Your Ref:
Our Ref: 5036759/23/MAS

8 July 2010

Ms S Walford Ext No: 5861
South Cambridgeshire District Council
South Cambs Hall
Cambourne Business Park
Cambourne
Cambridge
CB3 6EA

Dear Susan,

Former Bayer CropScience, Hauxton: Risk Assessment of Contaminants Not Previously Identified

Characterisation sampling and analysis to date identified 10 contaminants not previously identified (CNPIs) requiring further assessment. These CNPIs were notified to South Cambridgeshire District Council by Atkins (06.05.2010 and 24.05.2010) and by Harrow Estates (16.06.2010 and 29.06.2010). Upon further review of these compounds, two (2(1-methylpropyl)-phenol and 2-mathyl phenol) were in fact evaluated during the previous risk assessment in 2006. Both compounds were given a low risk score and not taken further as priority contaminants. The compounds have not been evaluated further as part of this exercise.

The grid squares in which the CNPIs have been identified and the treatment beds in which the materials have been placed are summarised in Table 1. The grid squares are shown of the enclosed Site Survey Reference Grid plan.

Table 1 – Contaminants Not Previously Identified

Contaminant	Grid squares	Treatment beds
2,6-bis(1-methylpropyl)-phenol	J16	TB1, TB4
2,6-bis(1,1-dimethylethyl)-4- (1-methylpropyl)-phenol	J16	TB1, TB4
2,4-Dichloro-o-cresol	L8, I9, H7, K10	TB6, TB17-18, TB23, TB30-31, TB50-51, TB59-60, TB69, TB71
Bis(2-ethylhexyl) maleate	L8	TB17-18, TB23, TB30-31
1,2-bis(2,4,6-trichlorophenoxy) ethane	H9, K7	TB9-10, TB15, TB60-63
Prochloraz	H9	TB60-63
2,3,6-Trichlorotoluene	I9	TB59-60
1-(2-Chloroethoxy)-2-(o-Tolyloxy)-ethane	I9	TB59-60

Toxicological assessments and human health and controlled waters risk assessments have been carried out for these CNPIs and, where sufficient toxicological, physical and chemical data is available, preliminary generic assessment criteria (GACs) have been derived for the specific compounds. The preliminary GACs will be provided to Vertase, who currently intend to use these as remedial targets for the CNPIs. Where there is insufficient toxicological, physical and chemical data available for assessment and modelling, suitable surrogate compounds for which

GACs have already been derived for the Hauxton site have been identified and selected based on chemical structures and toxicity data, see Table 2 overleaf.

Table 2 – Surrogates Used

Contaminant	Surrogates	
	Human Health	Controlled Waters
2,6-bis(1-methylpropyl)-phenol	2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol	4-chloro 2-methyl phenol
2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol	N/A	4-chloro 2-methyl phenol
2,4-Dichloro-o-cresol	N/A	4-chloro 2-methyl phenol
Bis(2-ethylhexyl) maleate	Benzene	N/A
1,2-bis(2,4,6-trichlorophenoxy) ethane	Vinyl chloride	N/A
Prochloraz	N/A	N/A
2,3,6-Trichlorotoluene	Vinyl chloride	4-chloro 2-methyl phenol
1-(2-Chloroethoxy)-2-(o-Tolyloxy)-ethane	Vinyl chloride	4-chloro 2-methyl phenol

The CNPIs, derived or surrogate GACs and required laboratory limits of detection (LODs) are summarised in Table 3 below. As for the previously identified contaminants of concern, four GACs have been derived for each CNPI: i) treated materials which will be placed within 20m of Riddy Brook (Inner Zone), ii) treated materials which will be placed at least 20m from Riddy Brook (Outer Zone), iii) treated materials which will be placed at least 1 m below final site levels (controlled waters risk driven) and iv) treated materials which will be placed within 1 m of final site levels (human health risk driven). The CNPIs and derived/surrogate GACs will be added to the list of Contaminants of Concern for the relevant grid square and treatment bed validation suites.

Table 3 – Preliminary Generic Assessment Criteria

Contaminant	GACs (□g/kg)				LOD (□g/kg)
	Greater than 1m depth		Less than1m depth		
	Outer Zone	Inner Zone	Outer Zone	Inner Zone	
2,6-bis(1-methylpropyl)-phenol	3170	2.25	2170	2.25	100[a]
2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol	3170	2.25	2170	2.25	100[a]
2,4-Dichloro-o-cresol	3170	2.25	3110	2.25	100[a]
Bis(2-ethylhexyl) maleate	LOD[c]	LOD[c]	LOD[c]	LOD[c]	LOD[d]
1,2-bis(2,4,6-trichlorophenoxy) ethane	>500,000	5100	5	5	100[b]
Prochloraz	5230	1.1	5230	1.1	100[a]
2,3,6-Trichlorotoluene	3170	2.25	5	2.25	100[b]
1-(2-Chloroethoxy)-2-(o-Tolyloxy)-ethane	3170	2.25	5	2.25	100[b]

a: An LOD of 100 □g/kg is acceptable for materials backfilled in the Outer Zone (at least 20 m from Riddy Brook). This LOD will be confirmed by the laboratory.
b: An LOD of 100 □g/kg is acceptable for materials backfilled in the Outer Zone (at least 20 m from Riddy Brook) and at depths greater than 1 m of final site levels. This LOD will be confirmed by the laboratory.
c: The calculated GACs were lower than the commercially available LODs and will therefore be set at an achievable LOD.
d: LOD to be confirmed by laboratory.

The data collected, methods and models used in the derivation of GACs and identification of surrogates are detailed in Annex 1: Toxicological Data, Annex 2: Physical and Chemical Data, Annex 3: Modelling, Annex 4: Derivation of Generic Assessment Criteria for the protection of Human Health and Annex 5: Derivation of Generic Assessment Criteria for the protection of Controlled Waters.

The treatability of these compounds has been reviewed by Vertase FLI and the remediation of the CNPIs will be dealt with by the existing treatment train identified in the Remediation Method Statement (Version 6) and detailed in the Environmental Permit Deployment Form for the site.

Yours sincerely
For and on behalf of Atkins Limited

Mark Smith
Project Manager

Cc Eileen Young – Environment Agency (with enclosures)
Nigel Blazeby - South Cambridgeshire District Council

Enc.

A1

Legend

Site Boundary

Rev.	Description	Revised By	Date
B	Text Rotated	JWH	21-04-10
A	Text added in Grid Squares	JWH	01-04-10
	FIRST ISSUE		19-02-10

Vertase F.L.I.

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Site Address:

Bayer Site
Hauxton
Cambridge

Rev: B

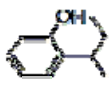
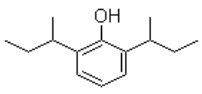
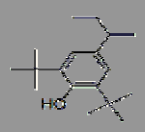
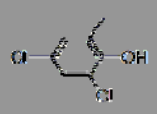
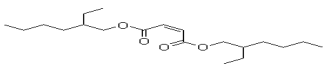
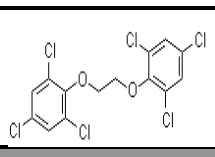
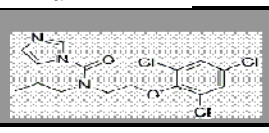
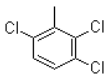
Title: Site Survey Reference Grid

Client: Harrow Estates

Drawn: JWH	Checked: JWH	Approved: CL
Dwg: D907_56	Contract: 907 BRI	Scale: 1:1250

Annex 1: Toxicological Data

- **Surrogate selection**
- **Prochloraz**
- **2,4-dichloro-o-cresol**
- **DTBSBP**

CNPIs	Structure	Synonym / CAS	Comments	Available tox data	Comment	Volatility	Suggested Surrogate	Comment
2(1-methylpropyl)-phenol		2-sec-Butylphenol 89-72-5	Insufficent data, surrogate to be identified. DTBSBP, ethylbenzene or phenol deemed most appropriate based on structure	LD50oral 320mg/kg bw LD50 inhal >290 (unit not given) LD50dermal 600mg/kg bw	Low acute toxicity	Not yet available	**Ethylbenzene**	Ethylbenzene has a more similar structure (benzene with alkyl group), and has more conservative tox data than phenol (benzene with -OH group). DTBSBP has the most conservative toxicity Differences in dermal absorption between phenol and ethylbenzene should still provide conservatism as limited data indicate low dermal toxicity
2,6-bis(1-methylpropyl)-phenol		2,6-Di-sec-butylphenol 5510-99-6	Insufficient data. Surrogate to be allocated. Phenol, toluene, ethylbenzene and DTBSBP suggested.	No suitable data	n/a	Not yet available	**DTBSBP**	DTBSBP has the most similar stucture (including previous pesticide structures evaluated for Hauxton). Also the most conservative toxicity data of those suggested
2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol		**DTBSBP** **17540-75-9**	**Taken forward for further evaluation**. Health Canada assessment - http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm					
2,4-Dichloro-o-cresol		2,4-dichloro-6-methylphenol 1570-65-6	Insufficient data. Data for mono-chloro-6-methylphenol available to be used as surrogate. **Needs to be taken forward for further evaluation**.					
Bis(2-ethylhexyl) maleate		142-16-5	Insufficient data. To be compared with benzene, or cyclohexanone as surrogate	Oral -14 000mg/kg	Very low acute toxicity	Not yet available	**Benzene**	Structure very different from both surrogates. Cyclohexanone also has a ketone group, but benzene has the more conservative toxicity
1,2-bis(2,4,6-trichlorophenoxy)ethane			Insufficent data. Chlorinated solvent surrogate to be adopted (PCE or vinyl chloride suggested). Dieldrin, MCPA and dicamba also chlorinated aromatics, although containing only one aromatic ring.	No data	n/a	Not yet available	**Vinyl chloride**	More similar to benzene structure, but vinyl chloride toxicity data more conservative. Also more conservative than dicamba, dieldrin and MCPA
Prochloraz		67747-09-5	**Taken forward for further evaluation** – oral RfD and cancer estimate (US EPA available as starting point, established pesticide constituent.					
2,3,6-Trichlorotoluene		2077-46-5	Insufficient data, to be compared with surrogate, benzene, toluene, vinyl chloride, dicamba (probable).	No data	n/a	a,a,a-trichlorotoluene HLC of 3.2E-3 (10°C)	**Vinyl chloride**	More similar to benzene structure, but vinyl chloride toxicity data more conservative. Dicamba also similar but relative toxicity makes vinyl chloride the most conservative option.
1-(2-Chloroethoxy)-2-(o-Tolyloxy)-ethane		21120-80-9	Insufficient data, to be compared with surrogate (benzene, vinyl chloride probable) .	No data	n/a	Not yet available	**Vinyl chloride**	More similar to benzene structure, but vinyl chloride toxicity dat more conservative

TOXICOLOGICAL DATA TEMPLATE

Chemical name: __Prochloraz_____

Common name: __BTS 40542_____

CAS RN: __67747-09-5_____

Chemical Identification:
Synonyms of prochloraz include BTS 40542 and n-propyl-N[2-(2,4,6-trichlorophenoxy)ethyl]-1H-=imidazole-1-carboxamide. Prochloraz is combustible, not auto flammable, not explosive, non-oxidising and has a flash point of ca. 160°C (IUCLID, 2000).

Sources
Prochloraz was synthesised for use as a fungicide in 1974 and commercially introduced in 1980 (JMPR, 2001).

Toxicokinetics
WHO report that prochloraz was extensively metabolised in rats with no unchanged parent compound being detected in urine. It was also detected in faeces and was the most abundant component on day 1 of the study undertaken (WHO, 2004). In addition, JMPR (2001) report several studies that show that urinary excretion is almost complete after 72-92 hours in studies on rats and mice.

Acute Toxicity
Acute oral toxicity studies undertaken on male and female Boots-Wistar rats reported an lethal dose $(LD)_{50}$ of 1600-2400 mg/kg bw/day (IUCLID 2000; JMPR, 2001). Studies on male CD-1 mice resulted in an LD_{50} of approximately 2400 mg/kg bw/day (IUCLID, 2000; JMPR 2001; TOXNET, 2010). The JMPR states that this study indicates that prochloraz was not acutely hepatotoxic (toxic to the liver) at doses up to and including the LD_{50} (JMPR, 2001).

