IDENTIFICATION OF PBT AND vPvB SUBSTANCE

RESULTS OF EVALUATION OF PBT / vPvB PROPERTIES

This dossier covers the substance manufactured and supplied as detailed below.

Substance name: Medium-chain chlorinated paraffins

EINECS number: 287-477-0

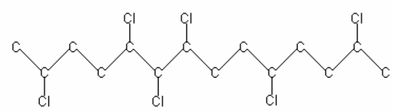
EINECS name: Alkanes, C_{14-17}, chloro

CAS number: 85535-85-9

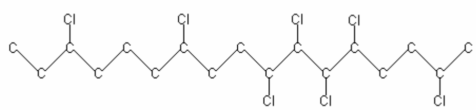
Registration number(s):

Molecular formula: $C_xH_{(2x-y+2)}Cl_y$, where x = 14-17 and y = 1-17

Structural formula: Example structures



$C_{14}H_{24}Cl_6$



$C_{17}H_{29}Cl_7$

Composition: Medium-chain chlorinated paraffins (MCCPs) is a complex substance containing a range of carbon chain lengths with variable chlorine contents

Summary of how the substance meets the CMR (Cat 1 or 2), PBT or vPvB criteria, or is considered to be a substance of an equivalent level of concern

A fish bioaccumulation study (OECD TG 305) was requested for MCCPs under Commission Regulation (EC) No. 466/2008, with a deadline of 30 November 2008. This study has now been completed and is summarised in this evaluation report, together with a further fish bioconcentration study with C_{13} chlorinated paraffins. These data are reasonably consistent with the existing data on bioconcentration of MCCPs in fish. In addition, biodegradation data for several chlorinated paraffins have become available, and these studies have also been reviewed.

The PBT assessment is complicated because both the biodegradability and bioconcentration factor of MCCP constituents depend on chlorine content and chain length, and the trends in these are opposite (i.e. persistence appears to increase with increasing chlorine content whilst the bioconcentration factor appears to decrease). The constituents of the commercial products that meet the P/vP criterion are not necessarily the same as those that meet the B/vB criteria and *vice versa*. For example, measured data for a C_{14}, 45% wt. Cl substance show that although it meets the vB criterion, it is not P. In other cases, there are no reliable data to determine whether one or more of the criteria will be met or not.

Based on a read-across and grouping analysis using all available data, the general picture emerges that for MCCP products containing about 50% chlorine by weight or higher, any chlorinated impurities with carbon chain lengths less than C_{14} ($C_{<14}$) might have a problematic P & B profile, especially at chlorination levels of 65% or more. In addition, some of the main constituents could also have problematic P & B profiles (i.e. the C_{14}- constituents, and C_{15}- constituents with chlorine contents in the range 50-55%). However, the C_{16} and C_{17} chain lengths do not appear to be of concern. The categorisation for some of the constituents is uncertain because of inherent limitations in the underlying data sets (particularly as predicted values have had to be used in many cases), so a definitive conclusion cannot yet be drawn.

This picture does not take account of the T criterion. This might be expected to be related to the bioaccumulation potential of the substances, since they are likely to act via a non-polar narcotic mode of action in invertebrates. It is clear that both a C_{14-17}, 52% wt. Cl substance and C_{10-13}, 58% wt. Cl substance meet the T criterion (the former on the basis of both aquatic and mammalian effects). Other chlorine content products could also be toxic, but this has not been established.

An important way forward to address some of the remaining uncertainty in the assessment would be to carry out further biodegradation testing of the constituents that potentially meet both the P and B criteria. It is understood that Industry is currently performing further enhanced ready biodegradation studies on a single chain length C_{14}- paraffin chlorinated in 5% increments between 45% and 70% by weight. This should provide further useful information for use in the read-across (provided that an appropriate inoculum is being used). However, if any constituent does not fulfil the ready biodegradation criteria, a sediment simulation test might still be needed to establish the environmental half-life.

It would also appear to be important to investigate the biodegradation potential of a C_{15} chlorinated paraffin with a chlorine content of around 51% by weight. This constituent is potentially persistent and the experimental BCF for a C_{15}, 51% wt. Cl substance is around 1,833-2,072 l/kg (i.e. borderline B). It is assumed to meet the T criterion based on the available evidence.

Depending on the outcome of this testing, there might still be a need to investigate the bioaccumulation potential of C_{14} chlorinated paraffins with chlorine contents of around 50% and higher. Additional information on the variation in long-term toxicity to *Daphnia magna* with chlorination level might also be useful for this chain length.

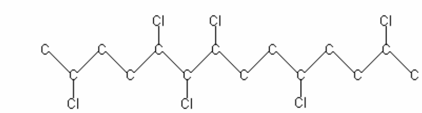
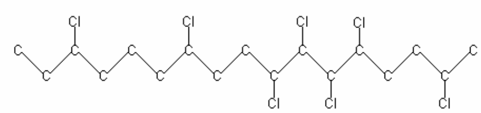
It is also important to ascertain the amounts of carbon chain lengths less than C_{14} present in a range of commercial MCCP products to determine if any of these impurities are present above 0.1% by weight. This information should be available from registration dossiers in due course.

CONTENTS

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifier of the substance

Name:	Medium-chain chlorinated paraffins
EC Number:	287-477-0
CAS Number:	85535-85-9
IUPAC Name:	Alkanes, C_{14-17}, chloro
Molecular Formula:	$C_xH_{(2x-y+2)}Cl_y$, where x = 14-17 and y = 1-17
Structural Formula:	 $C_{14}H_{24}Cl_6$  $C_{17}H_{29}Cl_7$
Molecular Weight:	300-600 approx.
Synonyms:	Chlorinated paraffin (C_{14-17}); chloroalkanes, C_{14-17}; chloroparaffin; chloroparaffine, C_{14-17}; medium-chain chlorinated paraffins; paraffine clorurate (C_{14-17}); paraffine clorurate a catena media.

The abbreviation MCCPs will be used for the substance throughout this dossier.

1.2 Composition of the substance

MCCPs contain constituents with varying chlorine content and carbon chain lengths (between C_{14} and C_{17}) and therefore can be considered to be a UVBC substance (i.e. a substance of unknown or variable composition, complex reaction products or biological materials). The percentage chlorine content of the commercially available products varies according to the applications they are used for. **Table 1** indicates the structural formulae of possible constituents of different MCCP products (adapted from information originally presented in EU (2000) and EU (2005)).

Table 1 Theoretical chlorine content of constituents in medium-chain chlorinated paraffins

Chlorine content, w/w	Constituent formula[a]							
	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}
<40%	$C_{10}H_{21}Cl$ & $C_{10}H_{20}Cl_2$	$C_{11}H_{23}Cl$ & $C_{11}H_{22}Cl_2$	$C_{12}H_{25}Cl$ to $C_{12}H_{27}Cl_3$	$C_{13}H_{27}Cl$ to $C_{13}H_{25}Cl_3$	$C_{14}H_{29}Cl$ to $C_{14}H_{27}Cl_3$	$C_{15}H_{31}Cl$ to $C_{15}H_{29}Cl_3$	$C_{16}H_{33}Cl$ to $C_{16}H_{30}Cl_4$	$C_{17}H_{35}Cl$ to $C_{17}H_{32}Cl_4$
40-45%	$C_{10}H_{19}Cl_3$	$C_{11}H_{21}Cl_3$	-	$C_{13}H_{24}Cl_4$	$C_{14}H_{26}Cl_4$	$C_{15}H_{28}Cl_4$	$C_{16}H_{29}Cl_5$	$C_{17}H_{31}Cl_5$
45-50%	$C_{10}H_{19}Cl_3$	$C_{11}H_{20}Cl_4$	$C_{12}H_{22}Cl_4$	$C_{13}H_{23}Cl_5$	$C_{14}H_{25}Cl_5$	$C_{15}H_{27}Cl_5$	$C_{16}H_{28}Cl_6$	$C_{17}H_{30}Cl_6$
50-55%	$C_{10}H_{18}Cl_4$	$C_{11}H_{19}Cl_5$	$C_{12}H_{21}Cl_5$	$C_{13}H_{22}Cl_6$	$C_{14}H_{24}Cl_6$	$C_{15}H_{26}Cl_6$ & $C_{15}H_{25}Cl_7$	$C_{16}H_{27}Cl_7$	$C_{17}H_{29}Cl_7$
55%-65%	$C_{10}H_{16}Cl_6$ & $C_{10}H_{17}Cl_7$	$C_{11}H_{18}Cl_6$ & $C_{11}H_{17}Cl_7$	$C_{12}H_{20}Cl_6$ to $C_{12}H_{18}Cl_8$	$C_{13}H_{21}Cl_7$ to $C_{13}H_{19}Cl_9$	$C_{14}H_{23}Cl_7$ to $C_{14}H_{21}Cl_9$	$C_{15}H_{24}Cl_8$ to $C_{15}H_{22}Cl_{10}$	$C_{16}H_{26}Cl_8$ to $C_{16}H_{23}Cl_{11}$	$C_{17}H_{28}Cl_8$ to $C_{17}H_{25}Cl_{11}$
>65%	$C_{10}H_{14}Cl_8$ and higher no. of Cl atoms	$C_{11}H_{16}Cl_8$ and higher no. of Cl	$C_{12}H_{17}Cl_9$ and higher no. of Cl atoms	$C_{13}H_{18}Cl_{10}$ and higher no. of Cl atoms	$C_{14}H_{20}Cl_{10}$ and higher no. of Cl atoms	$C_{15}H_{21}Cl_{11}$ and higher no. of Cl atoms	$C_{16}H_{22}Cl_{12}$ and higher no. of Cl atoms	$C_{17}H_{24}Cl_{12}$ and higher no. of Cl atoms

Note: a) The grey columns refer to potential impurities

The chlorine content of the commercially available products is generally within the range 40% by weight to around 63% by weight, but the majority of products have chlorine contents between 45% by weight and 52% by weight. The main constituents in the majority of products have between five and seven chlorine atoms per molecule. Nevertheless, it should be noted that percentage chlorine content only represents an average level of chlorination, and so a wider range of constituents may be present in any particular product.

Any impurities in commercial chlorinated paraffins are likely to be related to those present in the n-paraffin feedstocks, in which the major non-paraffinic impurity is a small proportion of aromatics, generally less than 100 mg/kg. The isoparaffin content of the feedstock is less than 1-2%. The producers of MCCPs (represented by Euro Chlor) have, since 1991, used paraffin feedstocks in the production process with a $C_{<14}$ content of <1% by weight and report that the actual levels are often much lower than this (EU, 2005).

Various stabilisers (for example long-chain epoxidised soya oil or glycidyl ethers at <1% by weight) are often added to commercial chlorinated paraffins in order to improve thermal stability or light stability (EU, 2005).

1.3 Physico-chemical properties

The physico-chemical property data are summarised in **Table 2**.

Table 2 Summary of physico-chemical properties

REACH ref Annex, §	Property	Value	Reference/comment
V, 5.1	Physical state at 20°C and 101.3 kPa	Liquid to semi-solid	EU (2005). Depends on chlorine content.
V, 5.2	Melting / freezing point	-45 to +25°C	EU (2005). Pour points, not distinct melting point. Value depends on chlorine content.
V, 5.3	Boiling point	>200°C	EU (2005). Decomposition with release of hydrogen chloride.
V, 5.5	Vapour pressure	2.27×10^{-3} Pa at 40°C (45% wt. Cl substance) 2.7×10^{-4} Pa at 20°C (52% wt. Cl substance)	EU (2005).
V, 5.7	Water solubility	0.005-0.027 mg/l at 20°C	EU (2005). Value is for a 51% chlorine content product. Little data available for other chlorine contents.
V, 5.8	Partition coefficient n-octanol/water (log value)	4.47-8.21 "typical" value ~7	EU (2005). Value depends on chlorine content and carbon chain length.
VII, 5.19	Dissociation constant	Not relevant	

2 MANUFACTURE AND USES

Not relevant for this type of this dossier.

3 CLASSIFICATION AND LABELLING

3.1 Hazard classification

Regulation (EC) No 1272/2008 (CLP Regulation):

Lact.; Hazard statement: H362, May cause harm to breast-fed children.

Supplemental hazard statement: EUH066, Repeated exposure may cause skin dryness or cracking.

Aquatic Acute 1; Hazard statement: H400, Very toxic to aquatic life.
Aquatic Chronic 1; Hazard statement: H410, Very toxic to aquatic life with long lasting effects.

Directive 67/548/EEC:

N; R50-53	Dangerous for the Environment. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
R64	May cause harm to breastfed babies.
R66	Repeated exposure may cause skin dryness or cracking.

4 ENVIRONMENTAL FATE PROPERTIES

The existing information on the environmental fate of MCCPs has been reviewed in detail in two environmental risk assessment reports produced under the Existing Substances Regulation (EU, 2005 and 2007a). In the following sections, the information from these previous reviews has been described only briefly under the heading *Summary of information from existing evaluation*. The new data are reported under the heading *New information*.

4.1 Degradation

4.1.1 Abiotic degradation

4.1.1.1 Summary of information from existing evaluation

The atmospheric half-life is estimated to be 1-2 days (EU, 2005).

4.1.1.2 New information

No new information is available.

4.1.2 Biotic degradation

4.1.2.1 Summary of information from existing evaluation

No standard ready or inherent biodegradation tests had been carried out for MCCPs, and no results from simulation tests were available. However, based on non-standard test data on biological oxygen demand (BOD), MCCPs were not expected to be readily biodegradable or inherently biodegradable within the meaning of standard ready biodegradation test systems (EU, 2005).

There is evidence that some microorganisms may be capable of degrading MCCPs in the environment in acclimated or cometabolic systems, but it is not possible to estimate a likely environmental degradation half-life from these data. The potential for biodegradation appears to decrease with increasing chlorine content, which implies that the more highly chlorinated MCCPs may be more persistent than the less chlorinated MCCPs. The most common types of MCCPs in commercial use have chlorine contents of ~45–52% by weight. Of these, the 52% wt. Cl products would be expected to be more persistent than the 45% wt. products (EU, 2005).

