: a major source of persistent organochlorines to subalpine Bow Lake in Banff National Park, Canada. Ambio 2001;30(7):410–5.

[Brooke L.T. 1991] Brooke, L.T.; „Results of Freshwater Exposures with the Chemicals Atrazine, Biphenyl,Butachlor, Carbaryl, Carbazole, Dibenzofuran, 3,3' - Dichlorobenzidine, Dichlorvos, 1,2 - Epoxyethylbenzene (Styrene Oxide), Isophorone, Isopropalin, Oxy"; Ctr.for Lake Superior Environ. Stud., Univ.of Wisconsin - Superior, Superior, WI :110 p. (1991).

[Chu and Kirsch 1972] Chu, J.P. and Kirsch, E.J. (1972) Metabolism of pentachloro-phenol by an axenic bacterial culture. Appl. Microbiol., 23: 1033-1035.

[Chung and Aust 1995] Chung, N. and S.D. Aust (1995) Degradation of pentachlorophenol in soil by *Phanerochaete chrysosporium*, Journal of Hazardous Materials 41: 177-183.

[Courtney 1979] Courtney, K.D. 1979. Hexachlorobenzene (HCB: A review. Environmental Research 20:225-266.

[Crosby et al. 1981] Crosby, D.G., Beynon, K.I., Greve, P.A., Korte, F., Still, G.G., & Vouk, J.W. (1981) Environmental chemistry of pentachlorophenol. Pure appl. Chem., 53: 1051 - 1080.

[Cserjesi and Johnson 1972] Csyerjesi AJ, Johnson EL (1972) Methylation of pentachlorophenol by Trichoderma virgatum. Can J Microbiol 18 (1): 45 .

[D´Angelo and Reddy 2000] D'Angelo, E.M.; Reddy, K.R. 2000 Aerobic and anaerobic transformations of pentachlorophenol in wetland soils. Soil Science Society of America Journal, 64 (3), 933 - 943 (2000).

[Deberts et al. 1981] Debets, F.M.H., J.H. Reinders, A.J.M. Debets, T.G. Lossbroek, J.J.T.W.A Strik and G. Koss. 1981. Biotransformation and porphyrinogenic action of hexachlorobenzene and its metabolites in primary liver cell culture. Toxicol. 19:185 - 196.

[Dieke et al. 1947] Dieke, S.H., Allen, G.S. and C.P. Richter (1947) The Acute Toxicity of Thioureas and related compounds to Wild and Domestic Norway Rats. J. Pharmakol. Exper. Ther., 90:260-270.

[Dobbs and Grant 1980] Dobbs, A.J. and C. Grant; Pesticide volatilization rates: a new measurement of the vapour pressure of pentachlorophenol at room temperature. Pestic. Sci. 11:29 - 32 (1980).

[EHC 41 1984] International Programme on Chemical Safety, Environmental Health Criteria 41, Quintozene, Published under the joint sponsorship of the United Nations Environment Programme,the International Labour Organisation,and the World Health Organization, http://www.inchem.org/documents/ehc/ehc/ehc41.htm

[EHC 71 1987] International Programme on Chemical Safety, Environmental Health Criteria 71, Pentachlorophenol, Published under the joint sponsorship of the United Nations Environment Programme,the International Labour Organisation,and the World Health Organization, http://www.inchem.org/documents/ehc/ehc/ehc71.htm

[EHC 124 1991] International Programme on Chemical Safety, Environmental Health Criteria 124, Lindane, Published under the joint sponsorship of the United Nations Environment Programme,the International Labour Organisation,and the World Health Organization, http://www.inchem.org/documents/ehc/ehc/ehc124.htm

[EHC 195 1997] International Programme on Chemical Safety, Environmental Health Criteria 195, Hexachlorobenzene, Published under the joint sponsorship of the United Nations Environment Programme,the International Labour Organisation,and the World Health Organization, http://www.inchem.org/documents/ehc/ehc/ehc195.htm

[Engel et al. 1966] Engel, C., De Groot, A.P. and Weurman, C. (1966) Tetra-chloroanisole: a source of musty taste in eggs and broilers. Science, 154: 270-271

[Engelhard et al. 1986] Engelhardt, G., Wallnöfer, P. R. , Mücke, W. and Renner, G. (1986) Transformations of pentachlorophenol, Toxicological & Environmental Chemistry, 11: 3, 233 — 252.

[Engst et al. 1979] Engst, R., Macholz, R.M. and M Kujawa (1975) Recent State of lindane metabolism, Part II. Res Rev. 72, pp. 71-95.

[Figueras et al. 1997] To_Figueras, M. Sala, R. Otero, C. Barrot, M. Santiago‐Silva, M. Rodamilans,m C., Herrero, J. Grimalt and J. Sunyer. Metabolism of hexachlorobenzene in humans: association between serum levels and urinary metabolites in a highly exposed population. 1997. Environ. Hlth. Perspectives 105: 78‐83.

[Frankovic et al. 1995] Frankovic, F., Khan, M.A.Q. and S.M. Al Ghai. 1995. Metabolism of Hexachlorobenzene in the Fry of Steelhead Trout, Salmo gairdneri (*Oncorhynchus mykiss*). Archives of Environmental Contamination and Toxicology. 28: 209-214.

[Glickman et al. 1977] Andrew H. Glickman, Charles N. Statham, Anthony Wu and John J. Lech, “Studies on the uptake, metabolism, and disposition of pentachlorophenol and pentachloroanisole in rainbow trout”, Toxicology and Applied Pharmacology, Volume 41, Issue 3, 649‐658 (1977).

[Government of Canada 2009] Risk Profile Document for PCA. Submitted to the LRTAP Task Force in May 2009. 25p.

[Haggblom et al. 1988] Haggblom MM, Nohynek LJ and Salkinoja-Salonen MS., Degradation and O-methylation of chlorinated phenolic compounds by Rhodococcus and Mycobacterium strains. Applied and Environmental Microbiology 54(12): 3043-3052 (1988).

[Haimi et al. 1992] Haimi J, Salminen J, Huhta V, Knuutinen J and Palm H.. 1992Bioaccumulation of organochlorine compounds in earthworms. Soil Biology and Biochemistry 24(12): 1699‐1703 (1992).

[Haimi et al. 1993] Haimi J, Salminen J, Huhta V, Knuutinen J and Palm H., 1993 Chloroanisoles in soil and earthworms. Science of the Total Environment, supplement 1993: 439 - 448 (1993).