Other studies report: an LD_{50} of 2400 mg/kg bw for male and female rats; a no observed adverse effect level (NOAEL) of 10 mg/kg bw and a lowest observed adverse effect level (LOAEL) of 100 mg/kg bw in beagle dogs following a single oral exposure; and a NOAEL of 50 mg/kg bw and LOAEL of 250 mg/kg bw for baboons given two single doses on day 1 and day 17 of the study (JMPR, 2001).

Two acute dermal toxicity studies are reported. The first, from 1987, on male and female Sprague-Dawley rats resulted in a LD_{50} of >2100mg/kg bw. The second, from 1979, on New Zealand white rabbits resulted in a LD_{50} of >3 ml/kg bw (IUCLID, 2000; JMPR, 2001; TOXNET, 2010).

JMPR reported one 4 hour inhalation study (whole body) using five male and five female rats exposed to an aerosol containing prochloraz which resulted in a LC_{50} of >2.2 mg/l (>2200 mg/m^3) air (JMPR, 2001).

Subacute Toxicity (short term repeat dose studies)
Several subacute toxicity studies were reported by JMPR (JMPR 2001) which are detailed in the following text.

Groups of 15 male and 15 female CD-1 mice were given diets containing technical-grade prochloraz (purity, 98.2%) at concentrations providing a dose of 6, 25, 100 or 400 mg/kg bw per day for 13 weeks. A control group comprised 24 mice of each sex. Further groups of 15 male and 15 female controls and mice treated at 400 mg/kg bw per day were kept for four weeks after the end of dosing, and, in addition, groups of nine males and nine females were treated for 6 weeks. The NOAEL was reported as 6 mg/kg bw per day on the basis of reversible effects on the liver at the next higher dose of 25 mg/kg bw/day (JMPR, 2001).

Studies on dogs resulted in a NOAEL of 2.5 mg/kg bw per day on the basis of effects on enzyme activity, liver size and weight and prostate and testes weights at the next highest dose in one study. These effects were reversible (JMPR, 2001). A NOAEL of 10mg/kg bw/day was reported in a separate study, on the basis of the increase in alkaline phosphatase activity (JMPR, 2001).

Technical-grade prochloraz (purity, 95.29%) was suspended in 10% aqueous acacia and given by gavage to groups of five male and five female CFLP mice at a dose of 96, 240 or 600 mg/kg bw per day for 21 days. Overt signs of toxicity occurred in males given 600 mg/kg bw per day; these included loss of condition, evidence of central nervous system depression (sedation or inactivity), piloerection (involuntary raising of hairs or 'goosebumps') and coolness to touch. Four males and one female given 600 mg/kg bw per day died during the study, but two of these deaths were attributable to administration accidents. The authors concluded that, as the dose of 600 mg/kg bw per day was not tolerated by the males, the appropriate highest dose for the 90-day study would be 400 mg/kg bw per day (JMPR, 2001).

Technical-grade prochloraz (purity, 92.7%) was emulsified in aqueous acacia and given by gavage to groups of five male and five female Boots-Wistar rats at a dose of 25, 100 or 400 mg/kg bw per day for 30 days; a control group of 10 males and 10 females received the vehicle alone. The dose of 100 mg/kg bw per day was tolerated by both sexes and the authors concluded that, on this basis, this would be the appropriate highest dose (JMPR, 2001).

Groups of 20 male and 20 female Boots-Wistar rats were given technical-grade prochloraz (purity, 97.5%) at a dose of 6, 25 or 100 mg/kg bw per day by gavage in 10% aqueous acacia suspension for 13 weeks; a control group of 20 males and 20 females received the vehicle alone. Further groups of 20 male and 20 female controls and rats at 100 mg/kg bw per day were kept for 4 weeks after the end of the dosing period. In addition, groups of 10 male and 10 female controls and rats at 6, 25 or 100 mg/kg bw per day were examined after 6 weeks. Various treatment-related effects were seen in all groups, the most important, apparently reversible, effects being increased liver weight and hepatocyte size. However, a NOAEL could not be identified (JMPR, 2001).

Subchronic Toxicity (longer-term/medium duration studies)

The IUCLID data sheet reported three 13 week repeated dose oral studies undertaken on Wistar rats, CD-1 mice and beagle dogs resulting in NOAELs of <6 mg/kg bw/day (where the lowest test concentration showed no adverse effects), 6 mg/kg bw/day and 2.27 mg/kg bw/day respectively. Effects included reduced/increased food consumption, haematological (blood parameter) effects, enlarged livers, decreased prostate size, mammary tissue effects, weight gain/reduction, kidney weight increase (IUCLID, 2000).

Chronic Toxicity (long-term toxicity data)

JMPR reported a number of long term studies involving mice, rats and dogs which resulted in NOAELS of 78 ppm (7.5 mg/kg bw/day), 38 ppm (1.3 mg/kg bw./day) and 30 ppm (0.90 mg/kg bw/day), respectively (JMPR, 2001[1]).

JMPR (2001) reported long term studies of toxicity and carcinogenicity in mice with liver-cell tumours contributing to the deaths of more males (20/52) and females (14/52) at 1300 ppm and more males at 325 ppm (13/52) than controls (9/104 males and 1/104 females). Many of these mice were in poor clinical condition when killed. The NOAEL was 78 ppm, equal to 7.5 mg/kg bw/day (JMPR, 2001).

[1] The studies reported present concentrations of test substance in the medium in which they are administered, in parts per million (ppm) – in a given study this could be concentration in diet or an oil such as corn oil. These concentrations are then converted to dose given per day, in the basis of a number of factors, such as amount of food intake per day in dietary studies, or quantity dosed by gavage. The body weight of the test subject is then used to calculate the dose per unit body weight per day, resulting in variations in the conversion of dose seen in ppm and mg/kg bw/day.

Another study, detailed by JMPR (2001) and involving rats, reported a NOAEL of 38 ppm (equivalent to 1.3 mg/kg bw/day prochloraz) on the basis of hepatic effects (periportal glycogen loss and centrilobular fat deposition) at the next highest dose. Groups of 60 male and 60 female Sprague-Dawley (CD) rats were fed a diet containing technical-grade prochloraz (purity, 95.1–97.0%) at a concentration of 38, 150 or 625 ppm, corresponding to mean achieved intakes of 1.3, 5.1 and 22 mg/kg bw per day for males and 1.6, 6.4 and 28 mg/kg bw per day for females for 115 weeks (males) and 111 weeks (females).

A third study reported by JMPR (2001) involved dogs and resulted in a NOAEL of 30 ppm (0.90 mg/kg bw/day), on the basis of effects on the liver in one dog at the next highest dose. The groups of five male and five female beagle dogs were fed diets containing technical-grade prochloraz (purity, 95.2–97.1%) at a concentration of 30, 135 or 600 ppm (increased to 1000 ppm from week 57) for 104 weeks. These concentrations corresponded to mean intakes of 0.90, 4.1, 18 and 28 mg/kg bw per day for females and 0.94, 4.5, 18 and 29 mg/kg bw/day for males. A LOAEL of 135 ppm (equal to 4.1 mg/kg bw/day) was also reported (JMPR, 2001).

Reproductive Toxicity

A two generation rat study (1982) using an oral feed with animals treated daily with doses of 0, 37.5, 150 or 625ppm prochloraz for 9 weeks resulted in reduced reproductive performance demonstrated by lower litter size and weight from birth to weaning in both mates and offspring at a dose of 625ppm prochloraz. Liver weights of F1A weanling females were increased at all concentrations. A concurrent control group with no treatment was used (IUCLID, 2001).

This study is described in further detail by JMPR (2001). The multi generation studies in rats involved mixing prochloraz (purity, 96.2–97%) into the diet at a concentration of 0, 38, 150 or 625 ppm, corresponding to mean achieved intakes of 3.1, 13 and 57 mg/kg bw per day for F0 (parent group) males and 3.5, 14 and 58 mg/kg bw per day for F0 females; 3.7, 16 and 70 mg/kg bw per day for F1 (first generation of off-spring from the parent group) males and 4.5, 18 and 81 mg/kg bw per day for F1 females. The parent animals were exposed to the fungicide for 9 weeks before mating, and representative offspring were retained to form a second generation. The initial animals were then re-mated with different males and females, and their offspring were discarded when they were about 3 weeks of age, after macroscopic examination post mortem. Reproductive performance was affected only at the highest dietary concentration, which was toxic to the parent animals. The NOAEL was 38 ppm, equal to 3.1 mg/kg bw per day and LOAEL was 150 ppm (equal to 13 mg/kg bw/day) for parental toxicity (JMPR, 2001). The conversions for offspring toxicity with regards to the NOAEL and LOAEL, were equal to 3.7 mg/kg bw per day and 16 mg/kg bw per day respectively (JMPR, 2001).

Developmental Toxicity

Two developmental studies suggest maternal toxicity and embryotoxicity, but no evidence of teratogenicity from prochloraz.

One oral gavage study reported in the IUCLID 2000 datasheet and by the JMPR (2001) indicated maternal toxicity and embryotoxicity but no teratogenicity at 160 mg/kg/day. This study used 16 female Chinchilla rabbits and a control group exposed over 6-18 days and treated daily at doses 0, 10, 40, 160mg/kg/day. This study resulted in a NOAEL of 40mg/kg bw/day. Effects included reduced weight gain and food consumption at 160 mg/kg, increased liver weight and liver/body weight ratios, a higher incidence of non-pregnant animals, animals with total litter loss and foetal resorption in dams with viable young, with maternal toxicity and embryotoxicity at 160 mg/kg (IUCLID, 2000). JMPR (2001) report both a NOAEL of 40 mg/kg bw/day and a LOAEL of 160 mg/kg bw/day for this study for maternal toxicity and embryo- and foetotoxicity.

A second study reported in the IUCLID 2000 data sheet and by JMPR (2001) used CD-1 rats with an exposure period of 0-19 days. Twenty female rats and a concurrent control group were treated daily over 20 days with doses of 6, 25 and 100mg/kg/day. Effects included increased salivation, reduced food consumption, lower bodyweight gain and liver enlargement at 25mg/kg/day and 100mg/kg/day. At 100 mg/kg/day, embryo-toxic markers, litter size, implantation index and viability index slightly decreased. Incidence of dead foetuses also

marginally increased. The placenta from treated dams was heavier than those from the untreated groups. There was no evidence of a teratogenic response (IUCLID 2000 and JMPR 2001). JMPR report a maternal toxicity NOAEL of 6 mg/kg bw/day and a LOAEL of 25 mg/kg bw/day, and an embryo- and foetotoxicity NOAEL of 25 mg/kg bw/day and LOAEL of 100 mg/kg bw/day.

Genotoxicity

Hamster, mice and human embryonic fibroblast in vitro studies reported in the IUCLID datasheet suggested prochloraz is not genotoxic (IUCLID, 2000). Although one assay for sister chromatid exchange in vitro in Chinese hamster ovary cells resulted in a slight increase in frequency in the presence and absence of metabolic activation at doses in the toxic range, this finding was supported by JMPR where the mutagenic and genotoxic potential of technical-grade prochloraz was investigated in a battery of tests in vitro and in vivo and results were negative (JMPR, 2001).

Carcinogenicity

IUCLID (2000) report that tumour incidence and distribution was unaffected by treatment with prochloraz. No evidence of carcinogenicity resulting from the chronic administration of prochloraz was identified during a CD-1 rat study lasting for 115 weeks. The study used an oral feed (doses 37.5, 150, 625ppm) in 60 male and 60 female rats, and a concurrent control group (no treatment). No clinical findings related to treatment were noted. Mortality rates for males were similar for treated and untreated animals, and treated females lived longer than untreated (IUCLID, 2000; US EPA 1989). JMPR (2001) reports a toxicity NOAEL of 38 ppm (equal to 1.3 mg/kg bw/day) and a LOAEL of 150 ppm (equal to 5.1 mg/kg bw/day), and a carcinogenicity NOAEL of 625 ppm (equal to 28 mg/kg bw/day).

A 121 week mouse study (52 males and 52 females) using daily treatment of doses of 0, 78, 325 and 1300 ppm noted that mortality rates were not treatment related, although liver tumours were noted in males and females at 1300 ppm, and in males at 325 ppm (IUCLID, 2000; JMPR, 2000; USEPA, 1989). The incidence of liver tumours was not significant at 78 ppm and the IUCLID and US EPA provide no further information (IUCLID, 2000; US EPA, 1989). JMPR (2001) report a NOAEL for this study of 78 ppm, equal to 7.5 mg/kg bw/day and a LOAEL of 325 ppm, equal to 33 mg/kg bw/day (for both toxicity and carcinogenicity).