In addition, biodegradation simulation studies using the OECD Test Guideline 308 were performed by Thompson and Noble (2007) for the related C_{10-13} chlorinated paraffins (short-chain chlorinated paraffins or SCCPs) and the results were summarised in EU (2007b). This study showed that both a C_{10}, 65% wt. Cl substance and a C_{13}, 65% wt. Cl substance had a long degradation half-life in sediment (335 and 680 days respectively in marine sediments and 1,340 and 1,790 days respectively in freshwater sediments).

4.1.2.2 New information

The biodegradability of a C_{14}, 45% wt. chlorinated paraffin has been tested using the OECD 301D Closed Bottle test methodology adapted to maximise the bioavailability of the test substance (AkzoNobel, 2010a).

The test substance had a purity of 99% and the average formula was $C_{14}H_{25.4}Cl_{4.6}$. The inoculum used was secondary activated sludge from a waste water treatment plant treating predominantly domestic waste water in the Netherlands. The test substance was administered to the test bottles as a suspension in water. The suspension was obtained by mixing 0.08 g of the test substance and 0.09 g of a polyalkoxylate alkylphenol in 80 ml of deionised water followed by ultrasonification for 10 minutes.

The final concentration of the test substance in the test bottles was 2.0 mg/l (which is above the expected water solubility). The inoculum concentration was not given in the test report (although AkzoNobel (2009) indicates that it was probably 2 mg dry weight/l). Both a control and polyalkoxylate controls were included in the experiment and sodium acetate was used as a positive control (at a concentration of 6.7 mg/l). The bottles were incubated at 24°C for up to 42 days and the dissolved oxygen concentration was analysed in duplicate bottles on day 7, 14, 21, 28 and 42 of the study.

The theoretical oxygen demand (ThOD) of the test substance was calculated to be 1.75 mg/mg. The dissolved oxygen concentrations and percentage degradation found during the test are summarised in **Table 3**.

Table 3 Results of the Closed Bottle test with a C_{14}, 45% wt Cl substance

Time (days)	Mean dissolved oxygen concentration (mg/l)				Percentage degradation	
	Control	Control with surfactant	Chlorinated paraffin with surfactant	Positive control (sodium acetate)	Chlorinated paraffin	Positive control (sodium acetate)
0	8.9	8.9	8.9	8.9	0%	0%
7	8.3	8.3	8.2	5.1	3%	62%
14	8.0	8.0	7.5	4.3	14%	71%
21	8.0	8.0	6.9	-	32%	-
28	7.8	7.7	5.5	-	64%	-
42	-	7.6	5.3	-	67%	-

The results showed around 64% biodegradation of the test substance had occurred by day 28, indicating that the test substance is readily biodegradable in this test system.

It should be noted that although the 10-day window is not met in the above test, the relevance of the 10-day window in this case has been questioned by AkzoNobel (2010a): although a single chain length substance was tested, it would still be a mixture of constituents with different numbers of chlorine atoms (the chlorine content given is in effect the average chlorine content). Thus the various constituents may not necessarily be degraded by a single microorganism, nor at the same rate. As the test generates a single biodegradation curve (effectively the sum of the individual biodegradation curves) it is possible that the 10-day window criterion is met for at least some of the constituents making up the curve. The REACH guidance document also indicates that the 10-day window is not applicable to tests carried out with a mixture of homologous substances (Chapter R.7B, p. 171).

AkzoNobel (2009) indicates that further studies have also shown this test substance to be readily biodegradable in similar test systems using a range of other inocula. A brief summary of these findings is given in **Table 4**. The inocula used were either activated sludge from a waste water treatment plant treating predominantly domestic waste water in the Netherlands (inoculum concentration 2 mg dry weight/l) or river water from the River Rhine near Heveadorp (used undiluted but spiked with mineral salts medium). Few other test details are currently available.

Table 4 Other Closed Bottle tests that have reportedly been carried out with a C_{14}, 45% wt Cl substance

Test system	**Percentage degradation**	
	at day 28	**at day 42**
Test concentration 1.0 mg/l, administered with dichloromethane. Activated sludge inoculum.	46%	101% (stated to be inaccurate)
Test concentration 2.0 mg/l, administered with dichloromethane. Activated sludge inoculum.	48%	65%
Test concentration 2.0 mg/l, administered with silicon oil. Activated sludge inoculum.	45%	60%
Test concentration 2.0 mg/l, administered with surfactant (polyalkoxylate alkylphenol). Activated sludge inoculum.	68%	74%
Test concentration unclear, administered with silicon oil and surfactant. Activated sludge inoculum.	66%	79%
Test concentration 2.0 mg/l, administered with dichloromethane. River water inoculum.	52%	65%
Test concentration 2.0 mg/l, administered with silicone oil. River water inoculum.	55%	60%
Test concentration 2.0 mg/l, administered with surfactant. River water inoculum.	64%	65%

These tests were carried out with a single carbon chain length substance. Further biodegradation tests have been carried out with a series of commercial chlorinated paraffins (medium-chain (C_{14-17}) and short-chain (C_{10-13}) chlorinated paraffins containing several different carbon chain lengths) using a similar methodology. The results are given below. The information on short-chain chlorinated paraffins is relevant as medium-chain chlorinated paraffins may contain chlorinated impurities with carbon chain lengths of C_{13} or below (see Section 1) and for read-across.

a) The first commercial MCCP tested was a 45.6% wt. Cl substance (AkzoNobel, 2010b). The purity of the substance was assumed to be 100 per cent in the test report (i.e. it was assumed that no stabilisers were present). The inoculum used in the test was secondary activated sludge from a plant treating predominantly domestic waste water in the Netherlands. The substance was tested as a suspension. A 1 g/l stock suspension was prepared by mixing 0.32 g of the test substance and 0.31 g of a polyalkoxylate alkylphenol in 310 ml of deionised water followed by ultrasonification for 5 minutes. This was then diluted in the nutrient medium used in the test bottles to give a final concentration of the test substance of 2.0 mg/l. The inoculum concentration was not given in the test report but, based on the studies reported above, was probably 2 mg dry weight/l. A control, a polyalkoxylate control and a positive control (sodium acetate at a concentration of 6.7 mg/l) were also included. The bottles were incubated at 22-24°C for up to 42 days and the dissolved oxygen concentration was analysed in duplicate bottles at intervals during the study.

The ThOD of the test substance was calculated to be 1.75 mg/mg[1]. The percentage degradation observed is summarised in **Table 5**.

Table 5 Results of the Closed Bottle test with a commercial C_{14-17}, 45.6% wt Cl substance

Time (days)	Mean dissolved oxygen concentration (mg/l)				Percentage degradation	
	Control	Control with surfactant	Chlorinated paraffin with surfactant	Positive control (sodium acetate)	Chlorinated paraffin	Positive control (sodium acetate)
0	8.8	8.8	8.8	8.8	0%	0%
7	8.3	8.3	8.3	4.4	0%	72%
14	7.8	7.9	7.6	3.7	9%	76%
21	7.8	7.9	6.8	-	31%	-
28	7.7	7.6	5.8	-	51%	-
35	-	7.7	5.6	-	60%	-
42	-	7.5	5.3	-	63%	-

The results showed that around 51 per cent biodegradation had occurred by day 28 but that further degradation occurred with prolonged incubation (60 per cent at day 35 and 63 per cent at day 42). Therefore, although the test substance cannot be considered to meet the criteria for ready biodegradation in this test, the results show that significant degradation was occurring in the study. The results of this test are discussed later in this section.

b) The second commercial MCCP tested was a C_{14-17}, 63.2% wt. Cl substance (AkzoNobel, 2010c). The test substance was presumed to have a purity of 100% and the test method was essentially the same as in the preceding test. The ThOD of the test substance was calculated to be 1.05 mg/mg. The percentage degradation observed is summarised in **Table 6**.

The extent of biodegradation was around 5-10 per cent after 60 days, so limited biodegradation was evident in this study.

[1] For a C_{14-17}, 45.6% wt. Cl substance the actual ThOD should be around 1.73 mg/mg. This is similar to, but slightly lower than, the value used in the test report (the lower value will lead to a slightly higher percentage degradation for a given oxygen consumption figure).

Table 6 Results of the Closed Bottle test with a commercial C_{14-17}, 63.2% wt Cl substance

Time (days)	Mean dissolved oxygen concentration (mg/l)				Percentage degradation	
	Control	Control with surfactant	Chlorinated paraffin with surfactant	Positive control (sodium acetate)	Chlorinated paraffin	Positive control (sodium acetate)
0	8.8	8.8	8.8	8.8	0%	0%
7	8.3	8.3	8.3	4.4	0%	72%
14	7.8	7.9	7.8	3.7	5%	76%
21	7.8	7.9	7.6	-	14%	-
28	7.7	7.6	7.5	-	5%	-
42	-	7.5	7.4	-	5%	-
60	-	7.2	7.0	-	10%	-

c) Similar biodegradation tests have also been carried out with a commercial short-chain (C_{10-13}) 49.8% wt. Cl chlorinated paraffin (AkzoNobel, 2010d). This was tested using a range of inocula and administration methods. A brief summary of the findings is given in **Table 7** (full test details of these studies are not yet available).

Table 7 Closed Bottle tests that have been carried out with a C_{10-13}, 49.8% wt Cl short-chain chlorinated paraffin

Test system	Percentage degradation		
	at day 28	at day 42	at day 56
Test concentration 2.0 mg/l, administered with dichloromethane[c]. Activated sludge inoculum[a].	31%	-	41%
Test concentration 2.0 mg/l, administered with silicone oil[d]. Activated sludge inoculum[a].	6%	-	22%
Test concentration 2.0 mg/l, administered with surfactant[e]. Activated sludge inoculum[a].	37%	55%	-
Test concentration 2.0 mg/l, administered with dichloromethane[c]. River water inoculum[b].	16%	-	32%
Test concentration 2.0 mg/l, administered with silicone oil[d]. River water inoculum[b].	9%	-	33%
Test concentration 2.0 mg/l, administered with surfactant[e]. River water inoculum[b].	63%	65%	-

Note: a) Secondary activated sludge from a plant treating predominantly domestic waste water in the Netherlands. The inoculum concentration was 2 mg dry weight/l.
b) River water from the River Rhine near Heveadorp, the Netherlands. The river water was used undiluted but spiked with nutrient minerals.
c) The test substance was firstly dissolved in dichloromethane and the solution added to the test bottle. The solvent was then allowed to evaporate overnight with rolling (resulting in the test substance being coated onto the wall of the test vessel) before the test medium was added.
d) Tested as a suspension in silicone oil.
e) Tested as a suspension with a surfactant (polyalkoxylate alkylphenol).

Discussion

It should be noted that these studies deviate in some respects from the OECD 301D Closed Bottle Test Guideline:

i) Ammonium chloride was omitted from the mineral medium prescribed in the test guideline to prevent oxygen consumption resulting from nitrification. It was reported that this omission did not result in nitrogen limitation as shown by the biodegradation of the reference compound. However, the degradation of the reference compound occurred over the first 14 days and so this comparison does not provide any information on potential nitrogen limitation on prolonged incubation.

ii) The inoculum used in some of the tests was secondary activated sludge from an activated sludge plant treating predominantly domestic waste water. Although full details are not available for all studies, it appears that the initial activated sludge (400 mg dry weight/l) was aerated for one week prior to use, and this was diluted to a concentration of 2 mg dry weight/l for use in the test. However, the introductory section to the OECD Test Guidelines on ready biodegradability indicates that for the Closed Bottle test method the preferred inoculum source is a coarsely filtered (or settled) secondary effluent from a domestic waste water treatment plant or laboratory-scale unit as a more dilute inoculum without sludge flocs is needed. The concentration of such an effluent-derived inoculum to be used is ≤5 ml/l (giving an approximate cell count of 10^4-10^6 cells/l). Based on the reported concentrations of activated sludge used it appears that around 5 ml/l of the activated sludge was added as the inoculum. However, it is not clear if, or how, the use of activated sludge in place of the preferred secondary effluent as inoculum would have affected the test (the cell counts present in the test medium were not reported).

iii) Undiluted river water was used for some of the tests (spiked with the appropriate nutrient minerals). The OECD Test Guideline for the Closed Bottle test does not give a preferred dilution for such inocula but indicates that the optimum volume (dilution) to be used may need to be determined by trial tests. The use of undiluted river water therefore does not seem to be precluded from use in the test.

Overall, although there are some deviations from the OECD Test Guideline, the tests appear to have been well carried out and show that in some cases, the chlorinated paraffin tested can be considered to be readily biodegradable in the particular enhanced test system. The use of the results from such enhanced ready biodegradation tests in the assessment of the persistence of a substance in relation to a PBT or vPvB assessment is discussed in detail in the REACH guidance. The main points from this guidance are summarised below:

- The very low concentrations (~2 mg/l) used for the closed bottle test can sometimes lead to an overestimate of the degradation owing to the poor signal to noise ratio (theoretical versus background) in the test (Chapter R.7b, p. 170).

- Substances that pass the ready biodegradation test are considered to be not persistent in terms of the PBT and vPvB criteria. The 10-day window is considered to be unnecessary in defining the pass criterion in this respect. In addition, in order to recognise that potential PBT and vPvB substances are often poorly soluble and present difficulties in carrying out standard ready biodegradation tests, modifications are permitted to improve the bioavailability (for example by use of a solubiliser (see Appendix 7.9-3 of Chapter R.7b of the REACH guidance); this is also allowable in the

OECD Test Guideline itself). The results of such modified tests are also acceptable in defining ready biodegradability for the purposes of the screening for persistence (Chapter R.7b, p. 191).

- However, enhanced screening studies, such as where the timescale has been increased to allow time for adaptation to occur should be carried out using a natural environmental medium as the source of inoculum (marine or freshwater). Enhanced screening studies using inocula derived from sewage treatment works cannot be used in persistence assessments (Chapter R.7b, p. 191).

- The REACH guidance recommends the use of a poorly soluble positive reference compound rather than the normal positive reference substance in tests with poorly soluble substances (Appendix 7.9-3 of Chapter R.7b of the REACH guidance (p. 223)).

These points indicate that although generally only one test was carried out, the results obtained at 28 days (which can be considered to be a standard ready biodegradation test modified to allow use of an emulsifier (this will be termed “modified ready test” in the following discussion)) should be treated separately from those from longer durations (which will be considered to be an “enhanced ready test” in the following discussion) within the same study. The available results are summarised in terms of a pass or fail for the 60 per cent degradation mark in **Table 8**.