[Herve et al. 1988] Herve S, Heinonen P, Paukku R, Knuutila M, Koistinen J and Paasivirta J, Mussel incubation method for monitoring organochlorine pollutants in watercourses. Four - year application in Finland. Chemo.17:1945 - 1961 (1988).

[Hinck et al. 2007] Hinck, J.E., V.S. Blazer, N.D. Denslow, K.R. Echols, T.S. Gross, T.W. May, P.J. Anderson, J.J., Coyle, D.E. Tillitt. 2007. Chemical contaminants, health indicators, and reproductive biomarker responses in fish from the Colorado River and its tributaries. Sci. Total Environ. 378:376 - 402.

[Hinck et al. 2008] Hinck, J.E., V.S. Blazer, N.D. Denslow, K.R. Echols, R.W. Gale, C. Wieser, T.W. Maya, M. Ellersieck, J.J. Coyle, D.E. Tillitt, Chemical contaminants, health indicators, and reproductive biomarker responses in fish from rivers in the Southeastern United States. Sci. Total Environ. 390 :538 - 557 (2008).

[Hoferkamp et al. 2010] Hoferkamp, L. M.H. Hermanson, and D.C.G. Muir; „Current use pesticides in Arctic media; 2000 - 2007"; Sci. Total Environ.408 (15): 2985-2994.

[Hung et al. 2005] Hung, H., P. Blanchard, C.J. Halsall, T.F. Bidleman, G. Stern, P. Fellin, D.C.G. Muir, L.A., Barrie, L.M. Jantunen, P.A. Helm, J. Ma and A. Konoplev; „Temporal and spatial variabilities of atmospheric polychlorinated biphenyls (PCBs), organochlorine (OC) pesticides and polycyclic aromatic hydrocarbons (PAHs) in the Canadian Arctic: Results from a decade of monitoring"; Sci. Tot. Environ. 342:119 - 144 (2005).

[Hung et al. unpublished] Hung et al., unpublished archive data, Environment Canada.

[Ide et al. 1972] Ide, A., Niki, J., Sakamoto, F., Watanabe, J., and H. Watanabe (1972) Decomposition of pentachlorophenol in paddy soil. Agric. biol. Chem., 36: 1937-1944.

[I.E.P. 2008] Institute of Environmental Protection, 2008. Pentachlorophenol: Dossier prepared in support of a proposal of pentachlorophenol to be considered as a candidate for inclusion in the Annex I of the Protocol to the 1979 Convention on Long-Range Transboundary Air Pollution on Persistent Organic Pollutants (LRTAP Protocol on POPs), Warsaw, May 2008, 87p.

[Ikeda et al. 1994] Ikeda GJ, Sapienza PP and Warr PI; "Disposition and metabolism of radiolabelled pentachloroanisole in rats and rabbits"; Food and Chemical Toxicology; 32, 1137 - 1146 (1994).

[Ikeda and Sapienza 1995] Ikeda, G.J. and P.P. Sapienza (1995) Distribution, Metabolism and Excretion of Pentachloroanisole in the Beagle Dog and Miniature Pig. Fd Chem. Toxic. 33 (5): 409-421.

[Jiang et al. 2000] Jiang X, Martens D, Schramm K‐W, Kettrup A, Xu SF and Wang LS. 2000. Polychlorinated organic compounds (PCOCs) in waters, suspended solids and sediments of the Yangtse River. Chemo. 41: 901‐905.

[Kasokat et al. 1989] Kasokat, T., Nagel, R. and K. Ulrich. 1989. Metabolism of chlorobenzene and hexachlorobenzene by the Zebra Fish, *Brachydanio rerio*. Bull Environ. Contam. Toxicol. 42:254-261.

[Kaufman 1978] Kaufman (1978) Degradation of Pentachlorophenol in Soil, and by Soil Microorganisms. *In* Pentachlorophenol: chemistry, pharmacology, and environmental toxicology. Edited by K. R. Rao. Plenum Press, New York. pp. 27-39.

[Kirsch and Etzel 1973] Kirsch, E.J. and J.E. Etzel (1973) Microbial decomposition of pentachlorophenol. J. Water Pollut. Control Fed., 45: 359-364.

[Klowskowski et al. 1981] Klowskowski, R., Scheunert, I., Klein, W. and F. Korte (1981) Laboratory screening of distribution, conversion and mineralization of chemicals in the soil-plant-system and comparison to outdoor experimental data. Chemosphere 10 (10): 1089-1100.

[Koss et al. 1976] Koss, G. W. Koransky and K. Steinbach. 1976. Studies on the toxicology of hexachlorobenzene. Arch. Toxicol. 35:107‐114.

[Koss et al. 1979] G. Koss, W. Koransky and K. Steinbach, Studies on the toxicology of hexachlorobenzene. IV. Sulphur-containing metabolites, Archs Toxic. 42 (1979), pp. 19–31

[Kogel et al. 1979] Kogel, W., Muller, W.F., Coulston, F. and F. Korte (1979) Biotransformation of Pentachloronitrobenzene-^{14}C in Rhesus Monkeys after Single and Chronic Oral Administration. Chemosphere 2: 97-105..

[Kujawa et al. 1977] Kujawa M, Engst R, & Macholz R (1977) On the metabolism of lindane. In: Proceedings of International Symposium on Industrial Toxicology, Environmental Pollution and Human Health, pp. 661-672.

[Kuwatsuka and Igarashi 1975] Degradation of PCP in Soils: The Relationship between the Degradation of PCP and the Properties of Soils, and the Identification of the Degradation Products of PCP. Japanese Society of Soil Science and Plant Nutrition 21(4): 405-414.

[Lamar et al. 1990] Lamar RT, Larsen MJ and Kirk T K. 1990 b. Sensitivity to and Degradation of Pentachlorophenol by Phanerochaete spp. Applied and Environmental Microbiology 56(11): 3519‐3526 (1990).

[Lamar and Dietrich 1990] Lamar, R.T. and D.M. Dietrich. 1990. In Situ depletion of pentachlorophenol from contaminated soil by Phanerochaete spp. Appl. Environ. Microbiol. 56 :3093‐3100.

[Li et al., 2002] Li Y-F, Macdonald RW, Jantunen LMM, Harner T, Bidleman TF, Strachan WMJ. The transport of β-hexachlorocyclohexane to the western Arctic Ocean: a contrast to α-

HCH. Sci Total Environ 2002;291:229–46.

[Lui and Sweeney 1975] Lui, H., and G.D. Sweeney (1975) Hepatic metabolism of hexachlorobenzene in rats. FEBS Lett 51:225-226.