The US EPA IRIS classification indicated a weight-of-evidence characterization classification of C (possible human carcinogen), based on the statistically significantly increased incidence, and dose-related trend, in liver adenomas and carcinomas (combined) in both sexes of one strain of mouse (US EPA, 1989).

Other Irritation and Sensitisation

Prochloraz was reported to be not irritating to skin and slightly irritating to eyes, based on tests on rabbits (1984), but is classified as not irritating to both skin and eyes by the EC (IUCLID, 2000). Tests on guinea pigs indicated no sensitising effects (IUCLID, 2000). Adverse effects in humans comprised – eye irritation, over exposure to formulation solvent, skin rash (person with multiple allergies) following accidental soaking with spray. (IUCLID, 2000; JMPR, 2001).

Background exposure (food, drinking water, air)

The UK Food Standards Agency refer to the Committee on Toxicity of Chemicals in Food, Consumer Products and the Environment to report the worst-case occurrence of multiple pesticide residues in different food commodities using data from the surveillance programmes from 1997 until 2001. The worst case residue occurrence for prochloraz was reported in mushrooms (COT, 2002).

WHO (2004) report an estimated intake range of 7-10 % of the maximum acceptable daily intake (ADI) of 0.01 mg/kg bw/day.

There are no data on ambient air concentrations of prochloraz in readily available literature sources.

Regulatory guidelines/ advisories/ guideline values

The US EPA (1989) reported a health based guidance value of 0.009 mg/kg bw/day based on an oral reference dose (RfD). The oral RfD is based on a NOAEL of 30 ppm (0.9 mg/kg bw/day) for adverse effects on the liver (increases in serum alkaline phosphatase, increased liver weights and changes in liver histopathology) in a 2-year dog feeding study, also applying an uncertainty factor of 100 and modifying factor of 1.

JMPR (2001) provide an ADI of 0.01 mg/kg bw/day based on two NOAELs for hepatic effects in 2 year studies – 0.9 mg/kg bw/day (dog) and 1.3 mg/kg bw/day (rat). An uncertainty factor of 100 was applied. This ADI was set in 1983 and reconfirmed in 2001 (JMPR, 2001).

JMPR (2001) and WHO (2004) report that the Meeting of the JMPR, held in September 2004, established an acute reference dose of 0.1 mg/kg bw, on the basis of a NOAEL of 10 mg/kg bw per day for effects on the liver at day 3 (increased serum alkaline phosphatase activity) in a 14-day study in dogs, and a safety factor of 100.

Selection of Health Criteria Value (HCV)

Oral Health Criteria Value (HCV)

The oral RfD derived by the US EPA (1989) of 9 µg/kg bw/day (0.009 mg/kg bw/day) has been selected for use as a Tolerable Daily Intake (TDI). This value is similar to that derived by JMPR (2001), who derived an ADI of 0.01 mg/kg bw/day. Both HCVs are based on the same long-term study in beagle dogs, but the JMPR appear to have rounded the value adopted, with supporting evidence from the NOAEL of 1.3 mg/kg bw/day in rats.

Oral Mean Daily Intake (**MDI)**

Food

The WHO (2004) reports an estimated intake range of 7-10 % of the maximum ADI of 0.01 mg/kg bw/day from dietary sources. This is, therefore, equal to a maximum daily intake of 0.001 mg/kg bw/day for a 70 kg adult. On this basis, the food MDI equals 70 µg/day (0.07 mg/day).

Drinking Water

The UK Water Quality (Water Supply) Regulations state that all other pesticides (with the exception of aldrin, dieldrin, heptachlor and heptachlor epoxide) should not exceed 0.1 µg/L in drinking water supplied to the consumer. Assuming an adult intake of 2L per day, this is equal to a maximum conservative intake of 0.2 µg of prochloraz per day, assuming that all 'other' pesticide is made up of prochloraz, for an adult consumer. This is equivalent to a dose of 0.00286 µg/kg bw/day (0.00000286 mg/kg bw/day).

The total MDI_{oral} for 70 kg adult is therefore:
(Dietary + drinking water intake) = (70 + 0.2) µg/day
= 70.2 µg/day

Therefore:

MDI_{oral} for 70 kg adult = 1.00286 µg/kg bw/day
= 0.00100286 mg/kg bw/day

Therefore, the Tolerable Daily Soil Intake $(TDSI)_{oral}$ for an adult is:
TDI – MDI = (9 – 1.00286) µg/kg bw/day
= 7.99714 µg/kg bw/day
= 0.007997 mg/kg bw/day

Inhalation Health Criteria Value

In the absence of data for long-term inhalation exposures, the data available for oral exposures will be extrapolated for use as a preliminary indicative health criteria value.

Therefore, the $TDI_{inhalation}$ is 9 µg/kg bw/day (0.009 mg/kg bw/day).

There are no readily available data on ambient air concentrations of prochloraz. However, as it is still approved for use in the UK, it has been assumed that it may be present in the environment. Background exposure is assumed to be 20% of the HCV, based on expert judgement as suggested in Environment Agency Science Report (SR) 2 (2009). This is equal to a value of 0.126 mg/day (126 µg/day). Therefore, the Tolerable Daily Soil Intake $(TDSI)_{inhalation}$ is 7.2 µg/kg bw/day (0.0072 mg/kg bw/day), which, based on a 70 kg adult.

Assuming the 70kg adult inhales 20m³ air per day, this is also equivalent to 0.0252 mg/m³ per day.

In the absence of other inhalation data, this HCV compares favourably with the acute inhalation exposure value, which is greater than four orders of magnitude above the long-term HCV derived here.

References

COT, 2002. Committee on Toxicity of Chemicals in Food, Consumer Products and the Environment. Risk Assessment of Mixtures of Pesticides and Similar Substances. September 2002. http://cot.food.gov.uk/pdfs/reportindexed.pdf Accessed 17th June 2010

Environment Agency (2009). Human Health Toxicological Assessment of Contaminants in Soil. Science Report SC050021/SR2

International Uniform Chemical Information Database (IUCLID) chemical data sheet ECB, 2000. IUCLID Chemical Data sheet. Available from: http://ecb.jrc.ec.europa.eu/esis/ Accessed 17th June 2010.

JMPR (Joint Meeting of the FAO Panel of Experts on Pesticide Residues in Food and the Environment and the WHO Core Assessment Group), 2001 IPCS INCHEM: http://www.inchem.org/documents/jmpr/jmpmono/2001pr11.htm

TOXNET ChemID plus http://toxnet.nlm.nih.gov/ Accessed 17th June 2010.

US EPA, 1989. US Environmental Protection Agency Integrated Risk Information System: Prochloraz. Available at: http://www.epa.gov/ncea/iris/subst/0378.htm

World Health Organisation (WHO), 2004. Pesticide Residues in Food. Report of the Joint Meeting of the FAO Panel of Experts on Pesticide Residues in Food and the Environment and the WHO Core Assessment Group on Pesticide Residues Rome, Italy, 20–29 September 2004. Available from: http://www.fao.org/ag/AGP/AGPP/Pesticid/JMPR/DOWNLOAD/2004_rep/report2004jmpr.pdf

TOXICOLOGICAL DATA TEMPLATE

Chemical name: _2,4-chloro-2-methylphenol **Common name:** _ 2,4-dichloro-o-cresol; DCOC

CAS RN: _1570-65-6

There are no readily available data for the primary chemical compound, 2,4-dichloro–o-cresol. Therefore, this summary is based on the data available for the structurally similar compound, 4-chloro-o-cresol (CAS RN 1570-64-5), commonly known as PCOC. ____

Chemical Identification
Synonyms include "4-chloro-o-cresol", "4-chloro-2-methylphenol" and "para-chloro-ortho-cresol (PCOC)".

Occurrence and Uses
2,4-dichloro-o-cresol is listed as an impurity in 4-chloro-o-cresol (PCOC) and is listed as being 2.0% of the weight[1] of PCOC (ECJRC, 2002). PCOC is used in the pesticide manufacturing industry as an intermediate in the synthesis of the phenoxy herbicides MCPA, MCPB and mecoprop (MCPP) (ECJRC, 2002).

The European Chemicals Bureau (ECB) states that PCOC may formerly have been used as a disinfectant, although no current evidence was found for the use of PCOC as such in products. They also state that direct exposure is likely to be restricted to those involved in the manufacture and handling of PCOC and in conjunction with its use in the manufacture of phenoxy herbicides (ECJRC, 2002).

The main exposure of human beings to PCOC is likely to be via production, or use of phenoxy herbicides which may contain it as an impurity (<1%), or as a breakdown product following exposure of herbicides to sunlight, or to their metabolic transformation to the substance (ECJRC, 2002).

Aquatic Toxicity
PCOC is very toxic to aquatic organisms (ECJRC, 2002).

Exposure
The OECD (OECD, 2005) this chemical (PCOC) is corrosive and toxic by inhalation. The OECD also report that it is "corrosive and toxic by inhalation but is only moderately toxic in acute mammalian tests by other routes" (OECD, 2005).

Workers' exposure is considered to be low because the substance is produced in a closed system as an intermediate for the manufacturing of phenoxyherbicides. Consumer exposure is considered to be negligible (OECD, 2005).

The most important sources of direct human exposure are assumed to be at production sites (with predicted exposures of up to 0.7 mg/kg/day) or in conjunction with the use of phenoxy herbicides where exposures of around 0.35 mg/kg/day are estimated (OECD, 2005). Indirect exposure is estimated as being several orders of magnitude lower than the above values at a regional level while consumer exposure to the substance as an impurity in lawn-treatment sprays may be as high as 0.07 mg PCOC /kg bw/event (OECD, 2005).

Toxicokinetics
Very little is known about the toxicokinetics, metabolism, distribution, and excretion of PCOC in humans and experimental animals. However, from the acute toxicity studies it can be inferred that PCOC can be taken up in the body through the gastrointestinal tract, the skin,

[1] 2% w/w

and via inhalation. There is no information on the metabolism and excretion of PCOC (ECB, 2002).

Acute Toxicity

The risk assessment by the ECB (ECB, 2002) reported the following LD_{50}s:

Acute Oral Toxicity

- Oral LD_{50} of 3,195 mg PCOC/kg bw (range 2,698 – 3,834 mg/kg bw) was found based on a study by Scantox (1982a) using five male and five female rats per group and dosing by gavage with the doses 1,728, 2,488, 3,583 and 5,160 mg/kg bw using oleum arachidis as vehicle;
- Oral LD_{50} of 1,190 mg/kg bw was derived based on a study by Hattula et al. (1979) using groups of ten male Wistar rats, 2-3 months of age, which were given 1,000, 1,100, or 1,200 mg PCOC/kg bw with the substance dissolved in olive oil. The animals were all killed 24 hours after dosing. Poor reporting of the Hattula study makes its interpretation difficult;
- Oral LD_{50} of 2,650 mg/kg bw derived based on a rat study by Hazleton Lab (1977); ;
- Oral LD_{50} of 2,700 mg/kg bw derived based on a mouse study by BASF AG (1978). This test report is not available, but the results are in accordance with the results of the study available (Scantox, 1982a);
- Oral LD_{50} of 1,330 mg/kg derived based on a rat study by Schrötter et al (1978). Few experimental details are provided.

The ECB report that, based on reliability of studies found, the oral LD_{50} of PCOC is above 2,000 mg/kg (ECB, 2002). The results also indicate that the vehicle used in administering PCOC may play an important role in determining absorption following oral administration (ECB, 2002).

The overall conclusion for acute oral toxicity is $LD_{50\ oral,}$rat is 2,650 – 3,195 mg/kg bw(ECB, 2002). PCOC not only shows corrosive properties but also properties resulting in systemic effects, i.e. effects on liver and kidney (ECB, 2002).

Acute Dermal Toxicity

The following data is available for acute dermal toxicity of PCOC:

- Dermal LD_{50} 2240 mg/kg based on a study by Scantox (1982b) of groups of five male and five female rats dermally dosed with 1,667, 2,000, 2,400, or 2,880 mg of PCOC using oleum arachidis as a dosing vehicle. A LD_{50} of 2240 mg/kg (range 2,023 – 2,484) was calculated from the observed deaths.