Table 8 Summary of modified and enhanced ready biodegradation test results

Substance tested	Inoculum	Administration method	Pass/fail	
			Modified ready test	Enhanced ready test
C_{10-13}, 49.8% wt. Cl	Activated sludge	Polyalkoxylate alkylphenol	Fail	Fail (but inoculum not appropriate for this type of study)
		Dichloromethane	Fail	Fail (but inoculum not appropriate for this type of study)
		Silicone oil	Fail	Fail (but inoculum not appropriate for this type of study)
	River water	Polyalkoxylate alkylphenol	Pass	Pass
		Dichloromethane	Fail	Fail
		Silicone oil	Fail	Fail
C_{14}, 45% wt. Cl	Activated sludge	Polyalkoxylate alkylphenol	Pass	Pass (but inoculum not appropriate for this type of study)
		Dichloromethane	Fail	Pass (but inoculum not appropriate for this type of study)
C_{14}, 45% wt. Cl	Activated sludge	Silicone oil	Fail	Pass (but inoculum not appropriate for this type of study)
		Silicone oil and polyalkoxylate alkylphenol	Pass	Pass (but inoculum not appropriate for this type of study)

Continued overleaf.

Table 8 continued

Substance tested	Inoculum	Administration method	Pass/fail	
			Modified ready test	**Enhanced ready test**
C_{14}, 45% wt. Cl	River water	Polyalkoxylate alkylphenol	Pass	Pass
		Dichloromethane	Fail	Pass
		Silicone oil	Fail	Pass
C_{14-17}, 45.6% wt. Cl	Activated sludge	Polyalkoxylate alkylphenol	Fail	Pass (but inoculum not appropriate for this type of study)
C_{14-17}, 63.2% wt. Cl	Activated sludge	Polyalkoxylate alkylphenol	Fail	Fail (but inoculum not appropriate for this type of study)

Based on Table 8 it can be concluded that the C_{10-13}, 49.8% wt. Cl substance (with river water) and the C_{14}, 45% wt. Cl substance (with both river water and activated sludge) are readily biodegradable in the modified ready test using the polyalkoxylate alkylphenol surfactant to increase bioavailability. Thus, these substances do not meet the Annex XIII criteria for a persistent substance. The alkane chains involved would typically have around five chlorine atoms per molecule at most.

The interpretation of the results for the C_{14-17}, 45.6% wt. Cl substance is less straightforward. It is not readily biodegradable in the modified ready test but more than 60 per cent degradation was seen in the enhanced (extended) ready test. The inoculum used in this test was derived from activated sludge, and the REACH guidance indicates that an enhanced test with such an inoculum is not suitable for use in an assessment of persistence. Therefore, although the results suggest that substantial degradation may occur, they are inconclusive as to whether the substance would degrade sufficiently rapidly so as not to meet the Annex XIII criteria. However, it should also be noted that, as a commercial substance containing different carbon chain lengths was tested, it is still possible that some constituents of the substance were readily biodegradable (for example, the C_{14}- constituents). The alkane chains involved would typically have around five to six chlorine atoms per molecule.

The results for the C_{14-17}, 63.2% wt. Cl substance (~7-11 chlorine atoms per molecule) show that the substance is not readily biodegradable under either the modified or enhanced conditions. Although this finding by itself is not sufficient to demonstrate that the Annex XIII criteria are met, the results are strongly suggestive of a relatively long degradation half-life in the environment. This is also supported by the fact that both a C_{10}, 65% wt. Cl substance (~6-7 chlorine atoms per molecule) and a C_{13}, 65% wt. Cl substance (~7-9 chlorine atoms per molecule) have a long degradation half-life in sediment (e.g. 335 and 680 days respectively in marine sediments). The longer chain lengths would be expected to be less water soluble and more adsorptive than the C_{10} and C_{13} substances, and so they are unlikely to have a shorter degradation half-life. On this basis, they are considered to meet the P and vP criteria of Annex XIII.

Other information

A recent study has investigated the levels of chlorinated paraffins, including MCCPs, in a dated sediment core from Lake Thun, Switzerland (Iozza *et al.*, 2008). The lake is located in a rural, densely populated alpine catchment area without any known point sources (e.g. metal or polymer industries). The sediment core was collected in May 2004 at a depth of 60 m and was sectioned into 1 cm slices. The core was dated using ^{137}Cs and ^{210}Pb analysis and the average sedimentation rate was determined to be 0.45 cm/year. The level of MCCPs in the sediment core showed an increasing trend from 1965 onwards reaching a level of 26 µg/kg dry weight in the surface layer (corresponding to 2004). Concentrations between 15 and 20 µg/kg dry weight were evident in the samples from the 1980s. The C_{14} carbon chain length was the most abundant constituent of the MCCPs present (accounting for 41 to 64 per cent of the total MCCPs). Analysis of the chlorine contents present indicated that there was a continuous increase in the chlorine contents of the MCCPs present in those parts of the sediment cores representing the last 20 years. The chlorine contents were generally between 53.3% and 56.6% by weight and a similar pattern of increase in the chlorine content was also seen with the short-chain chlorinated paraffins. Two possible explanations were given for this trend in chlorine content:

a) as a consequence of increased usage of chlorinated paraffins with higher chlorine contents in recent years; and/or

b) as a result of dechlorination/biotransformation of the higher chlorinated paraffins to lower chlorinated paraffins in the older sediment layers[2].

It was not possible to distinguish between these two possibilities.

Overall, although the data provide some possible evidence for dechlorination of chlorinated paraffins in the sediment core, the fact that measurable levels of MCCPs were present in the layers from the 1980s at concentrations of 15 to 20 µg/kg dry weight, when compared with the level of 26 µg/kg dry weight present in the surface layer, suggests that if degradation occurs it is likely to be very slow. This provides some strong, though indirect, evidence that the substance may be persistent (in terms of the REACH Annex XIII criteria) in these cores. It should be noted, however, that the conditions in the sediment core may vary with depth (e.g. aerobic versus anaerobic) and degradation mechanisms may also change accordingly. In addition, the levels found in the sediment layers will depend on the emissions to the environment occurring at the time the sediment layer was deposited. These factors therefore introduce uncertainties into the interpretation of the data.

4.1.3 Predicted data

The available degradation screening tests suggest that the persistence of MCCPs depends on the chlorine content of the substance. In order to explore the possible variation in degradation with structure, it is relevant to consider a weight of evidence approach based on read-across and quantitative structure-activity relationships (QSAR) (see the REACH Guidance, Chapter R.7b, p. 165).

The following criteria are given for identification of a persistent substance based on BIOWIN predictions:

---

[2] This would not be consistent with the results of the biodegradation screening studies which suggest that the lower chlorinated substances may be more degradable than the higher chlorinated substances. However, the conditions in the sediment layers are likely to be different to those in the screening studies (anaerobic versus aerobic).

BIOWIN 2 <0.5 or BIOWIN 6 <0.5 and BIOWIN 3 <2.2 – Persistent

BIOWIN 2 <0.5 or BIOWIN 6 <0.5 and BIOWIN 3 between 2.2 and 2.7 – more information needed.

BIOWIN[3] calculations have been carried out for example structures representing each possible chlorine content within the C_{13} to C_{17} range[4]. The results of these calculations are given in Appendix A. Based on these predictions, and the above suggested criteria from the REACH guidance, an estimate of the potential persistence (in relation to the REACH Annex XIII criteria) of each structure can be obtained. These are summarised in **Table 9**.

Table 9 Summary of predicted persistence for chlorinated paraffins

Carbon chain length	Chlorine content (% wt.)	BIOWIN Prediction			Assignment based on prediction	Modified assignment taking into account available screening data
		BIOWIN2	BIOWIN3	BIOWIN6		
C_{13}	28.1	0.0795	2.5915	0.0863	Further data needed	Not P
	37.0	0.0013	2.0438	0.0108	P	Not P
	44.1	0.0001	1.7945	0.0012	P	Not P
	49.8	0	1.5452	0.0001	P	Not P
	54.5	0	1.2959	0	P	P
	61.7	0	0.7973	0	P	P
C_{14}	26.6	0.0661	2.5605	0.0883	Further data needed	Not P
	35.3	0.0068	2.3112	0.011	Further data needed	Not P
	42.3	0.0001	1.7635	0.0013	P	Not P
	47.9	0	1.5142	0.0001	P	Not P
	52.6	0	1.2649	0	P	P
	62.8	0	0.5171	0	P	P
C_{15}	33.8	0.0055	2.2802	0.0113	Further data needed	Not P
	40.6	0.0005	2.0309	0.0013	P	Not P
	46.2	0	1.4832	0.0002	P	P
	50.8	0	1.234	0	P	P
	54.8	0	0.9847	0	P	P
	61.1	0	0.4861	0	P	P

Continued overleaf.

3 BIOWIN Version 4.02 were used for these calculations.

4 Although this evaluation concerns MCCPs (C_{14-17}), it is also relevant to consider C_{13} structures as they are potential impurities in the commercial MCCP products above 0.1% w/w (see Section 1).

Table 9 continued

Carbon chain length	Chlorine content (% wt.)	BIOWIN Prediction			Assignment based on prediction	Modified assignment taking into account available screening data[a]
		BIOWIN2	BIOWIN3	BIOWIN6		
C_{16}	32.3	0.0007	1.9508	0.0116	P	Not P
	39.0	0.0001	1.7016	0.0013	P	Not P
	44.5	0	1.4523	0.0002	P	P
	49.2	0	1.203	0	P	P
	53.2	0	0.9537	0	P	P
	62.2	0	0.2058	0	P	P
C_{17}	31.0	0.0006	1.9199	0.0118	P	Not P
	37.6	0.0001	1.6706	0.0014	P	Not P
	43.0	0	1.4213	0.0002	P	P
	47.7	0	1.172	0	P	P
	51.6	0	0.9227	0	P	P
	60.7	0	0.1748	0	P	P

Note: a) See text below for further explanation.

The REACH guidance interpretation of the BIOWIN predictions appears to be overly conservative when compared to the results of the available modified screening tests for chlorinated paraffins. This may partly be due to the fact that the guidance is based on the results of standard ready biodegradation tests rather than tests that have been modified to maximize the bioavailability of the test substance.

The available screening test results suggest that a C_{10-13}, 49.8% wt. Cl substance and the C_{14}, 45% wt. Cl substance can be considered to be readily biodegradable, whereas the C_{14-17}, 63.2% wt. Cl substance is potentially persistent. The results for the C_{14-17}, 45.6% wt. Cl substance were inconclusive. Comparing these test results with the predictions in Table 9, it can be seen that a BIOWIN3 prediction of around 1.4-1.5 would appear to represent a reasonable cut-off point between readily and not-readily biodegradable in the modified ready biodegradable test for these substances. The effects of this are shown in Table 9 (using a cut-off of 1.5). Based on this analysis, MCCPs with chlorine contents below around 45% by weight would not be expected to be persistent, whilst those with chlorine contents above around 50% by weight are potentially persistent. The predictions are less certain for the substances with chlorine contents between these values.

When considering these predictions, it is important to recognise that the number of actual screening test data available are limited compared with the possible number of constituents that could be present in commercial MCCP products. The predictions cannot therefore provide definitive proof of persistence or lack of persistence but rather provide reasonable indications of the components most likely to be potentially persistent or potentially not persistent.

4.1.4 Summary and discussion of persistence

The new data available show that a C_{14}, 45% wt Cl chlorinated paraffin is readily biodegradable in a standard test system (Closed Bottle Test) when measures are taken to maximise bioavailability. A C_{10-13}, 49.8% wt. Cl chlorinated paraffin is also readily biodegradable in a similar test system. Conversely, a more highly chlorinated C_{14-17}, 63.2% wt. Cl substance was not readily biodegradable in this test system, and by read across with data for shorter chain substances with similar degrees of chlorination, it is considered to be persistent.

There are insufficient data to draw conclusions for other MCCP constituents with intermediate levels of chlorination. The results of the biodegradation test with a C_{14-17}, 45.6% wt. Cl substance show that although substantial degradation may occur (especially for the shorter chain length constituents), it is not known whether it would degrade sufficiently rapidly so as not to meet the Annex XIII criteria. Monitoring evidence suggests that MCCPs with chlorine contents of around 55% by weight may persist for a long time in sediments.

A modelling exercise has been carried out in an attempt to provide a more complete picture based on the available data. This predicts that biodegradation potential depends on the chlorine content of the chlorinated paraffin. The modelling results suggest that MCCPs with chlorine contents below around 45% by weight would not be expected to be persistent, whilst C_{14}- chlorinated paraffins with chlorine contents above 50% by weight, C_{15}- and C_{16}-chlorinated paraffins with chlorine contents approaching 50% or above, and C_{17}-chlorinated paraffins with chlorine contents of around 45% or above are unlikely to be readily biodegradable and so are potentially persistent. However it should be noted that these estimates are uncertain, particularly in the 45–50% chlorine content range and, although considered useful for identifying constituents that potentially may meet or not meet the REACH Annex XIII criteria for persistence, they do not provide definitive proof of this.

4.2 Environmental distribution

4.2.1 Adsorption

4.2.1.1 Summary of information from existing evaluation

The substance has a high log K_{ow} value, with values ranging from around 4.5 up to around 8.2 depending on the chlorine content and carbon chain length, and a value of 7 was chosen for the EU risk assessment (EU, 2005 and 2007a). The K_{oc} estimated for MCCPs (based on a log K_{ow} of 7) is 588,844 l/kg (EU, 2005). In addition the substance has only limited solubility in water (around 0.005-0.027 mg/l; EU, 2005). These properties indicate that MCCPs are likely to adsorb onto sediment in aquatic environments. Therefore the persistence in sediment is more relevant than persistence in water.

4.2.1.2 New information

No new information is available.

4.2.2 Distribution modelling

Not relevant to this dossier.

4.3 Bioaccumulation

4.3.1 Screening data

MCCPs have log K_{ow} in the range 4.47-8.21 with a "typical" value around 7 (EU, 2005).

4.3.2 Measured bioaccumulation data

4.3.2.1 Summary of information from existing evaluation

A fish bioconcentration factor (BCF) of 1,087 l/kg was measured in rainbow trout (*Oncorhynchus mykiss*) for a C_{15}, 51% wt. Cl substance (EU, 2005). This substance would have had around six to seven chlorine atoms per molecule. The BCF value was based on radioactivity measurements, and so may represent accumulation of metabolites as well as the C_{15}-chlorinated paraffin. No lipid data are presented in the original study report, so it is not possible to lipid normalise this BCF. Subsequent further analysis of the data by the UK competent authority after publication of the EU (2005) assessment indicates that the growth-corrected BCF would be around 1,833-2,072 l/kg (see Appendix B).