[Lyr 1962] Lyr, H. (1962) [On the oxidative decomposition of chlorinated phenols.] Holztechnologie, 3: 201-208 (in German).

[Macdonald et al. 2000] Macdonald, R.W., L.A. Barrie, T.F. Bidleman et al. 2000. Contaminants in the Canadian Arctic : 5 years of progress in understanding sources, occurrence and pathways. Sci. Total Environ. 254:93‐234.

[Marco et al. 2006] Marco, J.A.M. and M.A. Kishimba, Pesticides and metabolites in cassava, eucalyptus, plum, and cashew leaves and roots in relation to a point source in Kibaha, Tanzania. Chemo. 64542‐548 (2006).

[Marco and Kishimba 2007] Marco Mahugija, J.A. and M. A. Kishimba. 2007. Organochlorine pesticides and metabolites in young leaves of Mangifera indica from sites near a point source in Coast region, Tanzania. Chemosphere 68:832‐837.

[Mayura et al. 1991] Mayura, K. E.E. Smith, B.A. Clement and T.D. Phillips.,"Evaluation of the developmental toxicity of chlorinated phenols utilizing Hydra attenuate and postimplantation rat embryos in culture.", Toxicol. Appl. Pharmacol. 108:253‐266 (1991).

[Mehendale et al. 1975] Mehendale, H.M., Fields, M. and H.B. Matthews 1975. Metabolism and Effects of Hexachlorobenzene on Hepatic Microsomal Enzymes in the Rat. J. Agr. Food Chem., 23 (2): 261-265.

[McCall et al. 1981] McCall, P.J., Laskowski, D.A., Swamm, R.L. and Dishburger, H.J. (1981). Measurements of sorption coefficients of organic chemicals and their use in environmental fate analysis. In Test Protocols for Environmental Fate and Movement of Toxicants. Proceedings of AOAC Symposium, AOAC, Washington, D.C.

[Metcalf et al. 1973] Metcalf, R.L, Kapoor, I.P., L. Po-Yung, Schuth, C.K. and P. Sherman. 1973. Model Ecosystem Studies of the Environmental Fate of Six Organochlorine Pesticides. Environmental Health Perspectives. p. 35-44.

[Mileski et al. 1988] Mileski, G.J, Bumpus, J.A., Jurek, M.A. and S.D. Aust (1988) Biodegradation of pentachlorophenol by the white rot fungi in batch culture. Wat. Res. 28:1533-1538.

[Muller et al. 1978] Muller, W.F., Scheunert, I., Rozman, K., Kogel, W., Freitag, D., Richter, E., Coulston, F., and F., Korte (1978) Comparative metabolism of hexachlorobenzene in plants, rats and Rhesus monkeys. Ecotoxicol. environ. Saf. 2: 437-445.

[Muir unpublished] Muir D,,.unpublished data, Environment Canada.

[Muir and Zheng 2007] Muir D, Zheng J. 2007. Environmental trends monitoring of new chemical contaminants in the Canadian High Arctic via ice and snow cores.“ In: Smith SL, Stow J, editors. Synopsis of research conducted under the 2006–2007, Northern Contaminants Program. Ottawa, ON: Indian and Northern Affairs Canada; p. 194–202 (2007).

[Muir et al. 2007] Muir D, Alaee M, Teixeira C, Pacepavicius G, Spencer C, Scott B, et al. „New contaminants in the Arctic and subarctic atmospheric and aquatic environments.“ CEPA resources report — FY 2006 2007. Burlington ON: Environment Canada, Aquatic Ecosystem Protection Research Division; 5 pp (2007).

[Murthy et al. 1979] Murthy NBK, Kaufman DD and Fries GF., Degradation of pentachlorophenol (PCP) in aerobic and anaerobic soil. Journal of Environmental Science and Health ‐ Part B Pesticides, Food Contaminants, and Agricultural Wastes 14 (1): 1 ‐ 14 (1979).

[Murthy and Kaufman 1978] Murthy, N.B.K. and D.D. Kaufman (1978). Degradation of Pentachloronitrobenzene (PCNB) in Anaerobic Soils. J.Agric., Food Chem., 26(5):1151-1156.

[Oh et al. 2005] Oh, J.R., H.K Choi, S.H. Hong, U.H. Yim, W.J. Shim and N. Kannan. 2005. A preliminary report of persistent organochlorine pollutants in the Yellow Sea. Mar. Pollut. Bulletin 50:208 ‐ 236.

[Okeke et al. 1993] Okeke, B.C., Smith, J.E., Peterson, A. and I.A. Watson-Craik (1993) Aerobic metabolism of pentachlorophenol by spent sawdust culture of “shiitake” mushroom (Lentinus edodes) in soil. Biotenchnology Letters 15 (10): 1077-1080.

[Okeke et al. 1994] Okeke, B.C., Paterson, A., Smith, J.E. and I.A. Watson-Craik (1994) Relationships between ligninolytic activities of *Lentinula* spp. and biotransformation of pentachlorophenol in sterile soil. Letters in Applied Microbiology 19 (4): 284-287.

[Okeke et al. 1997] Okeke BC, Paterson A, Smith JE and Watson ‐ Craik IA, Comparative biotransformation of pentachlorophenol in soils by solid substrate cultures of Lentinula edodes. Applied Microbiology and Biotechnology 48: 563 ‐ 569 (1997).

[Oliver and Niimi 1985] Oliver, B.G., and A.J. Niimi; „Bioconcentration Factors of Some Halogenated Organics for Rainbow Trout: Limitations in Their Use for Prediction of Environmental Residues“; Environ. Sci. Technol. 19 (9) 842 ‐ 849 (1985).

[Opperhuizen and Voors 1987] Opperhuizen, A., and P.I. Voors; „Uptake and Elimination of Polychlorinated Aromatic Ethers by Fish: Chloroanisoles“; Chemosphere 16 (5) 953 ‐ 962 (1987).

[Pierce and Victor 1978] R. H. Pierce and D.M. Victor (1978) the Fate of Pentachlorophenol in an Aquatic Ecosystem. *In* Pentachlorophenol: chemistry, pharmacology, and environmental toxicology. Edited by K. R. Rao. Plenum Press, New York. pp. 27-39.

[Rawn et al. 2001] Rawn, D.F.K., W.L. Lockhart, P. Wilkinson, D.A. Savoie, G.B. Rosenberg and D.C.G. Muir. 2001. Historical contamination of Yukon Lake sediments by PCBs and

organochlorine pesticides: influence of local sources and watershed characteristics. Sci. Total Environ. 280:17 – 37.