Acute Inhalation Toxicity

- Inhalation LC_{50} of 0.9 mg/l (900 mg/m³) based on a study by Scantox (1983) following OECD Guideline 403 of groups of five male and five female rats exposed to an aerosol containing 0, 5.79, 8.33, 9.11, or 10% PCOC in 50% alcohol for 4 hours.

The IUCLID datasheet (2000) presented various acute oral toxicity tests for rats and mice. Details of the test conditions are not provided. The acute oral LD_{50}s range from 1194 – 2700 mg/kg bw. Two acute inhalation studies are referenced, one with a LD_{50} of >30 mg/l based on a four hour exposure time, and the second test involving a seven hour test. However, no LD_{50} is provided for the second test. One acute rat dermal toxicity study is referenced which resulted in a LD_{50} of >5000mg/kg bw.

Irritation and sensitisation

A guinea pig maximisation test[2] involving 40 female albino guinea pigs carried out according to OECD guidelines PCOC caused no sensitisation. A provocation test[3] with 30% solution of

[2] The guinea pig maximisation test involved the application of test material to the skin of tests subjects, using an initial 'sensitising dose' (often intra-dermal or on broken skin), followed by other topical applications, known as the 'challenge dose' to determine the extent of reactions that occur as a response to the preliminary sensitising dose.

PCOC caused erythema. However, a further provocation test with 10% and 20% of PCOC applied on the left and right flank, respectively, was carried out a week later resulting in no clear differences between the control group and the test group (ECB, 2002). This is supported by the IUCLID datasheet (2000) which reports guinea pig tests to have negative sensitisation results and by OECD (2005) which reports that PCOC is "not a skin sensitizer".

The risk assessment final report (ECB, 2002) mentions another negative sensitisation study but concludes that the study does not seem to have been reported properly.

The IUCLID datasheet reports skin irritation tests on rabbits with positive results (corrosive and highly corrosive). Eye irritation tests on rabbits were also positive (irritating) and it is noted the EC classification is considered to be "risk of serious damage to eyes" (IUCLID, 2000).

Subacute Toxicity (short term repeat dose studies)

In 28-day repeat dose studies in rats, ECJRC state "the best no observed adverse effect limit (NOAEL) appears to be 200 mg/kg, with a lowest observed adverse effect limit (LOAEL) of 800 mg/kg where salivation after dosing and ruffled fur was seen in some animals" (ECJRC, 2002). Within this study groups of five male and five female rats were given 0, 50, 200, or 800 mg PCOC/kg bw by gavage for 28 days. No histopathological changes were seen in any organ at 800 mg/kg bw. The changes of liver enzymes (serum alanine aminotransferase) and liver weights in the 800 mg/kg bw group indicated mild toxicity to the liver. It was concluded in the test report that 800 mg/kg bw is a LOAEL, and that 200 mg/kg bw is a NOAEL (ECB, 2002).

OECD state "repeat dose toxicity is not likely to present a major health problem" and base margins of safety of 285 and 20,000 on a NOAEL of 200mg/kg bw/day for workers and consumers respectively (OECD, 2005). They do not explicitly derive a health criteria value.

Chronic dose studies

No chronic exposure data have been identified in readily available open literature sources for 2,4-dichloro-o-cresol or PCOC.

Reproductive Toxicity

The summary risk assessment report by the ECJRC (2002) states "There were no effects on reproduction according to OECD screening test 422 at doses of up to 600 mg/kg bw for a total of 40 days".

The final risk assessment report (ECB, 2002) provides further details on this study. Groups of 10 male and 10 female rats were given 0, 50, 200, or 600 mg PCOC/kg bw delivered in soybean oil by gavage for two weeks prior to mating and until day 20 of gestation. No toxic effects on any reproductive or developmental parameters were observed, resulting in a no effect level for these endpoints of 600 mg/kg bw.

Genotoxicity

Two studies (one in vitro study and one in vivo study) presented within the summary risk assessment report (ECJRB, 2002) were positive for mutagenicity. However, a repeat dose study, carried out and also repeated using current guidelines, produced unequivocally negative results and negative results respectively. The summary risk assessment report (ECJRB, 2002) therefore concluded there is not enough evidence that PCOC is a mutagen.

OECD concludes that PCOC does not appear to be genotoxic in valid Ames tests and therefore, based on current knowledge, PCOC is not considered to be a mutagen (OECD, 2005).

Carcinogenicity

[3] Use of a test substance to provoke a response, based on comparison with a control group.

No human or animal studies are available for PCOC. The IARC (1987) concluded that chlorophenoxy herbicides should be placed in group 2B (Possibly carcinogenic to humans) because of limited evidence for carcinogenicity to humans and because no adequate published data were available on the carcinogenicity of MCPA to animals. However, while PCOC is a breakdown product and possible contaminant of (impurity in) MCPA, the ECB state that the implications of these findings for the effects of PCOC itself can remain only speculative. (ECB, 2002).

Background exposures

There are no readily available data on the potential exposures to 2,4-dichloro-o-cresol or the surrogate compound PCOC. Further evaluation of background exposures is included in the MDI sections outlined below.

Regulatory guidelines/ advisories/ guideline values

The HSDB (2003) state the US Clean Water Act Requirements recommended a criterion level of 1,800 ug/l for PCOC.

The summary risk assessment by the ECJRC (2002) concluded that the results of acute studies do "not give rise to immediate concern, particularly considering that the substance (crystalline needles) is unlikely to form aerosols or dusts, and that personal protective equipment (PPE) is mandated during handling of the substance". They also report that for the population with the highest potential exposure (production workers assuming inhalation exposure at 5 mg/m^3 for eight hours) a margin of safety of 285 between the repeat dose NOAEL of 200 mg/kg bw/day and the predicted exposure of 0.7 mg/kg bw/day is obtained. Consumers may be exposed to 0.07 mg/kg/day once, or a few times yearly. All other exposure scenarios result in much higher margins of safety (ECJRC, 2002).

The final risk assessment report (ECB, 2002) states that no occupational exposure limits for PCOC have been found. PCOC is related to cresols and chlorophenols which have the following occupational exposure limits

- cresols: (8-hour threshold limit value (TLV) of 22 mg/m^3 set by the UK and DK authorities (all isomers); and
- chlorophenols (all isomers): the TLV is 0.5 mg/m^3 in e.g. Denmark (ECB, 2002).

Selection of Health Criteria Value

Oral Health Criteria Value

The NOAEL of 200 mg/kg bw/day for a 28 day sub-acute study in rats adopted by ECJRC for the surrogate compound PCOC has been taken forward for use a point of departure (POD) for derivation of an HCV for 2,4-dichloro–o-cresol.

Safety Factors applied:

5000 - 10 for inter-species differences;
- 10 for intra-species differences,
- 5 for extrapolation from short-term studies (based on the use of a well-run subacute study with a clearly defined no-effect level); and
- 10 for limitations in the database (a lack of data for the original compound as well as limited data for the surrogate chemical selected, particularly the lack of conclusive data on carcinogenicity).

Further safety factors are deemed unnecessary as the toxicity data for similar compounds indicates that the compound is unlikely to result in severe, irreversible adverse health effects such as genotoxicity.

TDI_{oral} = 200 mg/kg bw/day/5000
= **0.04 mg/kg bw/day**
= 40 µg/kg bw/day

MDI_{oral}

Food

There are no readily available data on the potential dietary exposures to 2,4-dichloro-o-cresol or the surrogate compound PCOC. As this product is intermediate to a known pesticide and produced under controlled conditions (OECD, 2005), although it could be present as an impurity, it is unlikely that it would be present in the food chain in large quantities. Therefore, background exposure via the diet is conservatively assumed to be 5% of the TDI, which is 0.002 mg/kg bw/day.

Drinking water
The UK Water Quality (Water Supply) Regulations state that all other pesticides (with the exception of aldrin, dieldrin, heptachlor and heptachlor epoxide) should not exceed 0.1 µg/L in drinking water supplied to the consumer. Assuming an adult intake of 2L per day, this is equal to a maximum conservative intake of 0.2 µg of 2,4-dichloro-o-cresol per day, assuming that all 'other' pesticide is made up of 2,4-dichloro-o-cresol, for an adult consumer. This is equivalent to a dose of 0.00286 µg/kg bw/day (0.00000286 mg/kg bw/day).

The total MDI_{oral} for an adult receptor is therefore:
Dietary + drinking water intake = (0.002 +0.00000286) mg/kg bw/day
= 0.00200286 mg/kg bw/day
= 2.00286 µg/kg bw/day (140.2 µg/day)

Therefore, the Tolerable Daily Soil Intake $(TDSI)_{oral}$ for an adult receptor is:
TDI – MDI = (0.04 – 0.00200286) mg/kg bw/day
= 0.037997 mg/kg bw/day
= 37.997 µg/kg bw/day

Inhalation Health Criteria Value (HCV)
In the absence of data for long-term inhalation exposures, the data available for oral exposures will be extrapolated for use as a preliminary indicative health criteria value.

Therefore, the $TDI_{inhalation}$ is 0.04 mg/kg bw/day (40µg/kg bw/day). Assuming a 70kg adult inhales 20m³ air per day, this is equivalent to an $TDI_{inhalation}$ of 0.14 mg/m³ per day.

$MDI_{inhalation}$
There are no readily available data on ambient air concentrations of 2,4-dichloro-o-cresol or the surrogate compound PCOC. However, as PCOC is an intermediate of a pesticide still approved for use in the UK (mecoprop) and contains 2,4-dichloro-o-cresol as an impurity and which is listed as being 2.0% (w/w) of PCOC (ECJRC, 2002), it has been assumed that it may be present in the environment. Background exposure is conservatively assumed to be 20% of the HCV, as this product would not be removed from the ambient environment in a manner assumed for oral exposure sources. Specifically, it would not be removed from ambient air, as it would be prior to distribution in drinking water or washed from food sources. This is equal to a value of 0.56 mg/day (560 µg/day).

This value is considered to be conservative due to the relatively minor composition of 2,4-dichlorocresol in PCOC, which is itself a chemical intermediate used in pesticide manufacture. Therefore, the Tolerable Daily Soil Intake $(TDSI)_{inhalation}$ is 0.032 mg/kg bw/day (0.112 mg/m³ per day), which is equivalent to 32 µg/kg bw/day.

In the absence of other inhalation data, this HCV compares favourably with the occupational exposure values reported by the EC for cresols, being less than three orders of magnitude below the occupational exposure limit reported for cresols. It is also approximately four times less than the occupational exposure limit for chlorophenols.

References

ECJRC, European Commission Joint Research Centre, 2002. 4-CHLORO-O-CRESOL Summary Risk Assessment Report. **http://ecb.jrc.ec.europa.eu/documents/Existing-Chemicals/RISK_ASSESSMENT/SUMMARY/pcocsum023.pdf** Accessed 22nd June 2010.

European Chemicals Bureau (ECB), 2002. European Union Risk Assessment Report 1st Priority List. 4-chloro-o-cresol. **http://ecb.jrc.ec.europa.eu/esis/** Accessed 22nd June 2010.

OECD, 2005. 4-chloro-2-methylphenol **http://www.inchem.org/documents/sids/sids/1570645.pdf** Accessed 22nd June 2010.

IUCLID datasheet, 2000. 4-chloro-o-cresol. **http://ecb.jrc.ec.europa.eu/esis/** Accessed 22nd June 2010.

HSDB, last revision date 15/10/2003. **http://toxnet.nlm.nih.gov/cgi-bin/sis/search** Accessed 22nd June 2010.

Hattula ML, Reunanen H, Arstila AU (1979). Toxicity of 4-Chloro-*o*-Cresol to Rat: I. Light Microscopy and Chemical Observations. Bull Environ Contam Toxicol, **21**, 492-497.

Scantox (1982a). Report No. 10150, 24th November 1982. Scantox, Ejby, Denmark.

Scantox (1982b). Report no. 10152, 26th November 1982. Scantox, Ejby, Denmark.

Scantox (1983). Report No. 10153, February 28th 1983. Scantox, Ejby, Denmark.

Schrötter E, Tschäpe M, Meister A (1977). Organische synthetica und ihre vermiziden Eigenschaften. 5. Mitteilung. Ovozide Phenolderivate. Pharmazie. 32: 171-174.