There are several other reported fish BCFs, but most of the studies are not reliable. Modelling and read-across approaches suggested that the non-growth corrected fish BCF is >2,000 l/kg for C_{14}, ~45% wt. Cl and C_{14}, ~52% wt. Cl example structures.

Feeding studies show that fish can take up MCCPs from their food. Accumulation factors (defined as the growth corrected concentration in fish on a lipid weight basis divided by the concentration in food on a lipid weight basis) in the range 1-3 were determined for several MCCPs of specific carbon chain lengths. However, since the experiments used radiolabelled test substances, the concentrations found do not necessarily represent those of the parent compound. The potential for uptake from food appears to reduce with increasing chlorine content.

High BCFs (above 2,000 l/kg) were also reported for marine molluscs, although the interpretation of these studies is not straightforward as there is a possibility that at least some of the exposure of the organisms resulted from direct ingestion of undissolved substance or the substance adsorbed to food particles (EU, 2005 and 2007a).

4.3.2.2 New information

An OECD 305 bioconcentration study has been carried out in accordance with Good Laboratory Practice (GLP) using a ^{14}C-labelled[5] 45% chlorinated n-tetradecane (C_{14}, 45% wt Cl) (AstraZeneca, 2010). This substance would have had around four to five chlorine atoms per molecule, and is the same compound that was tested in the modified ready biodegradation tests described in Section 4.1.2.2. The test substance had a purity of >98%. The test was carried out using rainbow trout (*Oncorhynchus mykiss*).

The dilution water used was dechlorinated tap water with a pH in the range 7.33 to 7.75 and mean total hardness of 44.3 mg/l as $CaCO_3$. A flow-through test system was used with a flow rate sufficient to provide 13.7 volume additions per 24 hours.

A single test concentration was used (nominally 0.5 µg/l). The substance was added to the test vessels as a solution in dimethyl formamide (the solvent concentration in the vessel was 0.004 ml/l). The exposure concentration was maintained over the duration of the uptake phase and the mean measured concentration was 0.34 µg/l (range was 0.26 to 0.44 µg/l), which was well below the expected water solubility for this substance. A solvent control was also included.

At the start of the test the fish were in the weight range 0.75 to 1.79 g (mean weight 1.21 g). The fish were exposed to the substance for 35 days followed by a 42-day depuration period. The test was carried out at 15°C and the concentrations in fish (and water) were determined at intervals by total ^{14}C-analysis.

A plot showing the uptake and depuration data is in **Figure 1**. The resulting BCFs (based on the mean whole body concentration measured at day 35 and the kinetic data) are summarised in **Table 10**.

The lipid contents of the fish were determined on day 0 and at the end of the depuration phase as 7.5% and 12.2% respectively. The mean lipid content was 10.3%. The REACH Guidance recommends that where possible the BCF data should be normalised to a 5% lipid content. The results of this normalisation are shown in Table 10.

The fish were found to grow significantly during this test and the rate constant for growth dilution was determined from the slope of a plot of the natural logarithm of the fish weight against time. The growth rate constants determined in the exposure group and solvent control group were 0.033 day^{-1} and 0.026 day^{-1} and the mean growth rate was 0.030 day^{-1}. These rate constants are significant compared with the overall depuration rate constant determined for the substance (0.0432 day^{-1}), implying that a major portion of the depuration seen resulted from growth dilution. The effect of growth correction on the resulting BCF values is shown in Table 10.

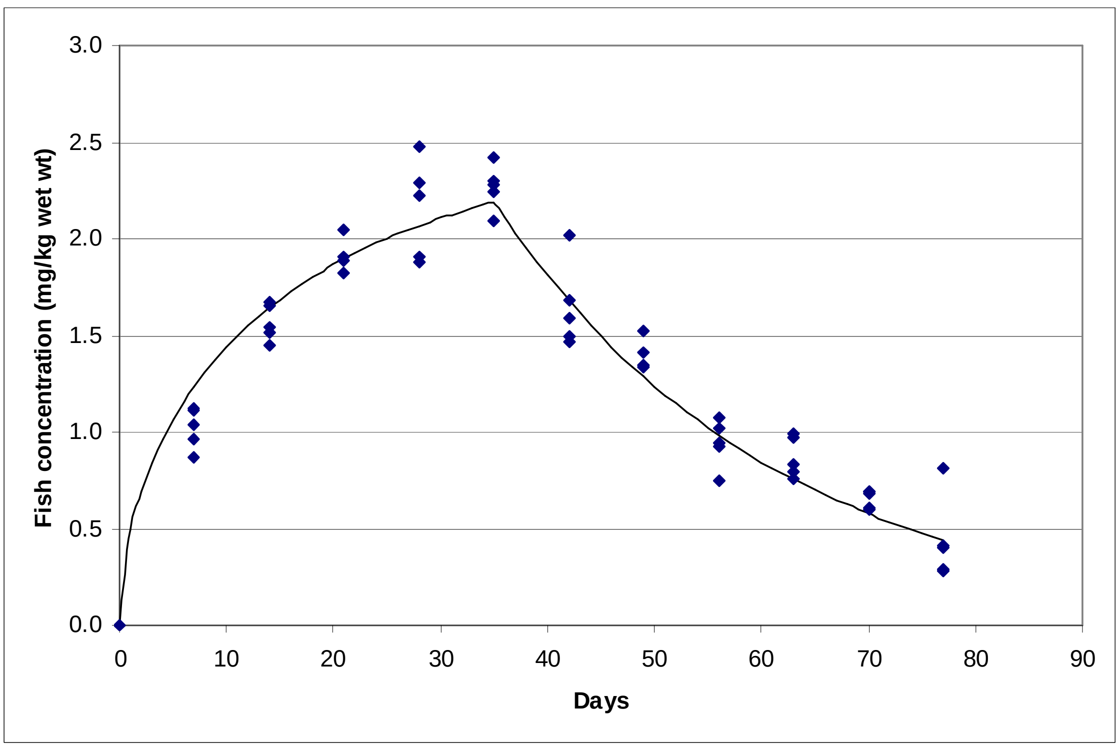
[5] The radio-label was in the 1-position on the carbon chain.

Table 10 Summary of BCF data for C_{14}, 45% wt Cl chlorinated paraffin

Endpoint	Value
Mean exposure concentration	0.34 µg/l
Mean measured concentration in fish at day 35	2,265 µg/kg
Uptake rate constant (k_1)	397 day^{-1}
Overall depuration rate constant (k_2)	0.0432 day^{-1}
Rate constant for growth dilution	0.030 day^{-1}
"Steady-state" BCF[a] at day 35 (as reported)	6,660 l/kg
"Steady-state" BCF at day 35 (normalised to 5% lipid)	3,230 l/kg
"Steady-state" BCF at day 35 (normalised to 5% lipid and corrected for growth)	~10,600 l/kg
Kinetic BCF at day 35 (as reported)	9,190 l/kg
Kinetic BCF at day 35 (normalised to 5% lipid)	4,460 l/kg
Kinetic BCF at day 35 (normalised to 5% lipid and corrected for growth)	~14,600 l/kg

Note: a) The "steady state" BCF was determined as the concentration in fish at day 35 divided by the concentration in water.

Figure 1 Uptake and depuration curve for the C_{14}, 45% wt Cl chlorinated paraffin (redrawn from the data reported in AstraZeneca (2010))



Overall, the new data for the C_{14}, 45% wt Cl chlorinated paraffin clearly show that the BCF is above 2,000 l/kg. Lipid normalisation of the data to a standard 5% lipid content results in a steady state BCF of 3,230 l/kg (based on the day 35 concentration) and a kinetic BCF of 4,460 l/kg. Growth dilution appears to account for a significant proportion of the depuration seen, and correcting for this results in BCFs of around 10,500-14,600 l/kg. This is important, because although the estimation method introduces some additional uncertainty, the resulting value is more likely to be appropriate for a fish that is not growing rapidly.

It should be noted that this study is based on total ^{14}C measurements and so the BCFs and kinetics obtained represent both the parent compound and any metabolites that are formed. Further analytical work has recently been carried out to investigate the extent of metabolism that occurred in the fish (Leonards and van Beuzekom, 2010). For the study, a method for extraction and separation of the chlorinated paraffin from polar metabolites in the fish was developed and validated. The fish used for the analysis were from the end of the depuration phase (day 77 of the study; a total of ten fish were available). The analysis showed that the ^{14}C-activity in the fish was associated mainly with the parent compound and little or no evidence of the presence of polar extractable metabolites was found. A minor part (around 21 per cent) of the radioactivity present was, however, found to be associated with non-extractable metabolites. Thus, the results of this analysis suggest that the majority of the radiolabel present in the fish was parent compound. It should be noted, however, that this analysis was carried out on fish at the end of the depuration phase and it is not clear if the same ratio between parent compound and metabolites would have been present during the uptake phase. Therefore it is possible that a higher (or indeed lower) percentage of metabolites could have been present at other times during the study, but it is not possible to infer from the available data whether or not this was the case[6].

If it were assumed that the parent substance was present in the fish samples at around 79% of the total radioactivity at the end of the uptake phase, the *minimum* lipid-normalised BCFs from this study would be in the range 2,500 – 3,500 l/kg (growth-corrected values would still be above 5,000 l/kg).

The apparently relatively low level of metabolism is surprising given the extensive microbial degradation apparent in the modified ready test using the same test material. The reasons for this difference are unknown.

Additional studies

A further bioconcentration study has been carried out with a C_{13} chlorinated paraffin[7]. The full study report is available in Japanese only (Mitsubishi, 2009) but an English summary is available (UNEP, 2009). The study was conducted in accordance with the test method prescribed under the Chemical Substances Control Law of Japan for testing new substances[8] and in compliance with GLP.

---

[6] Theoretically the amounts of metabolites present in the fish at any one time will be a balance between their rate of formation from MCCPs and the rate of elimination of the metabolites from the fish (or binding in the case of non-extractable metabolites). The effects of this will depend on the kinetics of the various processes.

[7] This is relevant to MCCPs both in terms of the possible presence of C_{13} impurities at >0.1% in the commercial products and the read-across of BCF data from other chlorinated paraffins to MCCPs.

[8] Bioconcentration test of chemical substances in fish and shellfish. Yakushokuhatsu No1121002, Heisei 15.11.3 Seikyoky No.2, Kanpokihatsu No.031121002, November 21, 2003; latest revision November 20, 2006.

The substance tested was a C_{13} chlorinated paraffin with a chlorine content of 48.7% wt. The average chemical formula was $C_{13}H_{23.2}Cl_{4.8}$ and the substance contained soyabean oil epoxide as an additive/stabiliser. Three main constituents of the test substance could be determined/distinguished during the test. These were $C_{13}H_{23}Cl_5$ (49.8% wt. Cl), $C_{13}H_{22}Cl_6$ (54.5% wt. Cl) and $C_{13}H_{21}Cl_7$ (58.4% wt. Cl) and the water solubilities of these constituents were determined as 0.05, 0.07 and 0.09 mg/l respectively.

The test was carried out using two nominal concentrations, 0.01 mg/l and 0.001 mg/l. The test system was a flow-through system and acetone (at 25 ppm by volume) was also present in the exposure solutions.

The fish used in the test were carp (*Cyprinus carpio*) which had an average lipid content of 3.9% at the start of the test. The test was carried out at 24°C and the exposure period was for 62 days.

Samples of water and fish were collected at various times during the test and analysed for the presence of the C_{13} chlorinated paraffins (by parent compound analysis). Steady state was found to be reached after approximately 28 days and the steady state BCF was determined based on the mean concentrations measured in fish over day 28 to 62 divided by the mean concentration in the water over the same time period. The steady state BCFs obtained are summarised in **Table 11**.

No kinetic evaluation of the data was carried out in the UNEP (2009) report and only data for the uptake phase were given. Therefore it is currently not possible to growth correct these data. The Mitsubishi (2009) report appears to contain some information on depuration (it appears that a 21-day depuration period was also included in the study), and elimination half-lives of 5.4-6.9 days (depuration rate constants (k_2) of 0.10-0.13 day^{-1}) for the $C_{13}H_{23}Cl_5$ constituent, 9.0-9.9 days (depuration rate constants (k_2) of 0.070-0.077) for the $C_{13}H_{22}Cl_6$ constituent and 13.7-11.4 days (depuration rate constants (k_2) of 0.051-0.061) for the $C_{13}H_{21}Cl_7$ constituent are given.

Some fish weight data are given in UNEP (2009) but these are few in number and show a large variability. However they appear to show that only limited growth of the fish occurred during the 62-day uptake period (a rate constant for growth dilutions of approximately 0.008 day^{-1} can be estimated from the data). Therefore growth correction does not appear to be so important in this study.

As the fish used in this test had a lipid content of 3.9% at the start of the exposure period, it is relevant to consider normalising the data to the "standard" lipid content of 5% as recommended in the REACH Guidance. The effect of this is shown in Table 11, assuming that the lipid content remained constant during the exposure phase (which, as the fish were not growing significantly during the test, seems to be reasonable).

Table 11 Summary of BCF data for C_{13} chlorinated paraffins

Constituent	Mean exposure concentration (day 28-62) (mg/l)	Mean concentration in fish (day 28-62) (mg/kg)	Steady state BCF (l/kg)	
			As reported	Normalised to 5% lipid content
$C_{13}H_{23}Cl_5$	0.000699	1.070	1,530	2,150
	0.00764	12.84	1,680	1,962
$C_{13}H_{22}Cl_6$	0.000764	1.256	1,640	2,100
	0.00799	15.72	1,970	2,530
$C_{13}H_{21}Cl_7$	0.000816	1.907	2,340	3,630
	0.00842	23.86	2,830	3,000

4.3.3 Other supporting information

4.3.3.1 Field bioaccumulation data

Summary of information from existing evaluation

Although very limited, the available monitoring data have shown MCCPs to be present in marine fish and marine mammals (including top predators such as porpoise (~3-7 µg/kg lipid) and fin whale (~144 µg/kg lipid)), and also in fish and birds from Arctic regions. Two studies investigating biomagnification in field situations suggest that a BMF above 1 might have been observed in an invertebrate-fish food chain, but not in a fish-seal food chain (EU, 2005). In general, the level of chlorination is not indicated in these studies.