[Reiner et al. 1978] Reiner, E.A., Chu, J.P. and E.J. Kirsch (1978) Microbial metabolism of pentachlorophenol. In: Rao, K.R., ed. Penta-chlorophenol: chemistry, pharmacology, and environmental toxicology, New York, London, Plenum Press, pp. 67-81.

[Renner 1981] Renner (1981) Biotransformation of the fungicides hexachlorobenzene and pentachloronitrobenzene. Xenobiotica 11(7): 435-446.

[Renner et al 1986] Renner G. Hopfer, C. and J.M. Gokel (1986) Acute toxicities of pentachlorophenol, pentachloroanisole, tetrachlorohydroquinone, tertrachlorocatechol, tetrachlororesorcinol and tertrachlorobenzendiol diacetates administered to mice"; Tox Environ Chem 11 (1): 37 – 50 (1986).

[Riedel et al. 2002] Riedel, R. D. Schlenk, D. Frank, B. Costa-Pierce. 2002. Analyses of organic and inorganic contaminants in Salton Sea fish. Mar. Pollut. Bull. 44:403-411.

[Rostad et al. 1999] Rostad, C.E., W.E. Pereira and T.J. Leiker; Distribution and transport of selected anthropogenic lipophilic organic compounds associated with Misssissippi River suspended sediment, 1989 – 1990. Arch. Environ. Contam. Toxicol. 36:248 – 255 (1999).

[Rott et al. 1979] Rott, B., Nitz, S. and F. Korte (1979) Microbial decomposition of sodium pentachlorophenolate. J. agric. food Chem., 27, 306-310.

[Salminen and Haimi 1991] J. Salminen and J. Haimi, Standardized toxicity test with earthworms used in EEC countries, Biol. Res. Rep. Univ. Jyväskylä 22 (1991), pp. 46–49.

[Sánchez-Bayo 2006] Sánchez – Bayo, F. (2006) Comparative acute toxicity of organic pollutants and reference values for crustaceans. I. Branchiopoda, Copepoda and Ostracoda. Environ. Pollut. 139:385 – 420 (2006).

[Sanborn et al. 1971] Sanborn, J.R. Childers, W.F. and LG. Hansen (1971) Uptake and Elimination of [^{14}C] Hexachlorobenzene (HCB) by the Green Sunfish, Lepomis cyanellus Raf., after Feeding Contaminated Food. J. Agric. Food Chem. 25 (3):551-553.

[Schmitt et al. 1990] Schmitt CJ, Zajicek JL and Peterman PH. (1990) National Contaminant Biomonitoring Program: Residues of Organochlorine Chemicals in U.S. Freshwater Fish, 1976 – 1984. Archives of Environmental Contamination and Toxicology 19: 748 – 781.

[Schreitmüller and Ballschmiter 1995] Schreitmüller, J. and K. Ballschmiter.1995 Air-water equilibrium of hexachlorocyclohexanes and chloromethoxybenzenes in north and south Atlantic; Environ. Sci. Technol. (29) pp 207-215 (1995).

[Su et al. 2008] Su, Y., Hung, H., Blanchard, P., Patton, G.W., Kallenborn, R., Knonplev, A., Fellin, P., Li, H., Geen, C., Stern, G., Rosenberg, B., and L.A. Barrie (2008) A circumpolar

perspective of atmospheric organochlorine pesticides (OCPs): Results from six Arctic monitoring stations in 2000-2003; Atmospheric Environment, 42 (19), pp. 4682‐4698.

[Suzuki 1983a] Suzuki, T. (1983) Metabolism of Pentachlorophenol (PCP) by Soil Microorganisms. Journal of Pesticide Science 8: 385-394. (English abstract)

[Suzuki 1983b] Suzuki, T. (1983) Methylation and hydroxylation of Pentachlorophenol by *Mycobacterium* sp. Isolated from Soil. Journal of Pesticide Science 8: 419-428.

[Swackhammer et al. 1988] Swackhammer, D.L. and R.A. Hites, Occurrence and bioaccumulation of organochlorine compounds in fishes from Siskiwit Lake, Isle, Royale, Lake Superior. Environ. Sci. Technol. 22:639‐648 (1988).

[Szokolay et al. 1980] Szokolay, A., Uhnak, J. and A. Mad'aric 1980 Dynamics of hexachlorobenzene residues in meat and eggs from chickens. Nahrung, 24 (4-5): 381-387. Abstract only as article in German.

[To-Figueras et al. 1997] To-Figueras, J., Sala, M., Otero, R., Barrot, C., Santiago-Silva, M., Rodamilans, M., Herroro, C., Grimalt, J. and J. Sunyer. 1997. Metabolism of Hexachlorobenzene in Humans: Association between Serum Levels and Urinary Metabolites in a Highly Exposed Population. Environmental Health Perspectives 105(1): 78-83.

[To-Figueras et al. 2000] To-Figueras, J., Barrot, C., Sala, M., Otero, R., Silva, M., Ozalla, M.D., Herrero, C., Corbella, J., Grimalt, J.O., and J. Sunyer. 2000. Excretion of hexachlorobenzene and metabolites in feces in a highly exposed human population. Environmental Health Perspectives 108:595-598.

[Tuomela et al. 1999] Tuomela, M.a , Lyytikäinen, M.b , Oivanen, P.a , Hatakka, A.a; "Mineralization and conversion of pentachlorophenol (PCP) in soil inoculated with the white‐rot fungus Trametes versicolor"; Soil Biology and Biochemistry, 31 (1), 65‐74 (1999).

[UNECE 2009] UNECE Task Force on Persistent Organic Pollutants (POPs)] (2009) Lead Reviewer's Track A Summary of Expert Reviews of Pentachlorophenol (PCP). April 14, 2009. Technical Report Series No. 414 (1993) NIH Publication No. 93‐3145.

[U.S. EPA 1992] U.S. EPA 1992. National Study of Chemical Residues in Fish Vol. II. EPA 823-R-92-008b

[U.S. EPA 2006] U.S. EPA 2006. Reregistration Eligibility Decision for Pentachloronitrobenzene. Office of Prevention, Pesticides and Toxic Substances. EPA OPP-2006-XXX. 102 pp.

[U.S. EPA 2008] U.S. EPA 2008. Pentachlorophenol environmental fate and transport assessment. Office of Prevention, Pesticides, and Toxic Substances. EPA‐HQ‐OPP‐2004‐0402‐0066. 21 pp. (2008).