TOXICOLOGICAL DATA TEMPLATE

Chemical name: __2-6-bis(1,1,-dimethylethyl)-4-(1-methylpropyl)-phenol_____

Common name: __DTBSBP_____

CAS RN: __17540-75-9_____

2-6-bis(1,1,-dimethylethyl)-4-(1-methylpropyl)-phenol is herein referred to as DTBSBP.

Chemical Identification

Health Canada and US EPA are the predominant sources of information regarding DTBSBP. Synonyms of DTBSBP include 2,6-Di-tert-butyl-4-sec-butylphenol and systematic names include "4-sec-Butyl-2,6-di-tert-butylphenol" and "Phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-" (Toxnet ChemID, 2010).

Uses and Occurence

DTBSBP is manufactured for use as an antioxidant and liquid stabiliser in plastics such as polyvinyl chloride (PVC) and polyurethane, as well as in brake fluids, ink resins and mineral/vegetable oils used in industrial applications. It is also used as an antioxidant in the petrochemical sector. Health Canada reports that inhalation of DTBSBP from consumer products is the main estimated route of exposure for the general population. (Health Canada, 2010).

Environmental Fate

Health Canada report DTBSBP to be a liquid under ambient conditions and, based on its physical and chemical properties, modelling suggests that it is expected to predominantly reside in air if released to air, in water and sediment if released to water, and in soil if released to soil (Health Canada, 2010).

It is not expected to degrade quickly in the environment and is persistent in water, soil and sediments (Health Canada, 2010). It is not persistent in air as it oxides rapidly (Health Canada, 2010). It also has the potential to accumulate in organisms and may biomagnify in food chains (Health Canada, 2010).

Acute Toxicity

Health Canada reports a low acute toxicity for DTBSBP with a LD_{50} of 4800 mg/kg bw (Health Canada, 2010).

In a 2002 report prepared for the US EPA, SII describes this study in more detail (SII, 2002). The study involved Sprague-Dawley CD rats (5 female and 5 male) and reported clear evidence of toxicity at all dose levels (3.4, 4.7, 6.6 and 9.3 g/kg bodyweight (bw)), resulting in a LD_{50}, with 95% confidence limits, of 4.8 (2.7-8.1) g/kg (4800 mg/kg bw/day (US EPA, September 2009)). Clinical signs of toxicity included decreased motor activity, diarrhoea, piloerection (involuntary lifting of hairs or 'goosebumps'), co-ordination loss, lethargy and irritation to the intestines.

Effects were reported at all dose levels:

- in the test group dosed at 3.4 g/kg bw macroscopic examination at the study termination revealed bright red lungs, dark red mottled liver, intestinal irritation, nasal and ocular haemorrhage (bleeding) and diarrhoea in males and wet ventral (front) surface in one female;
- in addition to these effects, in the test group dosed at 4.7 g/kg bw, slight hair loss was noted from ventral surface in one male and one female; and
- in the test group dosed at 6.6 g/kg bw and 9.3 g/kg bw necropsy examination revealed diarrhoea, lacrimation (tearing of eyes), wet ventral surface, stomach and intestinal irritation, hair loss from posterior ventral surface, bright red mottled lungs, small dark spots on thymus, and nasal and ocular haemorrhage in both males and females (SII, 2002).

The US EPA reports an acute dermal toxicity LD_{50} of >1000 mg/kg bw/day using the Screening Information Data Set (SIDS)(US EPA, September 2009), reporting a lack of data for the primary compound DTBSBP. The presented value value is based on the dermal LD_{50} of > 1000 mg/kg bw/day reported for the analogue 2,6-di-tert-butylphenol (CAS No. 128-39-2) (Health Canada, 2010).

Subacute Toxicity (short term repeat dose studies)

Health Canada examined data on several analogous substances to inform the understanding of the potential health effects associated with exposures to DTBSBP (Health Canada, 2010).

Health Canada reported one short term toxicity study using analogue 2,4,6-tris(1,1-dimethylethyl)-phenol (TTBP) (CAS No.: 732-26-3) carried out over 11 days using male beagle dogs. The dogs were fed 0, 49.2, 173 or 454 mg/kg bw/day of TTBP for 11 days. At exposure to doses of 454 mg/kg-bw/day (the highest dose tested), the dogs showed signs of behavioural abnormalities and increased liver enzyme function markers (glutamic-oxalacetic transaminase (GOT), glutamic-pyruvic transaminase (GPT) and alkaline phosphatase (ALP)) (Health Canada, 2010).

The lowest-observed-effect level (LOEL) of 173 mg/kg-bw/day was established based on the occurrence of diarrhoea and blood in the faeces which was observed at both 454 mg/kg bw/day and 173 mg/kg-bw/day doses (Health Canada, 2010).

Subchronic Toxicity (longer-term studies)

The US EPA reports a NOAEL of ~5 mg/kg bw/day and a LOAEL of ~15 mg/kg bw/day, for repeated dose toxicity based on read across (RA)[1] from other compounds as included in the SIDS (US EPA, September 2009).

Health Canada describes a 28-day gavage study of Wistar rats, originally reported by the US EPA above (US EPA, 2009). Rats were fed 0, 15, 100 or 600 mg/kg bw/day of a substitute, analogue 2,6-Di-tert-butylphenol (CAS 128-39-2). They report that no effects were observed at 100 mg/kg bw/day. However, at 600 mg/kg bw/day, increased liver weight and corresponding histopathology was observed in males and females (Health Canada, 2010).

Chronic Toxicity (long-term toxicity data)

Health Canada reported that chronic toxicity data for analogue TTBP (CAS 732-26-3), showed no statistically significant increased incidence of tumours compared to controls. The study comprised a 24 month feeding study in male and female rats exposed to 0, 30, 100, 300 or 1000 ppm of TTBP. No indicators of tumour formation were observed at 30 ppm (converted to 1.5 mg/kg bw/day). Increased liver weights and increased platelet count, phospholipids and total cholesterol were noted at 100 ppm and higher (Health Canada, 2010). The value of 30 ppm is adopted as the no observed effect level (NOEL) (Health Canada, 2010)

There are no data available on exposure to DTBSPB or similar compounds following chronic exposure via inhalation.

Developmental and Reproductive Toxicity

One combined developmental and reproductive study was found which was originally published by the US EPA (US EPA, September 2009) and noted by Health Canada (Health Canada, 2010). In a combined reproductive and developmental toxicity screening test, Wistar rats were administered 0, 30, 150 or 750 mg/kg bw/day of analogue 2,6-Di-tert-butylphenol (CAS 128-39-2) by gavage throughout the pre-mating and mating period. No reproductive effects were observed at any of the tested doses. At 150 mg/kg bw/day no adult systemic or developmental toxicity was observed. At 750 mg/kg bw/day, there were marginal effects on body weight in adults and reduced viability and weight gain in the pups. (US EPA, September 2009; Health Canada, 2010).

[1] Read across refers to data adopted from other compounds that are expected to have similar properties to the primary compound of concern.

The US EPA reports a NOAEL of 150mg/kg bw/day and a LOAEL of 750 mg/kg bw/day (RA) for developmental toxicity and a NOAEL of 750 mg/kg bw/day for reproductive toxicity using the SIDS as submitted under the U.S. Challenge Program: Summary of Human Health Data for Alkylphenols Category (US EPA, September 2009).

Genotoxicity

Both the US EPA and Health Canada report negative results from genotoxicity and mutagenicity studies.

Health Canada cited two genotoxicity studies reported by SII (SII, 2002). In the first study, DTBSBP was negative in in vitro mutagenicity assays in *Escherichia coli* (E. coli) strain WP_2 uvrA or *Salmonella typhimurium* (Salmonella) strains TA98, TA100, TA1535, TA1537 and TA1538, with or without metabolic activation with concentrations of up to 5000 µg/plate of test substance. In the second study, DTBSBP was negative for chromosomal aberrations in Chinese hamster ovary (CHO) cells with or without metabolic activation (Health Canada, 2010; SII, 2002). These studies led to the conclusion that DTBSBP is not genetically active in the Salmonella and E. coli assay, and it is considered negative for inducing chromosomal aberrations in CHO cells with and without metabolic activation.

Carcinogenicity

No carcinogenicity information was found for DTBSBP.

However, data has been identified for two substances that are considered by the respective reviewing bodies (as referenced below) to be analogous to it.

In a 24-month study where male and female Wistar rats (40 of each sex per dose concentration) were administered analogue TTBP (CAS No. 732-26-3) in the diet at 0, 30, 100, 300 and 1000 ppm (approximately 0, 1.5, 5, 15 and 50 mg/kg-bw/day) for 24 months, it was reported that there was no evidence of cancer in the treated animals (US EPA, 2009).

Health Canada also reported that another identified analogue BHT (CAS No. 128-37-0) has been assigned a threshold of 100 mg/kg-bw/day for possible carcinogenic and tumour-promoting effects (Health Canada, 2010; OECD, 2002).

Background exposure (food, drinking water, air)

Health Canada reports that no studies were identified reporting the presence of DTBSBP in food. However, DTBSBP has been approved by the U.S. Food and Drug Administration for use as an antioxidant in plasticised PVC for food packaging (US FDA 2008). Plasticised PVC may be used in films for wrapping fresh and frozen meat and produce (Health Canada, 2010).

A conservative upper-bound probable daily intake (PDI) of 0.0581 µg/kg bw/day was estimated for DTBSBP assuming that some plasticised PVC films may be used for wrapping meat (2009 email from Food Directorate, Health Canada, to Risk Management Bureau, Health Canada; unreferenced (Health Canada 2010)).
Mouthing of foam objects is also considered to be a potential source of exposure to infants and toddlers via the potential for mouthing of foam objects, packaging and furniture. Health Canada has undertaken a numerical evaluation of exposures. This is based on conservative assumptions and derived from experimental data on the structurally similar and more volatile antioxidant, butylated hydroxyl toluene (BHT). However, they state that it is '*uncertain whether DTBSBP is contained in common foam objects mouthed by toddlers and infants*' and '*confidence in the numerical results of the exposure estimations is low*'. Therefore, in combination with the fact that Atkins considers that it is less likely to occur based on parental supervision, it has not included this within the mean exposure assessment of intakes for children in this review.

There are no readily available data on occurrence of DTBSBP in drinking water. Health Canada state that laboratory testing indicates that DTBSBP is not extractable from rigid PVC (Health Canada, 2010), and exposure to this substance via rigid PVC associated applications is expected to be negligible.

Health Canada cite an investigation by Hillier et al. (2003) into volatile emissions from foam mattresses which found BHT emissions from one of five fresh foam mattress samples. DTBSBP was not identified in this study. As a conservative approach, they state that since DTBSBP is a less volatile substiuent than BHT, the extrapolated concentration of BHT is taken as the upper limit of DTBSBP atmospheric concentration from foam mattress emissions. Health Canada has therefore undertaken the following numerical evaluation of exposures:

- Considering an upper-bound-scenario whereby the maximum potential atmospheric concentration of DTBSBP (2.02 µg/m³) persists continually, the maximum potential inhalation chronic dose was calculated to be 0.178 µg/kg-bw per day for the 0.5–4 years age group. Potential volatile emissions from foam-filled furniture were also estimated and resulted in a mean event concentration of 2.69 µg DTBSBP/m^3 and a maximum potential inhalation chronic dose of 0.872 µg DTBSBP/kg-bw per day (0.5–4 years age group) as an upper-bounding scenario (Health Canada, 2010). They also state that '*since the volatility of DTBSBP is lower than that of BHT, studies that investigated the volatilization loss of BHT from foam mattresses and auto interior trim were considered in this assessment to screen the upper level of potential inhalation exposure to DTBSBP*'.

Regulatory guidelines/ advisories/ guideline values

Health Canada reports that inhalation of DTBSBP from consumer products is the main estimated route of exposure for the general population. However, health effects data available for DBSBP and its analogues were conducted via the oral route and there are no data on effects via inhalation exposures over a chronic exposure period. Therefore, risk characterisation for the inhalation route of exposure is based on a comparison with oral toxicity data, and the daily intake via inhalation was estimated from predicted air concentrations, rather than measured data for DTBSBP(Health Canada 2010).

The outputs of predictive models were also considered (comprising Derek, TopKat, CaseTox and Leadscope Model Applier). The predictions for carcinogenicity, genotoxicity, and developmental and reproductive toxicity were predominantly negative (Health Canada, 2010).