New information

No new information is available.

4.3.3.2 Predicted data

The predictions of the variation of BCF with chlorine content and carbon chain length originally discussed in detail in EU (2007a) have been adapted for this evaluation, using the following approach.

- Firstly, log K_{ow} values were estimated from the chemical structure for a range of chlorinated paraffins using the USEPA EPIWIN (version 3.12) software with SMILES notation as input. The structures chosen represented carbon chain lengths from C_{10} up to C_{18}, for three (approximately) constant chlorine contents of around 45%, 52% and 60% by weight (the chlorine contents were chosen to represent the main medium-chain chlorinated paraffins in commercial production).

- These log K_{ow} values were then used to estimate the fish BCFs using the following QSAR equations given in the REACH guidance Document (ECHA, 2008):

  For log K_{ow} up to 6, log $BCF_{fish} = 0.85 \times \log K_{ow} - 0.70$

  For log K_{ow} >6, log $BCF_{fish} = -0.20 \times (\log K_{ow})^2 + 2.74 \times \log K_{ow} - 4.72$

- The predicted BCF values were higher than the available measured BCF values for a C_{11}, ~58% wt. Cl substance (BCF of 7,816 l/kg; see EU, 2000) and a C_{15}, ~51% wt. Cl substance (BCF of 1,087 l/kg; see Section 4.3.2.1). (Note that these BCFs were not lipid normalised or growth corrected.) The predicted BCF values were therefore "scaled" as follows:

  Scaled BCF = Predicted BCF×1087/7186,

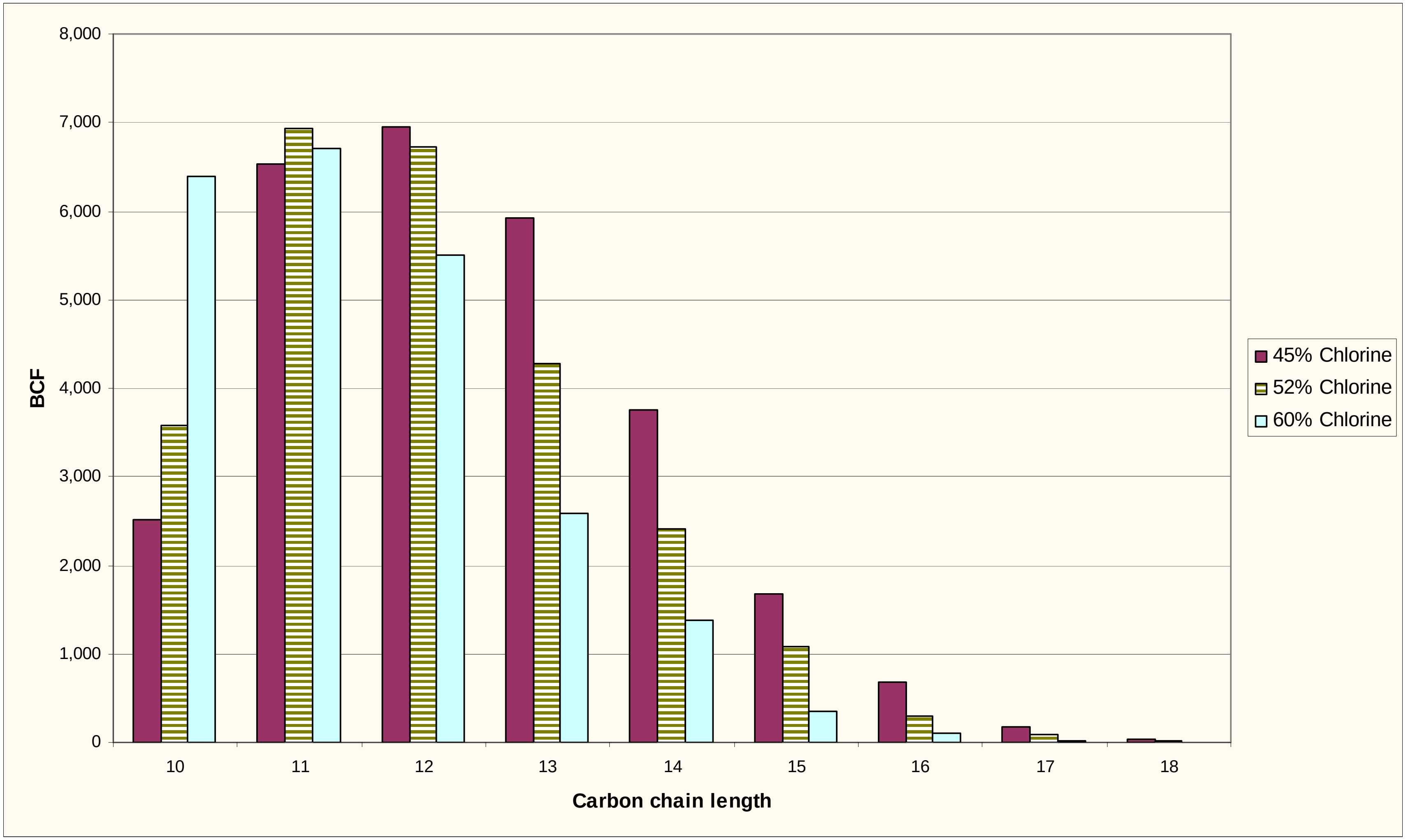
  where 7,186 represents the predicted BCF for a C_{15}, ~52% wt. Cl substance.

The results of this analysis are summarised in **Table 12** and **Figure 2**. The same approach has been used to estimate the non-growth corrected BCF for each possible combination of carbon chain length and chlorine content between C_{13} and C_{17}. The results are summarised in Appendix A.

Table 12 Estimated log K_{ow} and non-growth corrected BCF for a series of hypothetical chlorinated paraffin structures

Formula	Molecular weight (g/mol)	Chlorine content (% by weight)		SMILES notation used for estimating log K_{ow}	Log K_{ow} estimate (EPIWIN)	Predicted BCF - TGD method (l/kg)	Scaled predicted BCF (l/kg)
		Actual	Group				
$C_{10}H_{19}Cl_3$	245.5	43.4		CC(Cl)CC(Cl)CCC(Cl)CCC	5.79	16,653	2,519
$C_{11}H_{20}Cl_4$	294.0	48.3		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC	6.47	43,214	6,537
$C_{12}H_{22}Cl_4$	308.0	46.1		CC(Cl)CC(Cl)CC(Cl)CCCC(Cl)CC	6.96	45,928	6,947
$C_{13}H_{24}Cl_4$	322.0	44.1		CC(Cl)CC(Cl)CC(Cl)CCCCC(Cl)CC	7.45	39,129	5,919
$C_{14}H_{26}Cl_4$	336.0	42.3	45.0	C(Cl)CCCCC(Cl)CCCC(Cl)CC(Cl)CC	8.01	24,853	3,759
$C_{15}H_{27}Cl_5$	384.5	46.2		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CCCC(Cl)CC	8.61	11,091	1,678
$C_{16}H_{29}Cl_5$	398.5	44.5		CC(Cl)CC(Cl)CCC(Cl)CCC(Cl)CCC(Cl)CCC	9.10	4,487	679
$C_{17}H_{31}Cl_5$	412.5	43.0		C(Cl)CC(Cl)CC(Cl)CCCC(Cl)CCCC(Cl)CCCC	9.67	1,186	179
$C_{18}H_{32}Cl_6$	461.0	46.2		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CCC(Cl)CCC(Cl)CCC	10.26	218	33
$C_{10}H_{18}Cl_4$	280.0	50.7		CC(Cl)CC(Cl)C(Cl)CC(Cl)CCC	5.97	23,686	3,583
$C_{11}H_{19}Cl_5$	328.5	54.0		C(Cl)CC(Cl)CCC(Cl)CC(Cl)CC(Cl)C	6.72	45,827	6,932
$C_{12}H_{21}Cl_5$	342.5	51.8		CC(Cl)C(Cl)CC(Cl)CCC(Cl)CCC(Cl)C	7.14	44,430	6,721
$C_{13}H_{22}Cl_6$	391.0	54.5		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)C	7.88	28,335	4,286
$C_{14}H_{24}Cl_6$	405.0	52.6	52.0	C(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CC	8.37	15,937	2,411
$C_{15}H_{26}Cl_6$	419.0	50.8		C(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CCC	8.86	7,186	1,087
$C_{16}H_{27}Cl_7$	467.5	53.2		CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CCC(Cl)C(Cl)C	9.46	2,005	303
$C_{17}H_{29}Cl_7$	481.5	51.6		CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCC(Cl)CC(Cl)CC(Cl)CC	9.95	553	84
$C_{18}H_{31}Cl_7$	495.5	50.2		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CCCC(Cl)CCC	10.52	93	14
$C_{10}H_{16}Cl_6$	349.0	61.0		CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)	6.41	42,245	6,390
$C_{11}H_{17}Cl_7$	397.5	62.5		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)	7.15	44,310	6,703
$C_{12}H_{19}Cl_7$	411.5	60.4		C(Cl)CC(Cl)C(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)CC	7.57	36,376	5,503
$C_{13}H_{20}Cl_8$	460.0	61.7		C(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)CC(Cl)CC(Cl)CC(Cl)	8.32	17,073	2,583
$C_{14}H_{22}Cl_8$	474.0	59.9	60.0	C(Cl)CC(Cl)C(Cl)C(Cl)CC(Cl)CCC(Cl)CC(Cl)C(Cl)C	8.73	9,070	1,372
$C_{15}H_{23}Cl_9$	522.5	61.1		C(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C(Cl)C(Cl)CC(Cl)CC(Cl)C	9.41	2,258	342
$C_{16}H_{25}Cl_9$	536.5	59.6		C(Cl)CC(Cl)C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)C	9.89	655	99
$C_{17}H_{26}Cl_{10}$	585.0	60.7		C(Cl)CC(Cl)C(Cl)C(Cl)C(Cl)C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)CC	10.57	79	12
$C_{18}H_{27}Cl_{11}$	633.5	61.6		C(Cl)CC(Cl)CC(Cl)CC(Cl)CC(Cl)C(Cl)CC(Cl)C(Cl)C(Cl)CC(Cl)C(Cl)C	11.24	6	1

Figure 2 Plot of predicted non-growth corrected BCF against carbon number of a series of hypothetical chlorinated paraffin structures



This data scaling approach leads to a reasonably good prediction of the measured BCF for a C_{11}, 58% wt. Cl substance (a predicted value of around 6,700-6,900 l/kg is obtained for a C_{11}, 52-60% wt. Cl substance, compared with the experimental value of 7,816 l/kg). A comparison of the predicted BCF with the new experimentally determined BCFs (not growth corrected but normalised to 5% lipid) for C_{13} and C_{14} chlorinated paraffins is given below.

	Experimental BCF	**Predicted BCF**
$C_{13}H_{23}Cl_5$	1,962-2,150 l/kg	5,280 l/kg
$C_{13}H_{23}Cl_6$	2,100-2,530 l/kg	4,570 l/kg
$C_{13}H_{21}Cl_7$	3,000-3,630 l/kg	3,840 l/kg
C_{14}, 45% wt. Cl	3,230-4,460 l/kg	3,320-4,040 l/kg[9]

As can be seen, the predicted BCF is generally in reasonable agreement with the experimental BCF. However, it is recognized that the lack of lipid normalization adds a significant element of uncertainty, and that the scaling is based on a very small number of actual measured BCF values. For example, there are no data for highly chlorinated substances for comparison with the predictions.

For C_{13} chlorinated paraffins, the BCF using the data scaling approach is predicted to decrease slightly (from 5,280 to 3,840 l/kg) with increasing chlorine content, whereas the opposite trend is found experimentally (increases from 1,962-2,150 to 3,000-3,630 l/kg). This may suggest that the estimation approach is not totally in line with the available experimental data. However, when considering the predicted BCF it is important to recognise that there will be uncertainties in the actual experimental BCF values (for example the values obtained for the C_{13} substances are slightly different at the two different exposure concentrations, and the range of values obtained for two of the substances overlap). Therefore, precise agreement between predicted and experimental BCF should not always be expected. Despite this, the predictions are all within a factor of 2.7 of the experimental values, and in most cases are significantly closer than this.

The new BCF study with the C_{14}, 45% wt. Cl substance also allows a similar analysis to be carried out using growth-corrected data. Here the QSAR predictions have been normalised to the experimental growth-corrected BCF for the C_{15}, 51% wt. Cl substance (experimental BCF ~2,000 l/kg; QSAR predicted BCF ~7,186 l/kg). The results of this analysis are also shown in Appendix A. The predicted growth-corrected BCF for a C_{14}, 42-48% wt. Cl substance using this approach is in the range 6,300-7,700 l/kg, which compares reasonably well with the experimental growth-corrected and lipid-normalised BCF determined for a C_{14}, 45% wt. Cl substance of 10,600-14,600 l/kg.

Overall, the prediction method presented appears to provide reasonable estimates for both the growth corrected and non-growth corrected BCF for MCCPs. However, the limitations in the approach also need to be taken into account. For example, the general trend is for a slight over-prediction rather than under-prediction of the measured values. In particular the available database of experimental data for chlorinated paraffins is relatively limited and the

[9] Values for 42-48% wt. Cl.

extrapolation of these data to other carbon chain lengths and chlorine contents is likely to become increasingly uncertain for combinations of carbon chain lengths and chlorine contents that differ from those used to test the method. Thus although this modelling approach is useful as an indication of which constituents potentially have BCF values above or below the REACH Annex XIII criteria for B or vB, it does not provide definitive proof of this.

4.3.4 Summary and discussion of bioaccumulation

Consideration of growth dilution in the available bioconcentration study for a C_{15}, 51% wt Cl chlorinated paraffin suggests that it has a fish BCF close to 2,000 l/kg. The influence of lipid content on this result is unknown, and it is not possible to rule out a contribution from metabolites because of the analytical method that was used.