[U.S. EPA 2008b] U.S. EPA 2008. Reregistration Eligibility Decision for Pentachloronitrobenzene..Office of Prevention, Pesticides, and Toxic Substances. June 2006. 102 pp.

[U.S. EPA 2009] U.S. Environmental Protection Agency (USEPA); The National Study of Chemical Residues in Lake Fish Tissue; EPA‐823‐R-09-006; U.S. Environmental Protection Agency, Office of Water; Washington, DC. (2009); www.epa.gov/waterscience/fishstudy/

[U.S. EPA 2011] U.S. EPA. 2011. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.10. United States Environmental Protection Agency, Washington, DC, USA.

[Valo and Salkinoja-Salonen 1986] Valo and Salkinoja-Salonen, 1986. Bioreclamation of chlorophenol-contaminated soil by composting. Applied Microbiology and Biotechnology. 25:68-75.

[Van Ommen et al. 1985] van Ommen, B., P.J. Bladeren, J.H.M. Temmink and F. Müller. 1985. Formation of pentachlorophenol as the major product of microsomal oxida tion of hexachlorobenzene. Biochem. Biophys. Res. Communications 126:25□32.

[Van Ommen et al. 1986] van Ommen, B., A.E.P. Adang, L. Brader, M.A. Posthumus, F. Müller and P.J. Bladeren. 1986. The microsomal metabolism of hexachlorobenzene. 1986. Biochem. Pharmacol. 35:3233□3238.

[Vodicnik 1980] Vodicnik, M.J., Glickman, A.H., Rickert, D.E. and J.J. Lech. 1980. Studies on the Disposition and Metabolism of Pentachloroanisole in Female Mice. Toxicology and Applied Pharmacology 56: 311-316.

[Vorkamp et al. 2004] Vorkamp K, Rigetb F, Glasiusc M, Pécseli M and Lebeufd M., Chlorobenzenes, chlorinated pesticides, coplanar chlorobiphenyls and other organochlorine compounds in Greenland biota. Sci. Total Environ. 331: 157–175 (2004).

[Wade et al. 1998] Wade, T.L., J.L. Sericano, P.R. Gardinali, G. Wolff and L. Chambers. 1998. NOAA's 'mussel watch' project: current use organic compounds in bivalves. Mar. Pollut. Bull. 37:20□26.

[Walter et al. 2004] Walter M, Boul L, Chong R and Ford C., Growth substrate selection and biodegradation of PCP by New Zealand white□rot fungi. Journal of Environmental Management 71: 361–369 (2004).

[Walter et al., 2005] Walter, M, Boyd-Wilson, K., Boul, L., Ford, C., McFadden, D., Chong, B., and J. Pinfold. (2005) Field Scale bioremediation of pentachlorophenol by Trametes versicolor. International Biodeterioration and Biodegradation 56: 51-57.

[Walter et al. 2005b] Walter, M., Boyd-Wilson, K., McNaughton, D., and G. Northcott (2005) Laboratory trials on the bioremediation of aged pentachlorophenol residues. International Biodeterioration and Biodegradation 55: 121-130.

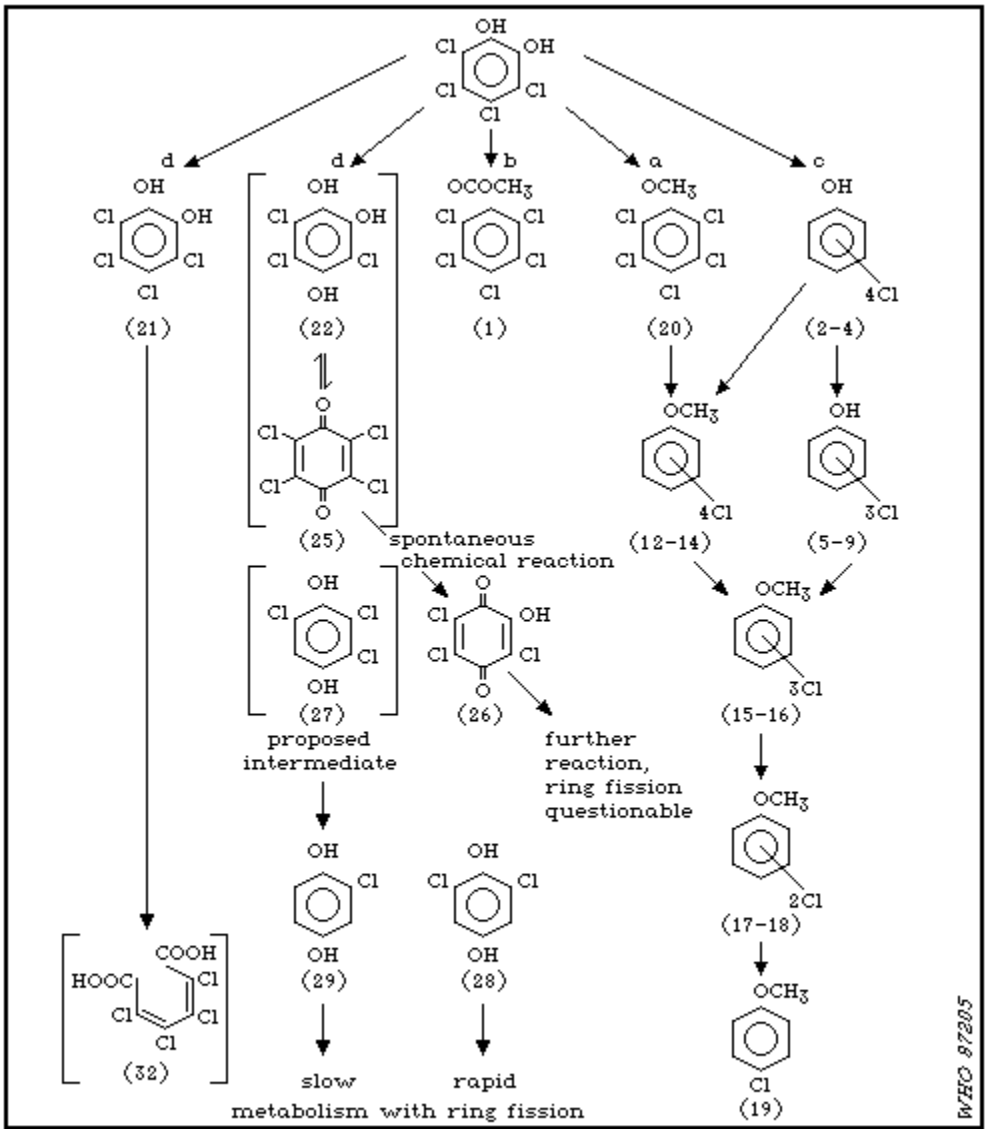
[Watanabe 1973] WATANABE I. (1973) Isolation of pentachlorophenol decomposing bacteria from soils. Soil Sci. PI. Nutr. 19, 109-116.