Comparison of the chronic no-observed-effects level (NOEL) of 30 ppm (1.5 mg/kg bw per day) for the analogue compound TTBP (CAS RN 732-26-3) via oral exposure with the upper-bounding estimate of daily intake of DTBSBP by toddlers through inhalation exposure of volatile emissions from foam-filled furniture (8.72×10^{-4} mg/kg-bw per day) results in a margin of exposure of approximately 1720.

A similar comparison of effects of the potential migration of DTBSBP from meat and produce plastic packaging yields a margin of exposure of approximately 25 800. This is based on the comparison of the chronic NOEL of 30 ppm) (1.5 mg/kg-bw per day) for the TTBP analogue (CAS RN 732-26-3) with the estimated probable daily intake (PDI) which is stated to be 0.0581 µg/kg bw.

Based on the information available, it is considered that the estimated margins of exposure are considered adequate to protect human health (Health Canada, 2010). It can be noted that due to the limited data available for DTBSBP, Health Canada considers the confidence in the toxicological dataset to be low (Health Canada, 2010).

Selection of Health Criteria Value

Oral Health Criteria Value

The NOEL of 1.5 mg/kg bw/day adopted by Health Canada for the surrogate compound TTBP has been taken forward for use a point of departure (POD) for *de novo* derivation of a health criteria value (HCV).

Safety Factors applied:
1000 - 10 for inter-species differences,

- 10 for intra-species differences; and
- 10 for limitations in the database. It is considered that a factor of 10 is more suitable than a factor of 5 (often adopted for data limitations) in order to account for a lack of chemical –specific data, as well as for limited data for the surrogate chemical selected.

TDI_{oral} = 1.5 mg/kg bw/day/1000
= **0.0015 mg/kg bw/day**
= **1.5 µg/kg bw/day**

MDI_{oral}
Food
A conservative upper-bound PDI of 0.0581 µg/kg bw/day (0.0000581 mg/kg bw/day) was estimated for DTBSBP based on intake from plasticised PVC films used for wrapping meat. This conservative estimate is deemed a suitable measure of mean daily intake (MDI) from all dietary sources.

Drinking water
Although there is no information on detected levels of DTBSBP in drinking waters, Atkins considers that it is likely to be present in plastic drinking water pipes, which would be in contact with drinking water for extended periods of time, However, Health Canada state that DTBSBP is unlikely to be released from rigid PVC, such as drinking water pipes and such exposure is expected to be negligible. Therefore, exposure to DTSBP via drinking water is assumed to be negligible.

The total oral MDI for an adult receptor is therefore:
(Dietary + drinking water intake) = (0.0000581 + 0) mg/kg bw/day
= 0.0000581 mg/kg bw/day
= 0.0581 µg/kg bw/day
= 4.07 µg/day

.

Therefore, the Tolerable Daily Soil Intake $(TDSI)_{oral}$ for an adult receptor is:
TDI – MDI = (0.0015 – 0.0000581) mg/kg bw/day
= 0.00144 mg/kg bw/day
= 1.44 µg/kg bw/day

Inhalation HCV
In the absence of data for long-term inhalation exposures, the data available for oral exposures will be extrapolated for use as a preliminary indicative health criteria value. This approach was also adopted by Health Canada in their risk evaluation for DTBSBP.

Therefore, the $TDI_{inhalation}$ is 0.0015 mg/kg bw/day (1.5 µg/kg bw/day). Assuming a 70kg adult inhales 20m³ air per day, this is equivalent to an $TDI_{inhalation}$ of 0.00525 mg/m³ per day.

$MDI_{inhalation}$
As a conservative measure, the sum of likely atmospheric concentrations of DTBSBP resulting from foam mattresses and foam filled furniture has been adopted as the basis for the derivation of the MDI for inhalation.

The maximum potential atmospheric concentration of DTBSBP from foam filled mattresses is 2.02 µg/m³. This is equivalent to a daily dose of 40.04 µg/day for a 70kg adult who inhales 20m³ air per day. The maximum potential atmospheric concentration of DTBSBP from foam filled furniture is 2.69 µg DTBSBP/m^3. This is equivalent to a daily dose of 53.8 µg/day, for a 70kg adult who inhales 20m³ air per day. Daily exposure is therefore estimated to total 93.8 µg/day.

This is equivalent to an MDI of 1.34 µg/kg bw/day (0.00134 mg/kg bw/day) for a 70 kg adult. This is greater than 50% of the TDI, and therefore the TDSI is set at 50% of the TDI, based on guidance available in SR2.

Therefore, the Tolerable Daily Soil Intake (TDSI)$_{inhalation}$ for an adult receptor is
50% of the TDI = (0.0015 x 0.5) mg/kg bw/day
= 0.00075 mg/kg bw/day (0.75 µg/kg bw/day)
= 0.002625 mg/m³

References

Health Canada. 1994. Human health risk assessment for priority substances: Appendix E Reference values for intakes and body weights of laboratory animals.[Internet]. Ottawa (ON): Health Canada, Environmental Health Directorate, Environmental Substances Division. [cited 2009 October 8]. 35 p. Available from: http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/approach/index-eng.php

Health Canada, 2010. Heatlh Canada Draft Screening Assessment for the Challenge. Phenol, 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)- DTSBP. Chemical Abstracts Service Registry Number 17540-75-9. Environment Canada. Health Canada. January 2010. Available from: http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm Accessed 18th June 2010

Hillier K, Schupp T, Carney I. 2003. An investigation into VOC emissions from polyurethane flexible foam mattresses. Cell Polym 22(4):237–259.

Matsumoto K, Ochiai T, Sekita K, Uchida O, Furuya T, Kurukawa Y. 1991 Chronic toxicity of 2, 4, 6-Tri-tert-butylphenol in rats. Journal of Toxicological Sciences 16: 167-179. [cited in US EPA 2009]. Available from: http://iaspub.epa.gov/oppthpv/Public_Search.PublicTabs?SECTION=1&epcount=2&v_rs_list=25034978,25034972

[OECD] Organisation for Economic Co-operation and Development. 2002. The Screening Information Data Set (SIDS) initial assessment report for SIAM 14 [Internet]. Paris (FR): OECD, Environment Directorate. [cited 2009 October 27]. Available from: http://www.chem.unep.ch/irptc/sids/OECDSIDS/128370.pdf Accessed 23rd June 2010.

[SII] Schenectady International, Inc. (now called SI Group). 2002. Alkylphenols Category. Section Two, Ortho-substituted Mono-alkylphenols, Chemical Right to Know Initiative, HPV Challenge Program. Report submitted to US Environmental Protection Agency, Office of Pollution Prevention and Toxics, HPV Challenge Program, Washington, D.C. Received 3 Apr. 2002. 565 pp. Available from: http://www.epa.gov/oppt/chemrtk/pubs/summaries/alkylphn/c13007rr.pdf

TOXNET ChemID http://toxnet.nlm.nih.gov/ Accessed 18th June 2010.

[US EPA] United States Environmental Protection Agency, September 2009. US EPA Hazard Characterization Document Screening-Level Hazard Characterization. Alkylphenols Category. http://www.epa.gov/hpvis/hazchar/Category_Alkylphenols_Sept2009.pdf Accessed 18th June 2010.

[US FDA] United States Food and Drug Administration. 2008. Inventory of Effective Food Contact Substance (FCS) Notifications: FCN No. 80. [Internet]. Washington (DC): US Food and Drug Administration, Center for Food Safety and Applied Nutrition, Office of Food Additive Safety. [cited 2008 April]. Available from: http://www.cfsan.fda.gov/~dms/opa-fcn.html USEPA, XXXX. Alkylphenols Category SECTION TWO Ortho-substituted Mono-alkylphenols. Chemical Right-to-Know Initiative. HPV Challenge Program. USEPA. http://www.epa.gov/HPV/pubs/summaries/alkylphn/c13007rr.pdf Accessed 18th June 2010.

Annex 2: Physical and Chemical Data

- **Prochloraz**
- **2,4-dichloro-o-cresol**
- **DTBSBP**
- **Calculations**

Prochloraz

http://srdata.nist.gov/solubility/

http://webbook.nist.gov/chemis http://cs3-hq.oecd.org/scripts/hpv/

	A		B	C	D		E	F	G	H	OTHER SOURCES
	HOWARD, 1990	IUPAC-NIST, 2006	LIDE, 2008	MACKAY et al, 2006	MERCK, 2006		MONTGOMERY, 2007	MONTGOMERY, 1997	NIST, 2005	OECD, 2000	
					Untis	Temp					
Relative Molecular Mass					376.67				376.6647	376.7 (ecb)	376.67 REF??? ONE OF Pete's sources, seeother spreadsheet
Henry's Law Constant (HLC)											
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)					5.5 mg/l					34.4mg/l at 25 oC (ecb)	
Chemical Boiling Point (ambient pressure)										208-210 oC (ecb)	263.4 (http://www.lookchem.com/cas-207/2077-46-5.html)
Chemical Melting Point (ambient pressure)										46.5-49.3 oC (ecb)	
Log Octanol - Water Coefficient (Kow)										log Pow = 4.12 at 25 oC (ecb)	
Molar Volume (Le Bas method)											
Enthalpy of Vaporisation at normal boiling point (EVNBP)											
Chemical Critical Point temperature (ambient pressure)											
Critical Pressure											
Diffusion Coefficient in Air											
Diffusion Coefficient in Water											
Log (organic carbon-water partition coefficient)(Koc)											
Vapour Pressure					$0.57x10^{-9}$ atorr	20degress				0.015 hpa at 25 degrees (ecb)	
Air-water partition coefficient (Kaw)											
Toxicity (fish)					1 mg/l (96 hour)					LC50 = 2.9mg/l over 96 hour exposure. LC50 = 1.5mg/l over 168 hour exposure (flow through). LC50 = 1.2mg/l (NOEC = 0.54) over 96 hour exposure period. LC50 = 2.2mg/l (NOEC = 0.78) over 96hour period (static) (ecb)	LD 0.008-0.042mg/l over 7 days (http://www.pesticideinfo.org/List_AquireAll.jsp?Rec_Id=PC36352)
Toxicity (invertebrate)										NOEC = 2.6mg/l for 48hr exposure, 0.31mg/l for 96 hr exposure (ecb)	
Toxicity (aquatic plant)										NOEC = 10ug/l for 14day exposure, and 0.05mg/l for 120 hour exposure (ecb)	LD 0.0241mg/l over 24 hours (http://www.pesticideinfo.org/List_AquireAll.jsp?Rec_Id=PC36352)
Half-life aerobic										Abiotic - 525 days at pH7, 639 days at pH 6 (at 30 oC), >30days at pH7, 78.9 days at pH 9 (at 22 oC). Biotic - 349 days at pH 7.8 (20 oC), 288 days at pH9 (20 oC).	
Half-life anaerobic											
Breakdown products											

2,4-Dichloro-o-cresol

http://srdata.nist.gov/solubility/

http://webbook.nist.gov/chemis http://cs3-hq.oecd.org/scripts/hpv/

	A	B	C	D	E	F	G	H	OTHER SOURCES
	HOWARD, 1990	IUPAC-NIST, 2006	LIDE, 2008	MACKAY et al, 2006	MERCK, 2006	MONTGOMERY, 2007	MONTGOMERY, 1997	NIST, 2005	OECD, 2000	
Relative Molecular Mass			177.028							
Henry's Law Constant (HLC)										
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)		$1.6x10^{3}$ mol dm^{-3}								
Chemical Boiling Point (ambient pressure)										225 REF???? FROM ONE OF THE SOURCES ON PETE'S SPREADSHEET
Chemical Melting Point (ambient pressure)			55 oC							
Log Octanol - Water Coefficient (Kow)										
Molar Volume (Le Bas method)										
Enthalpy of Vaporisation at normal boiling point (EVNBP)										
Chemical Critical Point temperature (ambient pressure)										
Critical Pressure										
Diffusion Coefficient in Air										
Diffusion Coefficient in Water										
Log (organic carbon-water partition coefficient)(Koc)										
Vapour Pressure										
Air-water partition coefficient (Kaw)										
Toxicity (fish)									LOEC 0.36mg/l (not timescale provided) (EnviChem	
Toxicity (invertebrate)									LC50 0.43mg/l (over 48hr exposure) (EnviChem)	
Toxicity (aquatic plant)										
Half-life aerobic										
Half-life anaerobic										
Breakdown products										