The results of a well conducted OECD 305 fish bioconcentration study indicate that a C_{14}, 45% wt Cl chlorinated paraffin has a kinetic BCF of ~4,460 l/kg and steady state BCF of 3,230 l/kg (both normalised to 5% lipid). At the end of the depuration phase, the majority of the radioactivity (around 79%) was associated with parent compound, with the remainder (around 21%) being associated with non-extractable metabolites. Taking this information into account suggests that the lipid-normalised BCF would still be in the range 2,500 – 3,500 l/kg as a minimum. A significant proportion of the depuration seen in this study appears to be related to growth dilution and the kinetic BCF corrected for growth dilution is 14,600 l/kg.

New steady state BCFs (normalised to a 5% lipid content) are also available for three C_{13} chlorinated paraffins (with chlorine levels between 49 and 58% by weight) as follows: 1,962-2,150 l/kg for a $C_{13}H_{23}Cl_5$ substance; 2,100-2,530 l/kg for a $C_{13}H_{22}Cl_6$ substance; and 3,000-3,630 l/kg for a $C_{13}H_{21}Cl_7$ substance.

It would not be ethical to collect measured fish BCF data for all of the potential constituents of MCCPs. Under these circumstances, modelling has been performed in an attempt to predict the BCFs based on the available data. This is complicated by the lack of lipid normalisation and the influence of growth on the different measured values that are available, and their limited number. The results should therefore be interpreted with caution. However, it seems reasonable to expect that the degree of bioaccumulation of the constituents will depend on their hydrophobicity and metabolism potential (and hence chain length and degree of chlorination).

4.4 Secondary poisoning

Not relevant for this dossier.

5 HUMAN HEALTH HAZARD ASSESSMENT

MCCPs are classified for human health hazards on the basis of effects seen in a one-generation dietary study in the rat (total treatment duration of 11-12 weeks). Neonatal vitamin K deficiency, mediated via lactation, was observed in rat pups (leading to internal haemorrhaging and death). The NOAEL was 47 mg/kg/day (ECHA, 2009). The test substance was an MCCP product with 52% chlorination.

6 HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICOCHEMICAL PROPERTIES

Not relevant for this dossier.

7 ENVIRONMENTAL HAZARD ASSESSMENT

The existing information on the environmental effects of MCCPs has been reviewed in detail in the environmental risk assessment produced under the Existing Substances Regulation (EU, 2005 and EU, 2007a). No further information has been provided since then and so in the following sections, the information in this existing evaluation has been reported only briefly.

7.1 Aquatic compartment (including sediment)

Aquatic toxicity testing is hampered by the low water solubility and complex nature of the test substance. Overall, the available toxicity data indicate that MCCPs are toxic to invertebrates over chronic exposures. No toxicity has been seen in the available experiments with fish or algae. The 21-day NOEC for *Daphnia magna* is 0.010 mg/l. In addition a 48-h EC_{50} for this species has been determined as 0.0059 mg/l and a further long-term study suggests that the long-term NOEC for *Daphnia magna* may be just below 0.010 mg/l (EU, 2007a). These studies used a C_{14-17}, 52% wt. Cl substance. The influence of varying degrees of chlorination on toxicity is not known.

For comparison, a 21-day NOEC values of 0.005 mg/l for *Daphnia magna* was obtained for a C_{10-13}, 58% wt. Cl substance (EU, 2000).

8 PBT AND vPvB

8.1 Comparison with criteria from Annex XIII

For the PBT and vPvB assessment it is necessary to take into account how the persistence, bioaccumulation potential and toxicity vary with carbon chain length and chlorine content. Only a few constituents of the commercial products have been tested and a modelling/read-across approach has to be considered, in addition to the available experimental data, to identify if any constituents have PBT or vPvB properties.

Persistence

The new data available indicate that some constituents of MCCPs are readily biodegradable (e.g. a C_{14}, 45% wt Cl chlorinated paraffin and a C_{10-13}, 49.8% wt. Cl substance) when measures are taken to maximise bioavailability. These constituents therefore do not meet the P criterion of Annex XIII. In contrast, a C_{14-17}, 63.2% wt. Cl chlorinated paraffin is considered to meet the P/vP criteria based on results in the same test system and by read across with shorter chain substances.

There are insufficient data to draw conclusions for other MCCP constituents with intermediate levels of chlorination. The results of the biodegradation test with a C_{14-17}, 45.6% wt. Cl substance show that although substantial degradation may occur (especially for the shorter chain length constituents), it is not known whether it would degrade sufficiently rapidly so as not to meet the Annex XIII criteria. Monitoring evidence suggests that MCCPs with chlorine contents of around 55% by weight may persist for a long time in sediments.

A modelling exercise has been carried out in an attempt to provide a more complete picture based on the available data. The modelling results suggest that MCCPs with chlorine contents below around 45% by weight would not be expected to be persistent, whilst C_{14}- chlorinated paraffins with chlorine contents above 50% by weight, C_{15}- and C_{16}- chlorinated paraffins with chlorine contents approaching 50% or above, and C_{17}-chlorinated paraffins with chlorine contents of around 45% or above are unlikely to be readily biodegradable and so are potentially persistent. However it should be noted that these estimates are uncertain, particularly in the 45–50% chlorine content range and, although considered useful for identifying constituents that potentially meet the REACH Annex XIII criteria for persistence, they do not provide definitive proof of this.

Overall, based on the information currently available, MCCPs with a chlorination level of around 63% w/w or higher are considered to be P or vP. MCCPs containing less than 40% chlorine by weight (i.e. with approximately 1 – 4 chlorine atoms per molecule) can be considered not to meet the criteria at the present time. It is possible that at least some constituents of MCCPs with intermediate levels of chlorination (particularly the longer chain lengths) will also meet the Annex XIII criteria for P or vP, but this cannot be elaborated further with any certainty for the time being.

Bioaccumulation

The results of a well conducted OECD 305 fish bioconcentration study with a C_{14}, 45% wt Cl chlorinated paraffin are available. This substance is identical to that found to be readily biodegradable under conditions of enhanced bioavailability (see above). The results confirm that this constituent of commercial MCCPs meets the Annex XIII criterion for B (the lipid-normalised BCFs are in the range 2,500 – 3,500 l/kg as a minimum and could be higher, depending how metabolites are considered). A significant proportion of the depuration seen in this study appears to be related to growth dilution and the kinetic BCF corrected for growth dilution is 14,600 l/kg which is significantly above the Annex XIII criterion for vB.

New data are also available on three C_{13} chlorinated paraffins (with chlorine levels between 49 and 58% by weight), and these show that the steady state BCF (normalised to a 5% lipid content) is above the Annex XIII B criterion (1,960-2,150 l/kg for a $C_{13}H_{23}Cl_5$ substance, 2,100-2,530 l/kg for a $C_{13}H_{22}Cl_6$ and 3,000-3,630 l/kg for a $C_{13}H_{21}Cl_7$). This is relevant, because commercial MCCP products may contain small amounts of C_{13} chlorinated paraffins as impurities.

Modelling has been performed in an attempt to predict the BCFs for all possible constituents of MCCPs, based on the available data. This is complicated by the lack of lipid normalisation and the influence of growth on the different measured values that are available, and their limited number. The results should therefore be interpreted with caution. However, it seems reasonable to expect that the degree of bioaccumulation of the constituents will depend on their hydrophobicity and metabolism potential (and hence chain length and degree of chlorination). The results of the modelling (in terms of whether the Annex XIII B or vB criteria are potentially met) are summarised in Table 13.

Table 13 Bioaccumulation predictions for constituents of MCCPs

Chlorine content, w/w	Constituent formula[a]							
	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}
45%	B	vB	vB	vB	B	Not B	Not B	Not B
52%	B	vB	vB	B	B	Not B	Not B	Not B
60%	vB	vB	vB	B	Not B	Not B	Not B	Not B

Note: a) The grey columns refer to potential impurities

Table 13 does not take account of the influence of growth dilution on the measured BCFs. When actual measured data are considered, the picture changes somewhat, with the C_{14}, 45% wt Cl chlorinated paraffin becoming vB, and the C_{15}, 51% wt Cl chlorinated paraffin becoming borderline B (recognising that the BCF result might include metabolites). This is a complicating factor which means that the modelling approach might be misleading for some constituents. It is therefore precautionary to consider the growth-corrected results for the final PBT assessment. These constituents have between 4 and 6 chlorine atoms per molecule.

Toxicity

A C_{14-17}, 52% wt. Cl substance has a 48-h EC_{50} of 0.0059 mg/l with *Daphnia magna*. The 21-day NOEC is around or below 0.01 mg/l. It is therefore concluded that this substance meets the T criterion. A C_{10-13}, 58% wt. Cl substance also meets the T criterion on the basis of toxicity to invertebrates. The influence of varying degrees of chlorination on toxicity is not known.

There is also evidence of relevant mammalian toxicity for an MCCP product with 52% chlorination. According to the REACH guidance (ECHA, 2007), where a substance has a chronic NOAEL below 50 mg/kg bw/day after repeated oral dosing, it might be considered as demonstrating an equivalent level of concern for the T criterion. In this case, a one-generation study showed adverse effects (internal haemorrhaging and death) in the offspring due to transfer of MCCPs or metabolites in the milk, with a NOAEL of 47 mg/kg/day.

8.2 Assessment of substances of an equivalent level of concern

Not relevant to this dossier.

8.3 Emission characterisation

An assessment of the emissions of MCCPs throughout the lifecycle is included in the environmental risk assessment carried out under the Existing Substances Regulation (EU, 2005 and 2007a) (one additional scenario was considered in the transition dossier (ECHA, 2009)).

8.4 Conclusion of PBT and vPvB or equivalent level of concern assessment

The PBT assessment is complicated because both the biodegradability and bioconcentration factor of MCCP constituents depend on chlorine content and chain length, and the trends in these are opposite (i.e. persistence appears to increase with increasing chlorine content whilst the bioconcentration factor appears to decrease). The constituents of the commercial products that meet the P/vP criterion are not necessarily the same as those that meet the B/vB criteria and *vice versa*. For example, measured data for a C_{14}, 45% wt. Cl substance show that although it meets the vB criterion, it is not P. In other cases, there are no reliable data to determine whether one or more of the criteria will be met or not. The influence of chlorine content on toxicity is not known.

The available information discussed in this evaluation is presented in **Table 14**, in terms of whether the Annex XIII criteria are likely to be met. The carbon chain lengths less than C_{14} are included as they may be impurities in the commercial MCCP products above 0.1% w/w.

The general picture emerges that for MCCP products containing about 50% chlorine by weight or higher, any $C_{<14}$ impurities might have a problematic P & B profile, especially at chlorination levels of 65% or more. In addition, some of the main constituents could also have problematic P & B profiles (i.e. the C_{14}- constituents, and C_{15}- constituents with chlorine contents in the range 50-55%). However, the C_{16} and C_{17} chain lengths do not appear to be of concern. Once again, it has to be noted that the categorisation for some of the constituents is uncertain because of inherent limitations in the underlying data sets, so a definitive conclusion cannot yet be drawn.

Table 14 Estimated P & B properties of potential constituents of MCCPs

Carbon no.	Chlorine content (w/w)			
	~40-50%	~50-55%	~55%-65%	>65%
10	Not P B	P? B	P? vB	P B or vB
11	Not P vB	P? vB	P? vB	P B or vB
12	Not P vB	P? vB	P? vB	P B or vB
13	Not P B or vB	P? B	P? B	P B
14	Not P vB	P? B	P? B?	P Not B?
15	P? Not B	P? Borderline B	P Not B	P Not B
16	P? Not B	P? Not B	P Not B	P Not B
17	P? Not B	P? Not B	P Not B	P Not B

Note: The shaded box represents constituent groups potentially meeting both the P and B/vB criteria.

This picture does not take account of the T criterion. This might be expected to be related to the bioaccumulation potential of the substances, since they are likely to act via a non-polar narcotic mode of action in invertebrates. It is clear that both a C_{14-17}, 52% wt. Cl substance and C_{10-13}, 58% wt. Cl substance meet the T criterion (the former on the basis of both aquatic and mammalian effects). Other chlorine content products could also be toxic, but this has not been established.

An important way forward to address some of the remaining uncertainty in the assessment would be to carry out further biodegradation testing of the constituents that potentially meet both the P and B criteria. It is understood that Industry is currently performing further enhanced ready biodegradation studies on a single chain length C_{14}- paraffin chlorinated in 5% increments between 45% and 70% by weight. This should provide further useful information for use in the read-across (provided that an appropriate inoculum is being used). However, if any constituent does not fulfil the ready biodegradation criteria, a sediment simulation test might still be needed to establish the environmental half-life.

It would also appear to be important to investigate the biodegradation potential of a C_{15} chlorinated paraffin with a chlorine content of around 51% by weight. This constituent is potentially persistent and the experimental BCF for a C_{15}, 51% wt. Cl substance is around 1,833-2,072 l/kg (i.e. borderline B). It is assumed to meet the T criterion based on the available evidence.

Depending on the outcome of this testing, there might still be a need to investigate the bioaccumulation potential of C_{14} chlorinated paraffins with chlorine contents of around 50% and higher. Additional information on the variation in long-term toxicity to *Daphnia magna* with chlorination level might also be useful for this chain length.

It is also important to ascertain the amounts of carbon chain lengths less than C_{14} present in a range of commercial MCCP products to determine if any of these impurities are present above 0.1% by weight. This information should be available from registration dossiers in due course.

INFORMATION ON USE, EXPOSURE, ALTERNATIVES AND RISKS

Information on the uses, exposure and risks of MCCPs throughout the lifecycle is included in the environmental risk assessment carried out under the Existing Substances Regulation (EU, 2005 & 2007a). Alternatives are described in the transition dossier (ECHA, 2009).

OTHER INFORMATION

REFERENCES

AkzoNobel (2009). Biodegradability of polychlorinated tetradecane: Closed Bottle Test Method. Confidential Memo, ECRA M09, AkzoNobel.

AkzoNobel (2010a). Biodegradability of polychlorinated tetradecane (45%) in the Closed Bottle Test. Confidential Report, Study Number T09050C, AkzoNobel.

AkzoNobel (2010b). Biodegradability of C_{14-17} chlorinated paraffin (45.6% Cl) in the closed bottle test. Confidential Report, Study Number T10007C, AkzoNobel.

AkzoNobel (2010c). Biodegradability of C_{14-17} medium chain chlorinated paraffin (63.2% Cl w/w) in the closed bottle test. Confidential Report, Study Number T10008C, AkzoNobel.