[Weiss et al. 1982] Weiss M.W., Scheunert, I., Klein W. and F. Korte. Fate of Pentachlorophenol-^{14}C in Soil under Controlled Conditions. Journal of Agriculture and Food Chemistry 30: 1191-1194.

[Weiss et al. 1982b] Weiss M.W., Moza, P., Scheunert, I., Haque, A. and F. Korte. Fate of Pentachlorophenol-^{14}C in Rice Plants under Controlled Conditions. Journal of Agriculture and Food Chemistry 30: 1186-1190.

[Welch et al. 1991] Welch HE, Muir DC, Billeck BN. 1991. Brown Snow:A long□range transport event in the Canadian Arctic. Environ Sci Technol.; 25:280–286.

APPENDIX I: Biotransformation Pathways of PCP (EHC 71 1987)



Metabolic pathways for the biodegradation of PCP. Adapted from: Kaufmann (1978), Reiner et al. (1978), and Rott et al. (1979). For a list of metabolites (numbers in parentheses), see Table 12.

Figure 9-1: Biotransformation pathways of PCP (EHC 71, 1997)

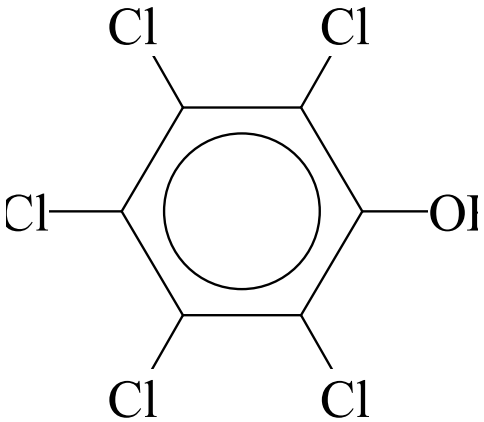
Table 9-1: Environmental Transformation Products of PCP as originally reported in EHC 71(1987) with corrections in red text.

Number	Chemical Name	Comment	Reference
1	Pentachlorophenol acetate		Rott et al. 1979
2	2,3,4,5-tetrachlorophenol		Ide et al. 1972; Kuwatsuka and Igarashi 1975; Murthy et al. 1979
3	2,3,5,6-tetrachlorophenol		Ide et al. 1972; Kuwatsuka and Igarashi 1975; Murthy et al. 1979
4	2,3,4,6-tetrachlorophenol		Ide et al. 1972; Kuwatsuka and Igarashi 1975
5	2,4,5-trichlorophenol		Ide et al. 1972; Kuwatsuka and Igarashi 1975
6	2,3,6-trichlorophenol		Kuwatsuka and Igarashi 1975; Murthy et al. 1979
7	2,3,4-trichlorophenol		Kuwatsuka and Igarashi 1975
8	2,3,5-trichlorophenol		Ide et al. 1972; Kuwatsuka and Igarashi 1975
9	2,4,6-trichlorophenol		Kuwatsuka and Igarashi 1975
10	3,4-dichlorophenol		Ide et al. 1972; Kuwatsuka and Igarashi 1975
11	3,5-dichlorophenol		Ide et al. 1972; Kuwatsuka and Igarashi 1975
12	2,3,4,5-tetrachloroanisole (acetate)	Note, Ide et al. (1972): The analytical methods included a methylation step with dimethyl sulphate. All chlorophenols were therefore measured as chloroanisoles. The methodology did not allow	~~Ide et al. 1972;~~ Rott et al. 1979b
13	2,3,5,6-tetrachloroanisole (acetate)		~~Ide et al. (1972);~~ Rott et al. 1979b
14	2,3,4,6-tetrachloroanisole (acetate)		Engel et al. 1966; ~~Ide et al. 1972~~; Rott et al. 1979b; Haimi et al. 1993
15	2,3,5-trichloroanisole		~~Ide et al. 1972~~
16	2,4,5-trichloroanisole		~~Ide et al. 1972~~
17	3,4-dichloroanisole		~~Ide et al. 1972~~
18	3,5 dichloroanisole		~~Ide et al. 1972~~
19	3-chloroanisole		~~Ide et al., 1972~~
20	Pentachloroanisole		Cserjesi & Johnson 1972; ~~Ide et al. 1972~~; Kuwatsaka & Igarashi 1975; Murthy et al. 1979; Rott et al.

Number	Chemical Name	Comment	Reference
		for distinguishing between the chlorophenols and chloroanisoles. The authors allotted all of the residues chlorophenols (not chloroanisoles).	1979
21	Tetrachlorocatechol (diacetate)		Suzuki 1977; Rott et al. 1979b
22	Tetrachlorohydroquinone		Suzuki 1977
23	Tetrachlororesorcinol (diacetate)		Rott et al. 1979b
24	Tetrachlorohydroquinone dimethylether (diacetate)		Rott et al. 1979
25	Trichlorobenzoquinone		Reiner et al. 1978
26	Trichlorohydroxybenzoquinone		Reiner et al. 1978
27	2,3,6-trichlorohydroquinone		Reiner et al. 1978
28	2,6-dichlorohydroquinone		Reiner et al. 1978
29	2-chlorohydroquinone		Reiner et al. 1978
30	CO_2		Chu and Kirsch 1972; Kirsch and Etzel 1973; Suzuki 1977
31	Cl^-		Watanabe 1973; Suzuki 1977
32	Tetrachloromuconic acid		Lyr 1962
33	beta-hydroxytrichloromuconic acid		Lyr 1962