2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol																					http://srdata.nist.gov/solubility/						
																					http://webbook.nist.gov/chemis			http://cs3-hq.oecd.org/scripts/hpv/			
	A						B			C			D			E			F			G			H			OTHER SOURCES		
	HOWARD, 1990			IUPAC-NIST, 2006			LIDE, 2008			MACKAY et al, 2006			MERCK, 2006			MONTGOMERY, 2007			MONTGOMERY, 1997			NIST, 2005			OECD, 2000					
Relative Molecular Mass																										262.43		
Henry's Law Constant (HLC)																										3.66x10-4 atm-cu m/mol (http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm)		
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)																								0.2479mg/l at 25 oC (epa)			2.47mg/l (http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm)		
Chemical Boiling Point (ambient pressure)																								275-330 oC (epa)			141-142, **275** (http://www.chemicalbook.com/ChemicalProductProperty_EN_CB6442327.htm), **http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm**		
Chemical Melting Point (ambient pressure)																								47-102 oC (epa)					
Log Octanol - Water Coefficient (Kow)																								Log Kow = 6.43 (epa)					
Molar Volume (Le Bas method)																													
Enthalpy of Vaporisation at normal boiling point (EVNBP)																													
Chemical Critical Point temperature (ambient pressure)																													
Critical Pressure																													
Diffusion Coefficient in Air																													
Diffusion Coefficient in Water																													
Log (organic carbon-water partition coefficient)(Koc)																										log koc 4.47[2] (http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm)		
Vapour Pressure																								0.0028 at 25 oC (epa)					
Air-water partition coefficient (Kaw)																													
Toxicity (fish)																								LC50 = 0.072mg/l over 96 hr exposure, LC50 = 0.22 over 48 hrs (epa)			LD 0.039-0.15mg/l over 96 hours and 0.007mg/l over 60days (http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm)		
Toxicity (invertebrate)																													
Toxicity (aquatic plant)																								EC50 = 0.016mg/l over 96 hrs exposure (epa)			LD 0.20mg/l over 96 hours and 0.09mg/l over 60days (http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm)		
Half-life aerobic																										2 days (http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm)		

Half-life anaerobic																												182 days (http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm)		
Breakdown products																															

Chemical Name	RANGE FOUND					value selected
Prochloraz	**Units**	**Source**	**cm3/cm3**	**Temp**		**Decision**
3.10E-10	dimensionl	henrywin	3.10E-10			
1.64E-08	atm/m3/mc	EPI	6.72E-07			Two values similar
1.64E-03	pa/m3/mol	Pesticide Handbook	6.64E-07			

2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol	**Units**	**Source**	**cm3/cm3**	**Temp**		**Decision**
0.000417	dimensionl	EPI	4.17E-04			
0.000366	atm·m3/mc	http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm (HENRYWIN)	1.50E-02			Most appropriate, similar to compounds with similar structure.
3.71	Pa.m3/mol	http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm (HENRYWIN)	1.50E-03	25		

2-4-Dichloro-o-cresol	**Units**	**Source**	**cm3/cm3**	**Temp**		**Decision**
2.09E-05	dimensionl	henrywin				only value and one of those methods recommended in SR7

	Units	**Source**	**cm3/cm3**	**Temp**		**Decision**

CoC	Mass
Prochloraz	376.67
2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol	262.44
2,4-Dichloro-o-cresol	177.03

Chemical Name	RANGE FOUND						value selected
Prochloraz	**Units**	**Source**	**mg/l**	**Temp**		**Decision**	
	3.44E+01	mg/l	PPDB	3.44E+01	25		
	5.5	mg/l	Mereck	5.5	not reported	at 25 degrees- based on merck. Newest value available. Also falling in the range of values which was 1mg/l (EPI) to 34.4mg/l(Ecb)	
	1.10E+00	mg/l	EPI	1.10E+00	25		
2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol	**Units**	**Source**	**mg/l**	**Temp**		**Decision**	
	0.2479	mg/l	OCED		25		
	2.47	mg/l	EC.gc.ca			values similar	
	0.248	mg/l	EPI		25		
	0.25	mg/l	EA - prioritisation of alkylphenols (based on EPI WIN)		unknown		
2-4-Dichloro-o-cresol	**Units**	**Source**	**mg/l**	**Temp**		**Decision**	
	1.60E+03	mol/dm3	IUPAC	2.83E+08		Selected	
	298.6	mg/l	EPI	298.6	25	the 298.6 mg/l	water solubility 2830 mg/L at 25OC
	2830	mg/l	Kovel.com	2830	25		
	Units	**Source**	**mg/l**	**Temp**		**Decision**	

Chemical Name	RANGE FOUND					value selected
Prochloraz	**Units**	**Source**	**Log kow**	**Temp**		**Decision**
4.12E+00	Log Pow	ecb	4.12E+00	25		log Pow is german term for log kow. Values are similar.
4.13	log kow	EPI	4.13			

2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol	**Units**	**Source**	**Log kow**	**Temp**		**Decision**
6.43	Log kow	OECD (SYRACUSE Chemical Properties Prediction Program. KOWWIN v 1.63.)	6.43			As it's the OCED reference and also quoted elsewhere, using the 6.43
6.1	Log kow	can	6.1			
6.43	Log kow					

2-4-Dichloro-o-cresol	**Units**	**Source**	**Log kow**	**Temp**		**Decision**
3.35E+00	log kow	EPI- KOWWIN	3.35E+00			Only value found

	Units	**Source**	**Log kow**	**Temp**	**Decision**

Chemical Name	RANGE FOUND					
Prochloraz	**Units**	**Source**	**Pa**	**Temp**		**Decision**
5.70E-10	torr	merck	7.60E-08		20	
0.015	hpa	OCED(estimate - 1990)	1.50E+00		25	Reference priority in SR7, also the EPI value is closer in range to it. The OCED value seems to not fit.
2.13E-06	pa	epi	2.13E-06		25	

2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol	**Units**	**Source**	**Pa**	**Temp**		**Decision**
0.0028	Pa	OCED (EPA) SYRACUSE Chemical Properties	2.80E-03		25	Two different sources (although based on the same calculation).
2.07E-05	mmHG	OCED (EPA)	2.76E-03			
0.35	pa	http://www.ec.gc.ca/substanc	3.50E-01		25	

2-4-Dichloro-o-cresol	**Units**	**Source**	**Pa**	**Temp**		**Decision**
0.724	Pa		7.24E-01		25	Only Value

	Units	**Source**	**Pa**	**Temp**

Prochloraz
Based on SR7 Section 2.4

	Answer	Calcs	Parameter
Eqn 2-13	0.037173		Mr
Eqn2.15	0.002076	0.002076	B'
Eqn 2.17	1.070394	1.070394	T*
eqn 2.16	1.393795	1.393795	Ω
eqn 2.14	**4.29E-06**	**4.29E-06**	**Da**
eqn 2.18	5.646405	5.646405	δAB
	265.2606	265.2606	Vb

Parameters

Mole Weight	376.67	
Boiling point	774.15	
Density	1.42	
tamb	283.15	

2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol

	Answer	Calcs	Parameter
Eqn 2-13	0.038329		Mr
Eqn2.15	0.002075	0.002075	B'
Eqn 2.17	1.213065	1.213065	T*
eqn 2.16	1.314746	1.314746	Ω
eqn 2.14	**4.43E-06**	**4.43E-06**	**Da**
eqn 2.18	5.765048	5.765048	δAB
	290.9534	290.9534	Vb

Parameters

Mole Weight	262.44		
Boiling point	602.76		
Density	0.902	g/m3	http://www.ec.gc.ca/substances/ese/eng/chall
tamb	283.15		

2-4-Dichloro-o-cresol

	Answer	Calcs	Parameter
Eqn 2-13	0.040167		Mr
Eqn2.15	0.002074	0.002074	B'
Eqn 2.17	1.30011	1.30011	T*
eqn 2.16	1.274583	1.274583	Ω
eqn 2.14	**#DIV/0!**	**#DIV/0!**	**Da**
eqn 2.18	#DIV/0!	#DIV/0!	δAB
	#DIV/0!	#DIV/0!	Vb

Parameters

Mole Weight	177.03	
Boiling point	524.75	
Density		
tamb	283.15	

In the absence of density, the structure of the compound and its molecular weight were taken into account. SR7 presents a value for 2,4 dichlorophenol which is similar structure and molecular weight. Therefore this value of 6.46e-6 was chosen.

lenge/batch8/batch8_17540-75-9.cfm

Based on equation in SR7 Section 2.4

Eqn 2.20		
Prochloraz	3.65E-10	
2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol	3.46E-10	
2-4-Dichloro-o-cresol	5.21E-10	
		In the absence of available data, the structure of the compound and its molecular weight were taken into account. SR7 presents a value for 2,4 dichlorophenol which is similar structure and molecular weight. Therefore this value of 5.21E-10 was chosen.

Annex 3: Modelling

- **Settings**
- **Outputs**

CLEA Software Version 1.06

Report generated 06/07/2010

Report title Hauxton - Residential with Homegrown Produce. 1% SOM, Sand.

Created by LM at Atkins

BASIC SETTINGS

Land Use Residential with homegrown produce

Building Small terraced house
Receptor Female (res) Start age class 1 End age class 6 Exposure Duration 6 years
Soil Sand

Exposure Pathways

Direct soil and dust ingestion	✓	Dermal contact with indoor dust	✓	Inhalation of indoor dust	✓
Consumption of homegrown produce	✓	Dermal contact with soil	✓	Inhalation of soil dust	✓
Soil attached to homegrown produce	✓			Inhalation of indoor vapour	✓
				Inhalation of outdoor vapour	✓

Land Use Residential with homegrown produce

Age Class	Exposure Frequencies (days yr^{-1})						Occupation Periods (hr day^{-1})		Soil to skin adherence factors (mg cm^2)		Direct soil ingestion rate (g day^{-1})
	Direct soil ingestion	Consumption of homegrown produce	Dermal contact with indoor dust	Dermal contact with soil	Inhalation of dust and vapour, indoor	Inhalation of dust and vapour, outdoor	Indoors	Outdoors	Indoor	Outdoor	
1	180	180	180	180	365	365	23.0	1.0	0.06	1.00	0.10
2	365	365	365	365	365	365	23.0	1.0	0.06	1.00	0.10
3	365	365	365	365	365	365	23.0	1.0	0.06	1.00	0.10
4	365	365	365	365	365	365	23.0	1.0	0.06	1.00	0.10
5	365	365	365	365	365	365	19.0	1.0	0.06	1.00	0.10
6	365	365	365	365	365	365	19.0	1.0	0.06	1.00	0.10
7	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
8	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
9	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
10	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
11	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
12	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
13	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
14	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
15	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
16	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
17	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
18	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00

Environment Agency

Receptor Female (res)

Age Class	Body weight (kg)	Body height (m)	Inhalation rate (m^3 day^{-1})	Max exposed skin factor: Indoor (m^2 m^{-2})	Max exposed skin factor: Outdoor (m^2 m^{-2})	Total skin area (m^2)	Consumption rates (g FW kg^{-1} BW day^{-1}): Green vegetables	Root vegetables	Tuber vegetables	Herbaceous fruit	Shrub fruit	Tree fruit
1	5.60	0.7	8.5	0.32	0.26	3.43E-01	7.12	10.69	16.03	1.83	2.23	3.82
2	9.80	0.8	13.3	0.33	0.26	4.84E-01	6.85	3.30	5.46	3.96	0.54	11.96
3	12.70	0.9	12.7	0.32	0.25	5.82E-01	6.85	3.30	5.46	3.96	0.54	11.96
4	15.10	0.9	12.2	0.35	0.28	6.36E-01	6.85	3.30	5.46	3.96	0.54	11.96
5	16.90	1.0	12.2	0.35	0.28	7.04E-01	3.74	1.77	3.38	1.85	0.16	4.26
6	19.70	1.1	12.2	0.33	0.26	7.94E-01	3.74	1.77	3.38	1.85	0.16	4.26
7	22.10	1.2	12.4	0.22	0.15	8.73E-01	3.74	1.77	3.38	1.85	0.16	4.26
8	25.30	1.2	12.4	0.22	0.15	9.36E-01	3.74	1.77	3.38	1.85	0.16	4.26
9	27.50	1.3	12.4	0.22	0.15	1.01E+00	3.74	1.77	3.38	1.85	0.16	4.26
10	31.40	1.3	12.4	0.22	0.15	1.08E+00	3.74	1.77	3.38	1.85	0.16	4.26
11	35.70	1.4	12.4	0.22	0.14	1.19E+00	3.74	1.77	3.38	1.85	0.16	4.26
12	41.30	1.4	13.4	0.22	0.14	1.29E+00	3.74	1.77	3.38	1.85	0.16	4.26
13	47.20	1.5	13.4	0.22	0.14	1.42E+00	3.74	1.77	3.38	1.85	0.16	4.26
14	51.20	1.6	13.4	0.22	0.14	1.52E+00	3.74	1.77	3.38	1.85	0.16	4.26
15	56.70	1.6	13.4	0.21	0.14	1.60E+00	3.74	1.77	3.38	1.85	0.16	4.26
16	59.00	1.6	13.4	0.21	0.14	1.63E+00	3.74	1.77	3.38	1.85	0.16	4.26
17	70.00	1.6	14.8	0.33	0.27	1.78E+00	2.94	1.40	1.79	1.61	0.22	2.97
18	70.90	1.6	12.0	0.33	0.27	1.80E+00	2.94	1.40	1.79	1.61	0.22	2.97