AkzoNobel (2010d). Biodegradability of chlorinated n-alkanes C_{10-13} (50%) (SCCP): Closed Bottle Test Method. Doc. No. 2.423.536, AkzoNobel.

AstraZeneca (2010). [^{14}C]-Chlorinated n-tetradecane: Determination of the bioconcentration in rainbow trout (*Oncorhynchus mykiss*). Brixham Environmental Laboratory Study Number 09-0133/B, Report No. BR0088/B, AstraZeneca UK Limited.

ECHA (2007). Guidance for the preparation of an Annex XV dossier on the identification of substances of very high concern. June 2007.

ECHA (2008). Guidance on information requirements and chemical safety assessment. May 2008.

ECHA (2009). ANNEX XV RESTRICTION REPORT for Medium chain chlorinated paraffins (MCCPs). European Chemicals Agency.

EU (2000). European Union Risk Assessment Report: Alkanes, C_{10-13}, chloro-. 1st Priority List, Volume 4. European Commission Joint Research Centre, EUR 19101 EN.

EU (2005). European Union Risk Assessment Report: Alkanes, C_{14-17}, chloro-. 3rd Priority List, Volume 58. European Commission Joint Research Centre, EUR 21640 EN.

EU (2007a). European Union Risk Assessment Report: Alkanes, C_{14-17}, chloro-. Draft environmental update assessment, R331_0807_env, August 2007.

EU (2007b). European Union Risk Assessment Report: Alkanes, C_{10-13}, chloro-. Final Combined Draft updated risk assessment, R010_0704_env_hh, April 2007.

Iozza S, Müller C E, Schmid P, Bogdal C and Oehme M (2008). Historical profiles of chlorinated paraffins and polychlorinated biphenyls in a dated sediment core from Lake Thun (Switzerland). Environ. Sci. Technol., **42**, 1045-1050.

Leonards P E G and van Beuzekom S (2010). Analysis of ^{14}C-labeled polychlorinated tetradecane exposed fish. Report R-10/06-1, IVM Institute for Environmental Studies.

Mitsubishi (2009). Bioconcentration study of TPX-13C48 with carp. Study No A090084, Mitsubishi Chemical Corporation.

Thompson R S and Noble H (2007). Short-chain chlorinated paraffins (C_{10-13}, 65% chlorinated): Aerobic and anaerobic transformation in marine and freshwater sediment systems. Final Report No BL8405/B. Brixham Environmental Laboratory, AstraZeneca UK Limited.

UNEP (2009). Additional information on short-chain chlorinated paraffins: bioconcentration study of a chlorinated paraffin (C=13). UNEP/POPS/POPRC.5/INF/23, Stockholm Convention on Persistent Organic Pollutants.

Appendix A Modelling and read-across for persistence and bioaccumulation

The predictions of persistence and bioaccumulation are summarised in the following table for each combination of carbon chain length and chlorine content.

- The summary of persistence is based on the Biowin 3 prediction. A prediction of >1.5 is considered to be not persistent, a prediction <1.4 is considered to be potentially persistent and a prediction between 1.4 and 1.5 is considered to be not clear.
- The log K_{ow} and biodegradation predictions have been carried out using the EPIWIN model (v3.12).
- The predictions of BCF are based on the REACH Guidance methodology using the predicted log K_{ow} and have been scaled to the available BCF data on a C_{15}, 51% wt. Cl substance.

The shaded boxes represent cases where the substance is predicted to be persistent (or is not clear on persistence) and is predicted to meet the B or vB criteria.

Formula			Smiles used	Cl content (% wt.)	EPI Predictions						BCF predictions (TGD method – normalised to C_{15}, 51% wt. Cl		Summary of persistence	Summary of B based on non-growth corrected BCF	Summary of B based on growth-corrected BCF
C	H	Cl			log Kow	Biowin 1	Biowin 2	Biowin 3	Biowin 5	Biowin 6	Not growth corrected	Growth corrected			
13	28	0	CCCCCCCCCCCCC	0.0	6.73	0.8766	0.9833	3.3884	0.708	0.8772	6,940	13,229	Not P	vB	vB
13	27	1	CCCC(CL)CCCCCCCCC	16.2	6.91	0.6404	0.4731	2.8408	0.5066	0.4511	6,975	13,295	Not P	vB	vB
13	26	2	CCCC(CL)CCC(CL)CCCCCC	28.1	7.09	0.5126	0.0795	2.5915	0.3051	0.0863	6,803	12,968	Not P	vB	vB
13	25	3	CCCC(CL)CCC(CL)CCC(CL) CCC	37.0	7.27	0.2764	0.0013	2.0438	0.1036	0.0108	6,441	12,278	Not P	vB	vB
13	24	4	CC(CL)CC(CL)CCC(CL)CCC(CL)CCC	44.1	7.45	0.1486	0.0001	1.7945	-0.0979	0.0012	5,919	11,282	Not P	vB	vB
13	23	5	CC(CL)CC(CL)CC(CL)C(CL)C CC(CL)CCC	49.8	7.63	0.0208	0	1.5452	-0.2993	0.0001	5,279	10,063	Not P	vB	vB
13	22	6	CC(CL)CC(CL)CC(CL)C(CL)C C(CL)C(CL)CCC	54.5	7.81	-0.107	0	1.2959	-0.5008	0	4,570	8,711	Potentially P	B	vB
13	21	7	CC(CL)CC(CL)CC(CL)C(CL)C C(CL)C(CL)CC(CL)C	58.4	7.99	-0.2347	0	1.0466	-0.7023	0	3,840	7,320	Potentially P	B	vB
13	20	8	CC(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)CC(CL)C	61.7	8.17	-0.3625	0	0.7973	-0.9037	0	3,132	5,969	Potentially P	B	vB
13	19	9	CC(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)C(CL)C(CL) C	64.6	8.35	-0.4903	0	0.5481	-1.1052	0	2,479	4,725	Potentially P	B	B
13	18	10	C(CL)C(CL)C(CL)C(CL)CC(C L)C(CL)CC(CL)C(CL)C(CL)C(CL)C	67.1	8.6	-0.6181	0	0.2988	-1.1576	0	1,705	3,250	Potentially P	Not B	B
13	17	11	C(CL)C(CL)C(CL)C(CL)C(CL) C(CL)C(CL)CC(CL)C(CL)C(C L)C(CL)C	69.3	8.78	-0.7459	0	0.0495	-1.3591	0	1,257	2,396	Potentially P	Not B	B
13	16	12	C(CL)C(CL)C(CL)C(CL)C(CL) C(CL)C(CL)C(CL)C(CL)C(CL) C(CL)C(CL)C	71.2	8.97	-0.8737	0	-0.1998	-1.5606	0	882	1,681	Potentially P	Not B	Not B
13	15	13	C(CL)C(CL)C(CL)C(CL)C(CL) C(CL)C(CL)C(CL)C(CL)C(CL) C(CL)C(CL)C(CL)	73.0	9.22	-1.0015	0	-0.4491	-1.6129	0	526	1,002	Potentially P	Not B	Not B

MCCPs PBT/vPvB EVALUATION

Formula			Smiles used	Cl content (% wt.)	EPI Predictions						BCF predictions (TGD method – normalised to C_{15}, 51% wt. Cl		Summary of persistence	Summary of B based on non-growth corrected BCF	Summary of B based on growth-corrected BCF
C	H	Cl			log Kow	Biowin 1	Biowin 2	Biowin 3	Biowin 5	Biowin 6	Not growth corrected	Growth corrected			
14	30	0	CCCCCCCCCCCCCC	0.0	7.22	0.87	0.9797	3.3574	0.7157	0.8799	6,559	12,503	Not P	vB	vB
14	29	1	CCCC(CL)CCCCCCCCCC	15.3	7.4	0.6337	0.4239	2.8098	0.5143	0.4572	6,078	11,585	Not P	vB	vB
14	28	2	CCCC(CL)CCCCC(CL)CCCCC	26.6	7.58	0.5059	0.0661	2.5605	0.3128	0.0883	5,466	10,419	Not P	vB	vB
14	27	3	CCCC(CL)CCC(CL)CC(CL)CCCCC	35.3	7.76	0.3782	0.0068	2.3112	0.1113	0.011	4,771	9,095	Not P	B	vB
14	26	4	CCCC(CL)CCC(CL)CC(CL)CCC(CL)CC	42.3	7.94	0.1419	0.0001	1.7635	-0.0902	0.0013	4,042	7,705	Not P	B	vB
14	25	5	CCCC(CL)C(CL)CC(CL)CC(CL)CCC(CL)CC	47.9	8.12	0.0142	0	1.5142	-0.2916	0.0001	3,324	6,336	Not P	B	vB
14	24	6	CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CCC(CL)CC	52.6	8.3	-0.1136	0	1.2649	-0.4931	0	2,653	5,057	Potentially P	B	vB
14	23	7	CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C(CL)CC	56.5	8.48	-0.2414	0	1.0157	-0.6946	0	2,055	3,918	Potentially P	B	B
14	22	8	C(CL)C(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C(CL)CC	59.9	8.73	-0.3692	0	0.7664	-0.747	0	1,372	2,615	Potentially P	Not B	B
14	21	9	C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)C(CL)CC(CL)C(CL)CC	62.8	8.91	-0.497	0	0.5171	-0.9484	0	990	1,887	Potentially P	Not B	Not B
14	20	10	C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC	65.4	9.1	-0.6248	0	0.2678	-1.1499	0	679	1,294	Potentially P	Not B	Not B
14	19	11	C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC	67.6	9.28	-0.7526	0	0.0185	-1.3514	0	461	878	Potentially P	Not B	Not B
14	18	12	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC	69.6	9.46	-0.8804	0	-0.2308	-1.5529	0	303	578	Potentially P	Not B	Not B
14	17	13	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C	71.4	9.64	-1.0082	0	-0.4801	-1.7543	0	194	369	Potentially P	Not B	Not B

Formula			Smiles used	Cl content (% wt.)	EPI Predictions						BCF predictions (TGD method – normalised to C_{15}, 51% wt. Cl		Summary of persistence	Summary of B based on non-growth corrected BCF	Summary of B based on growth-corrected BCF
C	H	Cl			log Kow	Biowin 1	Biowin 2	Biowin 3	Biowin 5	Biowin 6	Not growth corrected	Growth corrected			
14	16	14	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)	73.0	9.89	-1.1359	0	-0.7294	-1.8067	0	99	189	Potentially P	Not B	Not B
15	32	0	CCCCCCCCCCCCCCC	0.0	7.71	0.8633	0.9754	3.3264	0.7234	0.8824	4,970	9,473	Not P	B	vB
15	31	1	CCCCCC(CL)CCCCCCCCC	14.4	7.89	0.7355	0.7921	3.0771	0.5219	0.4633	4,245	8,092	Not P	B	vB
15	30	2	CCCCCC(CL)CCCCC(CL)CCCC	25.3	8.07	0.6077	0.2681	2.8278	0.3205	0.0903	3,520	6,710	Not P	B	vB
15	29	3	CC(CL)CCCC(CL)CCCCC(CL)CCCC	33.8	8.25	0.3715	0.0055	2.2802	0.119	0.0113	2,833	5,400	Not P	B	vB
15	28	4	CC(CL)CCCC(CL)CC(CL)CCC(CL)CCCC	40.6	8.43	0.2437	0.0005	2.0309	-0.0825	0.0013	2,213	4,218	Not P	B	B
15	27	5	CC(CL)CCCC(CL)CC(CL)CCC(CL)CC(CL)CC	46.2	8.61	0.0075	0	1.4832	-0.284	0.0002	1,678	3,198	Not clear	Not B	B
15	26	6	CC(CL)CC(CL)CC(CL)CC(CL)CCC(CL)CC(CL)CC	50.8	8.79	-0.1203	0	1.234	-0.4854	0	1,235	2,353	Potentially P	Not B	B
15	25	7	CC(CL)C(CL)C(CL)CC(CL)CC(CL)CCC(CL)CC(CL)CC	54.8	8.97	-0.2481	0	0.9847	-0.6869	0	882	1,681	Potentially P	Not B	Not B
15	24	8	CC(CL)C(CL)C(CL)CC(CL)CC(CL)CC(CL)C(CL)CC(CL)CC	58.2	9.15	-0.3759	0	0.7354	-0.8884	0	611	1,165	Potentially P	Not B	Not B
15	23	9	CC(CL)C(CL)C(CL)CC(CL)CC(CL)CC(CL)C(CL)CC(CL)C(CL)C	61.1	9.33	-0.5037	0	0.4861	-1.0899	0	411	784	Potentially P	Not B	Not B
15	22	10	CC(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CC(CL)C(CL)C	63.7	9.51	-0.6315	0	0.2368	-1.2913	0	269	512	Potentially P	Not B	Not B
15	21	11	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CC(CL)C(CL)C	66.0	9.77	-0.7593	0	-0.0125	-1.3437	0	138	262	Potentially P	Not B	Not B
15	20	12	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)C(CL)C	68.1	9.95	-0.887	0	-0.2618	-1.5452	0	84	159	Potentially P	Not B	Not B