APPENDIX II: EpiSuite v. 4.10 Summary Output for PCP and PCA

EPI Suite Results For CAS 000087-86-5




```
SMILES : Oc(c(c(c(c1CL)CL)CL)CL)c1CL
CHEM   : Phenol, pentachloro-
MOL FOR: C6 H1 CL5 O1
MOL WT : 266.34
------------------------------ EPI SUMMARY (v4.10) -------------------------
Physical Property Inputs:
Log Kow (octanol-water):   ------
Boiling Point (deg C)  :   ------
Melting Point (deg C)  :   ------
Vapor Pressure (mm Hg) :   ------
Water Solubility (mg/L):   ------
Henry LC (atm-m3/mole) :   ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) =  4.74
Log Kow (Exper. database match) =  5.12
Exper. Ref:  HANSCH,C ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C):  311.71  (Adapted Stein & Brown method)
Melting Pt (deg C):  106.77  (Mean or Weighted MP)
VP(mm Hg,25 deg C):  1.08E-005  (Modified Grain method)
VP (Pa, 25 deg C) :  0.00144  (Modified Grain method)
MP  (exp database):  174 deg C
BP  (exp database):  309.5 deg C
VP  (exp database):  1.10E-04 mm Hg (1.47E-002 Pa) at 25 deg C
Subcooled liquid VP: 0.00327 mm Hg (25 deg C, exp database VP )
: 0.436 Pa  (25 deg C, exp database VP )

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L):  3.09
log Kow used: 5.12 (expkow database)
```

```
no-melting pt equation used
Water Sol (Exper. database match) =  14 mg/L (25 deg C)
Exper. Ref:  YALKOWSKY,SH & DANNENFELSER,RM (1992)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) =  45.051 mg/L

ECOSAR Class Program (ECOSAR v1.00):
Class(es) found:
Phenols

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method :   1.25E-007  atm-m3/mole  (1.27E-002 Pa-m3/mole)
Group Method:   2.94E-007  atm-m3/mole  (2.98E-002 Pa-m3/mole)
Exper Database: 2.45E-08  atm-m3/mole  (2.48E-003 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC:  not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC:  1.225E-006 atm-m3/mole  (1.241E-001 Pa-m3/mole)
VP:   1.08E-005 mm Hg (source: MPBPVP)
WS:   3.09 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used:  5.12  (exp database)
Log Kaw used:  -5.999  (exp database)
Log Koa (KOAWIN v1.10 estimate):  11.119
Log Koa (experimental database):  None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model)         :  -0.1755
Biowin2 (Non-Linear Model)     :   0.0000
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model):   1.6340  (recalcitrant)
Biowin4 (Primary Survey Model) :   2.6765  (weeks-months)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model)    :   0.0149
Biowin6 (MITI Non-Linear Model):   0.0031
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): -1.0946
Ready Biodegradability Prediction:   NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled):  0.436 Pa (0.00327 mm Hg)
Log Koa (Koawin est  ): 11.119
Kp (particle/gas partition coef. (m3/ug)):
Mackay model           :  6.88E-006
Octanol/air (Koa) model:  0.0323
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model     :  0.000248
Mackay model           :  0.00055
Octanol/air (Koa) model:  0.721

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant =   0.5505 E-12 cm3/molecule-sec
```

Half-Life =   19.430 Days (12-hr day; 1.5E6 OH/cm3)
Ozone Reaction:
No Ozone Reaction Estimation
Reaction With Nitrate Radicals May Be Important!
Fraction sorbed to airborne particulates (phi):
0.000399 (Junge-Pankow, Mackay avg)
0.721 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc   : 4959 L/kg (MCI method)
Log Koc: 3.695   (MCI method)
Koc   : 1.17E+004 L/kg (Kow method)
Log Koc: 4.068   (Kow method)
Experimental Log Koc: 3.7 (database)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 3.045 (BCF = 1110 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.3423 days (HL = 2.199 days)
Log BCF Arnot-Gobas method (upper trophic) = 2.405 (BCF = 254)
Log BAF Arnot-Gobas method (upper trophic) = 2.406 (BAF = 254.7)
log Kow used: 5.12 (expkow database)

Volatilization from Water:
Henry LC: 2.45E-008 atm-m3/mole (Henry experimental database)
Half-Life from Model River: 3.9E+004 hours   (1625 days)
Half-Life from Model Lake : 4.256E+005 hours   (1.773E+004 days)

Removal In Wastewater Treatment:
Total removal: 81.16 percent
Total biodegradation: 0.70 percent
Total sludge adsorption: 80.46 percent
Total to Air: 0.00 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)	
Air	0.0377	466	1000
Water	4.12	4.32e+003	1000
Soil	93.7	8.64e+003	1000
Sediment	2.18	3.89e+004	0

Persistence Time: 7.81e+003 hr

....

BIOWIN-PCP

SMILES : Oc(c(c(c(c1CL)CL)CL)CL)c1CL
CHEM :
MOL FOR: C6 H1 CL5 O1
MOL WT : 266.34
---------- BIOWIN v4.10 Results ----------

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast
Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin3 (Ultimate Biodegradation Timeframe): Recalcitrant
Biowin4 (Primary Biodegradation Timeframe): Weeks-Months
Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable
Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable
Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast
Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.1158	0.1158
Frag	5	Aromatic chloride [-CL]	-0.1824	-0.9121
MolWt	*	Molecular Weight Parameter		-0.1268
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		-0.1755

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.9086	0.9086
Frag	5	Aromatic chloride [-CL]	-2.0155	-10.0775
MolWt	*	Molecular Weight Parameter		-3.7820
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0564	0.0564
Frag	5	Aromatic chloride [-CL]	-0.2066	-1.0330
MolWt	*	Molecular Weight Parameter		-0.5886
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		1.6340

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0397	0.0397
Frag	5	Aromatic chloride [-CL]	-0.1653	-0.8267
MolWt	*	Molecular Weight Parameter		-0.3843

Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		2.6765

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0642	0.0642
Frag	5	Aromatic chloride [-CL]	0.0062	0.0309
MolWt	*	Molecular Weight Parameter		-0.7924
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.0149

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.4884	0.4884
Frag	5	Aromatic chloride [-CL]	-0.2191	-1.0957
MolWt	*	Molecular Weight Parameter		-7.6889
RESULT		Biowin6 MITI Non-Linear Biodeg Probability		0.0031

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

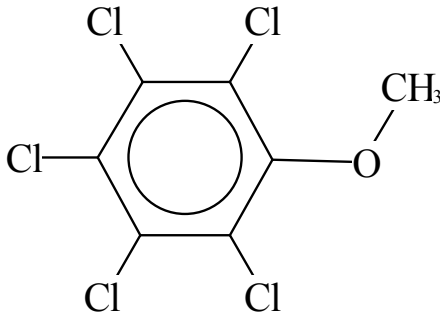
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aromatic alcohol [-OH]	0.0807	0.0807
Frag	5	Aromatic chloride [-CL]	-0.4023	-2.0114
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-1.0946