Formula			Smiles used	Cl content (% wt.)	EPI Predictions						BCF predictions (TGD method – normalised to C_{15}, 51% wt. Cl		Summary of persistence	Summary of B based on non-growth corrected BCF	Summary of B based on growth-corrected BCF
C	H	Cl			log Kow	Biowin 1	Biowin 2	Biowin 3	Biowin 5	Biowin 6	Not growth corrected	Growth corrected			
15	19	13	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C(CL)C	69.9	10.13	-1.0148	0	-0.5111	-1.7467	0	49	94	Potentially P	Not B	Not B
15	18	14	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C	71.5	10.31	-1.1426	0	-0.7604	-1.9481	0	28	54	Potentially P	Not B	Not B
15	17	15	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)	73.0	10.56	-1.2704	0	-1.0097	-2.0005	0	12	24	Potentially P	Not B	Not B
16	34	0	CCCCCCCCCCCCCCCC	0.0	8.2	0.8566	0.9701	3.2954	0.7311	0.8849	3,018	5,753	Not P	B	vB
16	33	1	CCCC(CL)CCCCCCCCCCCC	13.6	8.38	0.6204	0.3307	2.7478	0.5296	0.4694	2,377	4,531	Not P	B	B
16	32	2	CCCC(CL)CCCCCCCCC(CL)CCC	24.1	8.56	0.3842	0.0075	2.2001	0.3282	0.0923	1,817	3,464	Not P	Not B	B
16	31	3	CCCC(CL)CCCCC(CL)CCCC(CL)CCC	32.3	8.74	0.2564	0.0007	1.9508	0.1267	0.0116	1,348	2,570	Not P	Not B	B
16	30	4	CC(CL)CC(CL)CCCCC(CL)CCCC(CL)CCC	39.0	8.92	0.1286	0.0001	1.7016	-0.0748	0.0013	971	1,851	Not P	Not B	Not B
16	29	5	CC(CL)CC(CL)CC(CL)CCC(CL)CCCC(CL)CCC	44.5	9.1	0.0008	0	1.4523	-0.2763	0.0002	679	1,294	Not clear	Not B	Not B
16	28	6	CC(CL)CC(CL)CC(CL)CCC(CL)CC(CL)CC(CL)CCC	49.2	9.28	-0.127	0	1.203	-0.4777	0	461	878	Potentially P	Not B	Not B
16	27	7	CC(CL)CC(CL)CC(CL)CCC(CL)CC(CL)CC(CL)CC(CL)C	53.2	9.46	-0.2548	0	0.9537	-0.6792	0	303	578	Potentially P	Not B	Not B
16	26	8	CC(CL)CC(CL)CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C	56.6	9.64	-0.3826	0	0.7044	-0.8807	0	194	369	Potentially P	Not B	Not B
16	25	9	CC(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C	59.6	9.82	-0.5104	0	0.4551	-1.0822	0	120	229	Potentially P	Not B	Not B

Formula			Smiles used	Cl content (% wt.)	EPI Predictions						BCF predictions (TGD method – normalised to C_{15}, 51% wt. Cl		Summary of persistence	Summary of B based on non-growth corrected BCF	Summary of B based on growth-corrected BCF
C	H	Cl			log Kow	Biowin 1	Biowin 2	Biowin 3	Biowin 5	Biowin 6	Not growth corrected	Growth corrected			
16	24	10	C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C	62.2	10.08	-0.6381	0	0.2058	-1.1345	0	57	109	Potentially P	Not B	Not B
16	23	11	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)CC(CL)CC(CL)C	64.5	10.26	-0.7659	0	-0.0435	-1.336	0	33	63	Potentially P	Not B	Not B
16	22	12	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)CC(CL)C	66.6	10.44	-0.8937	0	-0.2928	-1.5375	0	18	35	Potentially P	Not B	Not B
16	21	13	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C	68.4	10.62	-1.0215	0	-0.5421	-1.739	0	10	19	Potentially P	Not B	Not B
16	20	14	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C	70.1	10.8	-1.1493	0	-0.7914	-1.9404	0	5	10	Potentially P	Not B	Not B
16	19	15	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C	71.6	10.98	-1.2771	0	-1.0407	-2.1419	0	3	5	Potentially P	Not B	Not B
16	18	16	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)	73.0	11.23	-1.4049	0	-1.29	-2.1943	0	1	2	Potentially P	Not B	Not B
17	36	0	CCCCCCCCCCCCCCCCC	0.0	8.69	0.8499	0.9638	3.2644	0.7388	0.8874	1,469	2,801	Not P	Not B	B
17	35	1	CCCCCCCCCCC(CL)CCCCCC	12.9	8.87	0.7221	0.719	3.0151	0.5373	0.4755	1,067	2,034	Not P	Not B	B
17	34	2	CCCC(CL)CCCCCCC(CL)CCCCCC	23.0	9.05	0.4859	0.0375	2.4675	0.3358	0.0944	752	1,434	Not P	Not B	Not B
17	33	3	CCCC(CL)CCCCCCC(CL)CCC(CL)CCC	31.0	9.23	0.2497	0.0006	1.9199	0.1344	0.0118	514	981	Not P	Not B	Not B
17	32	4	CCCC(CL)CCC(CL)CCCC(CL)CCC(CL)CCC	37.6	9.41	0.1219	0.0001	1.6706	-0.0671	0.0014	342	651	Not P	Not B	Not B
17	31	5	CC(CL)CC(CL)CCC(CL)CCCC(CL)CCC(CL)CCC	43.0	9.59	-0.0059	0	1.4213	-0.2686	0.0002	220	420	Not clear	Not B	Not B

Formula			Smiles used	Cl content (% wt.)	EPI Predictions						BCF predictions (TGD method – normalised to C_{15}, 51% wt. Cl		Summary of persistence	Summary of B based on non-growth corrected BCF	Summary of B based on growth-corrected BCF
C	H	Cl			log Kow	Biowin 1	Biowin 2	Biowin 3	Biowin 5	Biowin 6	Not growth corrected	Growth corrected			
17	30	6	CC(CL)CC(CL)CCC(CL)CC(CL)CC(CL)CCC(CL)CCC	47.7	9.77	-0.1337	0	1.172	-0.4701	0	138	262	Potentially P	Not B	Not B
17	29	7	CC(CL)CC(CL)CCC(CL)CC(CL)CC(CL)CC(CL)C(CL)CCC	51.6	9.95	-0.2615	0	0.9227	-0.6715	0	84	159	Potentially P	Not B	Not B
17	28	8	CC(CL)CC(CL)CCC(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CCC	55.0	10.13	-0.3892	0	0.6734	-0.873	0	49	94	Potentially P	Not B	Not B
17	27	9	CC(CL)CC(CL)CC(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CCC	58.0	10.31	-0.517	0	0.4241	-1.0745	0	28	54	Potentially P	Not B	Not B
17	26	10	CC(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CCC	60.7	10.5	-0.6448	0	0.1748	-1.276	0	15	29	Potentially P	Not B	Not B
17	25	11	CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)CC(CL)C(CL)CCC	63.0	10.68	-0.7726	0	-0.0745	-1.4774	0	8	16	Potentially P	Not B	Not B
17	24	12	CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)CCC	65.1	10.86	-0.9004	0	-0.3238	-1.6789	0	4	8	Potentially P	Not B	Not B
17	23	13	CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)CC(CL)C	67.0	11.04	-1.0282	0	-0.5731	-1.8804	0	2	4	Potentially P	Not B	Not B
17	22	14	CC(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C	68.7	11.22	-1.156	0	-0.8224	-2.0818	0	1	2	Potentially P	Not B	Not B
17	21	15	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)CC(CL)C(CL)C(CL)C(CL)C	70.3	11.47	-1.2838	0	-1.0717	-2.1342	0	0	1	Potentially P	Not B	Not B
17	20	16	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C	71.7	11.65	-1.4116	0	-1.321	-2.3357	0	0	0	Potentially P	Not B	Not B
17	19	17	C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)C(CL)	73.0	11.91	-1.5393	0	-1.5703	-2.3881	0	0	0	Potentially P	Not B	Not B

Appendix B Growth correction of the BCF for a C_{15}, 51% wt. Cl substance

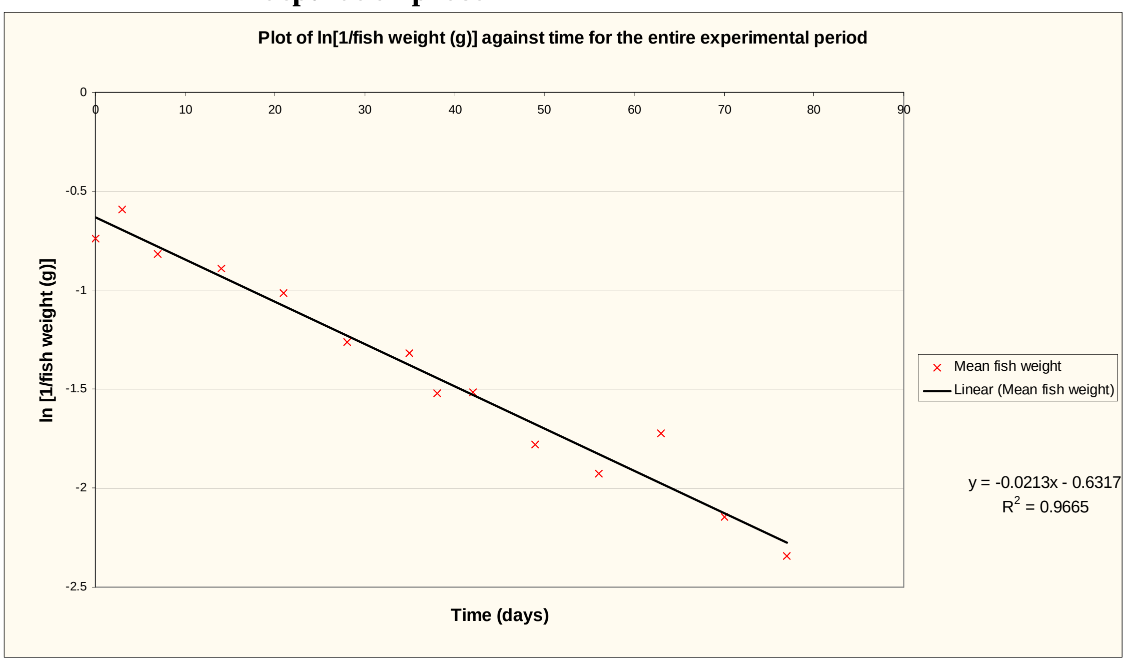
The background to the corrections made in this appendix is discussed in detail in EA (*in prep.)*. The study performed by Thompson *et al*. (2000) was originally summarised in EU (2005). The relevant kinetic parameters are summarised in Table B1.

Table B1 Summary of kinetic parameters from the Thompson *et al.* (2000) study

Exposure concentration (mg/l)	Uptake rate constant k_{uptake} (l/kg/day)	Overall depuration rate constant $k_{depuration\_overall}$ (day^{-1})	Kinetic BCF (l/kg)
0.00093	48.7	0.0448	1,087
0.0049	14.2	0.0407	349

The fish weights were determined at various time points during the uptake phase (days 0 to 35) and the depuration phase (days 38 to 77). The rate constant for growth dilution (k_{growth}) can be obtained from a plot of ln [1/fish weight] against time. The slope of such a plot is the negative of the growth dilution constant ($-k_{growth}$). Such a plot is shown in Figure B1 for the entire duration of the experiment (uptake and depuration phase). Similar plots were also constructed for the depuration period (day 35 to day 77 and day 38 to 77).

Figure B1 Determination of growth rate constant over the uptake and depuration phase



Based on these plots the following growth rate constants are determined:

For the entire experiment duration (day 0 to 77) k_{growth} = 0.0213 day^{-1} (R^2=0.97)

For depuration period days 35 to 77 k_{growth} = 0.0209 day^{-1} (R^2=0.88)

For depuration period days 38 to 77 k_{growth} = 0.0197 day^{-1} (R^2=0.84)

As can be seen, the rate constant for growth dilution appears to have been relatively constant over the entire period of the experiment. As the growth correction is applied to the depuration rate constant, the rate constant for growth dilution determined over the depuration period is most relevant to the analysis. However, the correlation (as measured by the R^2 value) is slightly better for the growth rate constant determined over the entire experimental period than those determined during the depuration phase. Therefore the effect of the growth rate constants obtained using all three datasets are considered here.

The growth corrected depuration rate constant can be obtained from the following equation assuming additivity of first order rate constants.

$$k_{depuration\_overall} = k_{depuration\_growth\ corrected} + k_{growth}$$

thus $k_{depuration\_growth\ corrected} = k_{depuration\_overall} - k_{growth}$.

The growth corrected rate constants and growth corrected BCF values are summarised in Table B2.

Table B2 Summary of growth corrected kinetic parameters from the Thompson *et al.* (2000) study

Exposure concentration (mg/l)	Uptake rate constant k_{uptake} (l/kg/day)	Rate constant for growth dilution k_{growth} (day^{-1})	Growth corrected depuration rate constant $k_{depuration\_growth\ corrected}$ (day^{-1})	Kinetic BCF (l/kg)
0.00093	48.7[a]	0.0197	0.0251	1,940
		0.0209	0.0239	2,038
		0.0213	0.0235	2,072
0.00093	46.0[b]	0.0197	0.0251	1,833
		0.0209	0.0239	1,925
		0.0213	0.0235	1,957
0.0049	14.2	0.0197	0.0210	676
		0.0209	0.0198	717
		0.0213	0.0194	732

Notes: a) Value taken from the Thompson *et al.* (2000) test report. The value has been estimated by forcing the curve fitting routine to pass through the measured concentration in fish at day 35.
b) Value recalculated by Euro Chlor without constraint of the day 35 value.

The uptake rate constant of 48.7 l/kg/day given in the Thompson *et al.* (2000) study was estimated from the uptake curve by forcing the curve fitting routine through the point for the concentration measured at day 35 of the uptake period (the concentration measured at this time point was 0.80 mg/kg). There is some rationale for this approach as a larger number of fish samples were analysed on day 35 (and also day 28) of the study compared with the earlier time points[1]. Thus it could be argued that the actual concentration in fish is known more reliably at day 35 (and day 28) than the earlier time points and so fitting the curve through this point is appropriate. However, it has been pointed out by Euro Chlor (2009) that a better overall fit to the data is obtained if the curve fitting is carried out without the constraint of the day 35 point. When this is carried out the uptake rate constant for the 0.00093 mg/l treatment group was 46.0 l/kg/day (and the estimated concentration in fish at day 35 from the regression was 0.76 mg/kg). The effect of using this uptake rate constant on the predicted growth corrected BCF is shown in Table B2 – the estimated BCF is slightly lower.

References

EA (*in prep.*). Estimation of fish bioconcentration factor (BCF) from depuration data. Environment Agency, Bristol.

Euro Chlor (2009). Comments from the Chlorinated Paraffins Sector Group of Euro Chlor on: Growth correction of the BCF from medium-chain chlorinated paraffins determined in the OECD 305 method, February 2009.

Thompson R S, Caunter J E and Gillings E (2000). Medium-chain chlorinated paraffins (51% chlorinated, n-pentadecane-8-14C): Bioconcentration and elimination by rainbow trout (*Oncorhynchus mykiss*). AstraZeneca Confidential Report BL6869/B.

[1] Eight fish were sampled on each of day 35 and day 28 of the study compared with four fish on each of days 21, 14, 7, and 3 of the study.