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

EPI Suite Results For CAS 001825-21-4




```
SMILES : COc1c(CL)c(CL)c(CL)c(CL)c1CL
CHEM   : Pentachloroanisole
MOL FOR: C7 H3 CL5 O1
MOL WT : 280.37
------------------------------ EPI SUMMARY (v4.10) -------------------------
Physical Property Inputs:
Log Kow (octanol-water):   ------
Boiling Point (deg C)  :   ------
Melting Point (deg C)  :   ------
Vapor Pressure (mm Hg) :   ------
Water Solubility (mg/L):   ------
Henry LC (atm-m3/mole) :   ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) =  5.30
Log Kow (Exper. database match) =  5.45
Exper. Ref:  OPPERHUIZEN,A & VOORS,PI (1987)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C):  297.85  (Adapted Stein & Brown method)
Melting Pt (deg C):  84.27  (Mean or Weighted MP)
VP(mm Hg,25 deg C):  0.000344  (Modified Grain method)
VP (Pa, 25 deg C) :  0.0458  (Modified Grain method)
MP  (exp database):  107-109 deg C
Subcooled liquid VP: 0.00219 mm Hg (25 deg C, Mod-Grain method)
: 0.292 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L):  0.3535
log Kow used: 5.45 (expkow database)
no-melting pt equation used

Water Sol Estimate from Fragments:
```

```
Wat Sol (v1.01 est) =  0.78504 mg/L

ECOSAR Class Program (ECOSAR v1.00):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method :   7.12E-005  atm-m3/mole  (7.21E+000 Pa-m3/mole)
Group Method:   1.94E-003  atm-m3/mole  (1.97E+002 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC:  not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC:  3.590E-004 atm-m3/mole  (3.638E+001 Pa-m3/mole)
VP:   0.000344 mm Hg (source: MPBPVP)
WS:   0.353 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used:  5.45  (exp database)
Log Kaw used:  -2.536  (HenryWin est)
Log Koa (KOAWIN v1.10 estimate):  7.986
Log Koa (experimental database):  None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model)         :  -0.1661
Biowin2 (Non-Linear Model)     :   0.0002
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model):   1.4885  (recalcitrant)
Biowin4 (Primary Survey Model) :   2.6937  (weeks-months)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model)    :   0.1046
Biowin6 (MITI Non-Linear Model):   0.0049
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): -1.0768
Ready Biodegradability Prediction:   NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled):  0.292 Pa (0.00219 mm Hg)
Log Koa (Koawin est  ): 7.986
Kp (particle/gas partition coef. (m3/ug)):
Mackay model           :  1.03E-005
Octanol/air (Koa) model:  2.38E-005
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model     :  0.000371
Mackay model           :  0.000821
Octanol/air (Koa) model:  0.0019

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant =   1.0945 E-12 cm3/molecule-sec
Half-Life =     9.773 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life =   117.274 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
0.000596 (Junge-Pankow, Mackay avg)
```

0.0019 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc   : 2474 L/kg (MCI method)
Log Koc: 3.393   (MCI method)
Koc   : 1.38E+004 L/kg (Kow method)
Log Koc: 4.140   (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):
Log BCF from regression-based method = 3.263 (BCF = 1832 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 1.8390 days (HL = 69.03 days)
Log BCF Arnot-Gobas method (upper trophic) = 4.137 (BCF = 1.371e+004)
Log BAF Arnot-Gobas method (upper trophic) = 5.619 (BAF = 4.155e+005)
log Kow used: 5.45 (expkow database)

Volatilization from Water:
Henry LC: 0.00194 atm-m3/mole (estimated by Group SAR Method)
Half-Life from Model River: 2.214 hours
Half-Life from Model Lake :   164.6 hours   (6.856 days)

Removal In Wastewater Treatment:
Total removal: 88.89 percent
Total biodegradation: 0.68 percent
Total sludge adsorption: 83.56 percent
Total to Air: 4.65 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)	
Air	3.39	235	1000
Water	5.94	4.32e+003	1000
Soil	89.3	8.64e+003	1000
Sediment	1.39	3.89e+004	0

Persistence Time: 1.73e+003 hr

….

SMILES : COc1c(CL)c(CL)c(CL)c(CL)c1CL
CHEM   :
MOL FOR: C7 H3 CL5 O1
MOL WT : 280.37
--------------------------- BIOWIN v4.10 Results ----------------------

   Biowin1 (Linear Model Prediction)   : Does Not Biodegrade Fast
   Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast
   Biowin3 (Ultimate Biodegradation Timeframe): Recalcitrant
   Biowin4 (Primary Biodegradation Timeframe): Weeks-Months
   Biowin5 (MITI Linear Model Prediction)   : Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast
   Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	5	Aromatic chloride [-CL]	-0.1824	-0.9121
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1319	0.1319
MolWt	*	Molecular Weight Parameter		-0.1335
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		-0.1661

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	5	Aromatic chloride [-CL]	-2.0155	-10.0775
Frag	1	Aromatic ether [-O-aromatic carbon]	2.2483	2.2483
MolWt	*	Molecular Weight Parameter		-3.9812
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.0002

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	5	Aromatic chloride [-CL]	-0.2066	-1.0330
Frag	1	Aromatic ether [-O-aromatic carbon]	-0.0581	-0.0581
MolWt	*	Molecular Weight Parameter		-0.6196
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		1.4885

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	5	Aromatic chloride [-CL]	-0.1653	-0.8267
Frag	1	Aromatic ether [-O-aromatic carbon]	0.0771	0.0771
MolWt	*	Molecular Weight Parameter		-0.4045
Const	*	Equation Constant		3.8477

RESULT	Biowin4 (Survey Model - Primary Biodeg)		2.6937

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	5	Aromatic chloride [-CL]	0.0062	0.0309
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1952	0.1952
Frag	1	Methyl [-CH3]	0.0004	0.0004
MolWt	*	Molecular Weight Parameter		-0.8341
Const	*	Equation Constant		0.7121
RESULT	Biowin5 (MITI Linear Biodeg Probability)			0.1046

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	5	Aromatic chloride [-CL]	-0.2191	-1.0957
Frag	1	Aromatic ether [-O-aromatic carbon]	1.3227	1.3227
Frag	1	Methyl [-CH3]	0.0194	0.0194
MolWt	*	Molecular Weight Parameter		-8.0938
RESULT	Biowin6 (MITI Non-Linear Biodeg Probability)			0.0049

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	5	Aromatic chloride [-CL]	-0.4023	-2.0114
Frag	1	Aromatic ether [-O-aromatic carbon]	0.1780	0.1780
Frag	1	Methyl [-CH3]	-0.0796	-0.0796
Const	*	Equation Constant		0.8361
RESULT	Biowin7 (Anaerobic Linear Biodeg Prob)			-1.0768

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.