Building Small terraced house

Soil Sand

Building footprint (m^2)	2.80E+01
Living space air exchange rate (hr^{-1})	5.00E-01
Living space height (above ground, m)	4.80E+00
Living space height (below ground, m)	0.00E+00
Pressure difference (soil to enclosed space, Pa)	3.10E+00
Foundation thickness (m)	1.50E-01
Floor crack area (cm^2)	4.23E+02
Dust loading factor ($\mu g\ m^{-3}$)	5.00E+01

Porosity, Total ($cm^3\ cm^{-3}$)	5.40E-01
Porosity, Air-Filled ($cm^3\ cm^{-3}$)	3.00E-01
Porosity, Water-Filled ($cm^3\ cm^{-3}$)	2.40E-01
Residual soil water content ($cm^3\ cm^{-3}$)	7.00E-02
Saturated hydraulic conductivity ($cm\ s^{-1}$)	7.36E-03
van Genuchten shape parameter *m* (dimensionless)	3.51E-01
Bulk density ($g\ cm^{-3}$)	1.18E+00
Threshold value of wind speed at 10m ($m\ s^{-1}$)	7.20E+00
Empirical function (F_x) for dust model (dimensionless)	1.22E+00
Ambient soil temperature (K)	2.83E+02
Soil pH	7.00E+00
Soil Organic Matter content (%)	1.00E+00
Fraction of organic carbon ($g\ g^{-1}$)	5.80E-03
Effective total fluid saturation (unitless)	3.62E-01
Intrinsic soil permeability (cm^2)	9.83E-08
Relative soil air permeability (unitless)	7.68E-01
Effective air permeability (cm^2)	7.54E-08

Environment Agency

Soil - Vapour Model

Depth to top of source (no building) (cm)	0
Depth to top of source (beneath building) (cm)	65
Default soil gas ingress rate?	**No**
Soil gas ingress rate ($cm^3\ s^{-1}$)	3.54E+01
Building ventilation rate ($cm^3\ s^{-1}$)	1.87E+04
Averaging time surface emissions (yr)	6
Finite vapour source model?	No
Thickness of contaminated layer (cm)	200

Air Dispersion Model

Mean annual windspeed at 10m ($m\ s^{-1}$)		5.00
Air dispersion factor at height of 0.8m *		2400.00
Air dispersion factor at height of 1.6m *		0.00
Fraction of site cover ($m^2\ m^{-2}$)		0.75

* Air dispersion factor in $g\ m^{-2}\ s^{-1}$ per $kg\ m^{-3}$

Soil - Plant Model

	Dry weight conversion factor	Homegrown fraction		Soil loading factor	Preparation correction factor
		Average	High		
	g DW g^{-1} FW	dimensionless		g g^{-1} DW	dimensionless
Green vegetables	0.096	0.05	0.33	1.00E-03	2.00E-01
Root vegetables	0.103	0.06	0.40	1.00E-03	1.00E+00
Tuber vegetables	0.210	0.02	0.13	1.00E-03	1.00E+00
Herbaceous fruit	0.058	0.06	0.40	1.00E-03	6.00E-01
Shrub fruit	0.166	0.09	0.60	1.00E-03	6.00E-01
Tree fruit	0.157	0.04	0.27	1.00E-03	6.00E-01

Gardener type Average

CLEA Software Version 1.06

Report generated	06-Jul-10
Report title	Hauxton - Residential with Homegrown Produce. 1% SOM, Sand.
Created by	LM at Atkins

Environment Agency

RESULTS

Environment Agency

		Assessment Criterion (mg kg^{-1})			Ratio of ADE to HCV			Saturation Limit (mg kg^{-1})	50% rule?	
		oral	inhalation	combined	oral	inhalation	combined		Oral	Inhal
1	Prochloraz	8.49E+00	2.23E+04	8.49E+00	1.00	0.00	1.00	1.16E-01 (vap)	Yes	Yes
2	2,6-bis(1,1-dimethyl)-4-(1-methylpr	2.28E+01	2.38E+02	2.17E+01	0.95	0.05	1.00	1.87E+01 (sol)	No	Yes
3	2,4-Dichloro-o-cresol	3.13E+01	2.44E+03	3.11E+01	0.99	0.01	1.00	8.61E+02 (sol)	No	Yes
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Environment Agency

	Assessment Criterion (mg kg^{-1})			Ratio of ADE to HCV			Saturation Limit (mg kg^{-1})	50% rule?	
	oral	inhalation	combined	oral	inhalation	combined		Oral	Inhal
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Environment Agency

		Soil Distribution				Media Concentrations													
		Sorbed	Dissolved	Vapour	Total	Soil	Soil gas	Indoor Dust	Outdoor dust at 0.8m	Outdoor dust at 1.6m	Indoor Vapour	Outdoor vapour at 0.8m	Outdoor vapour at 1.6m	Green vegetables	Root vegetables	Tuber vegetables	Herbaceous fruit	Shrub fruit	Tree fruit
		%	%	%	%	mg kg^{-1}	mg m^{-3}	mg kg^{-1}	mg m^{-3}	mg m^{-3}	mg m^{-3}	mg m^{-3}	mg m^{-3}	mg kg^{-1} FW	mg kg^{-1} FW	mg kg^{-1} FW	mg kg^{-1} FW	mg kg^{-1} FW	mg kg^{-1} FW
1	Prochloraz	96.8	3.2	0.0	100.0	8.49E+00	8.86E-04	4.24E+00	3.61E-09	0.00E+00	1.62E-06	4.12E-07	0.00E+00	8.14E+00	1.12E+01	3.03E+00	0.00E+00	0.00E+00	1.13E+00
2	2,6-bis(1,1-dimethyl)-4-(1-methy	99.7	0.3	0.0	100.0	2.17E+01	1.20E-01	1.08E+01	9.23E-09	0.00E+00	7.33E-05	1.04E-06	0.00E+00	3.68E-01	2.88E+00	1.99E+00	0.00E+00	0.00E+00	1.56E-03
3	2,4-Dichloro-o-cresol	92.9	7.1	0.0	100.0	3.11E+01	2.25E-01	1.55E+01	1.32E-08	0.00E+00	2.75E-04	3.32E-06	0.00E+00	4.43E+01	6.44E+01	1.57E+01	0.00E+00	0.00E+00	1.97E+01
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Environment Agency

	Soil Distribution				Media Concentrations												
	Sorbed	Dissolved	Vapour	Total	Soil	Soil gas	Indoor Dust	Outdoor dust at 0.8m	Outdoor dust at 1.6m	Indoor Vapour	Outdoor vapour at 0.8m	Outdoor vapour at 1.6m	Green vegetables	Root vegetables	Tuber vegetables	Herbaceous fruit	Shrub fruit	Tree fruit
	%	%	%	%	mg kg^{-1}	mg m^{-3}	mg kg^{-1}	mg m^{-3}	mg m^{-3}	mg m^{-3}	mg m^{-3}	mg m^{-3}	mg kg^{-1} FW	mg kg^{-1} FW	mg kg^{-1} FW	mg kg^{-1} FW	mg kg^{-1} FW	mg kg^{-1} FW
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Environment Agency

		Average Daily Exposure (mg kg^{-1} bw day^{-1})							Distribution by Pathway (%)							
		Direct soil ingestion	Consumption of homegrown produce and attached soil	Dermal contact with soil and dust	Inhalation of dust	Inhalation of vapour	Background (oral)	Background (inhalation)	Direct soil ingestion	Consumption of homegrown produce and attached soil	Dermal contact with soil and dust	Inhalation of dust	Inhalation of vapour (indoor)	Inhalation of vapour (outdoor)	Background (oral)	Background (inhalation)
1	Prochloraz	6.29E-05	4.91E-03	8.08E-05	2.00E-07	1.51E-06	3.95E-03	7.64E-03	0.70	54.49	0.90	0.00	0.02	0.00	43.87	0.02
2	2,6-bis(1,1-dimethyl)-4-(1-methy	1.61E-04	8.44E-04	2.07E-04	5.10E-07	6.79E-05	2.29E-04	5.69E-03	10.20	53.51	13.10	0.03	4.30	0.00	14.52	4.34
3	2,4-Dichloro-o-cresol	2.30E-04	3.14E-02	2.96E-04	7.31E-07	2.54E-04	7.89E-03	3.39E-02	0.57	77.86	0.73	0.00	0.63	0.00	19.57	0.63
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Environment Agency

	Average Daily Exposure (mg kg^{-1} bw day^{-1})							Distribution by Pathway (%)							
	Direct soil ingestion	Consumption of homegrown produce and attached soil	Dermal contact with soil and dust	Inhalation of dust	Inhalation of vapour	Background (oral)	Background (inhalation)	Direct soil ingestion	Consumption of homegrown produce	Dermal contact with soil and dust	Inhalation of dust	Inhalation of vapour (indoor)	Inhalation of vapour (outdoor)	Background (oral)	Background (inhalation)
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Environment Agency

		Oral Health Criteria Value (µg kg^{-1} BW day^{-1})		Inhalation Health Criteria Value (µg kg^{-1} BW day^{-1})		Oral Mean Daily Intake (µg day^{-1})	Inhalation Mean Daily Intake (µg day^{-1})	Air-water partition coefficient (K_{aw}) (cm^3 cm^{-3})	Coefficient of Diffusion in Air (m^2 s^{-1})	Coefficient of Diffusion in Water (m^2 s^{-1})	log K_{oc} (cm^3 g^{-1})	log K_{ow} (dimensionless)	Dermal Absorption Fraction (dimensionless)	Soil-to-dust transport factor (g g^{-1} DW)	Sub-surface soil to indoor air correction factor (dimensionless)	Relative bioavailability via soil ingestion (unitless)	Relative bioavailability via dust inhalation (unitless)
1	Prochloraz	TDI	9	TDI	9	70.2	126	6.72E-07	4.29E-06	3.65E-10	3.031	4.13	0.25	0.5	1	1	1
2	2,6-bis(1,1-dimethyl)-4-(1-methy	TDI	1.5	TDI	1.5	4.07	93.8	4.17E-04	4.43E-06	3.46E-10	4.112	6.43	0.25	0.5	1	1	1
3	2,4-Dichloro-o-cresol	TDI	40	TDI	40	140.2	560	2.09E-05	6.46E-06	5.21E-10	2.665	3.35	0.25	0.5	1	1	1
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Environment Agency

	Oral Health Criteria Value (µg kg^{-1} BW day^{-1})		Inhalation Health Criteria Value (µg kg^{-1} BW day^{-1})		Oral Mean Daily Intake (µg day^{-1})	Inhalation Mean Daily Intake (µg day^{-1})	Air-water partition coefficient (K_{aw}) (cm^3 cm^{-3})	Coefficient of Diffusion in Air (m^2 s^{-1})	Coefficient of Diffusion in Water (m^2 s^{-1})	log K_{oc} (cm^3 g^{-1})	log K_{ow} (dimensionless)	Dermal Absorption Fraction (dimensionless)	Soil-to-dust transport factor (g g^{-1} DW)	Sub-surface soil to indoor air correction factor (dimensionless)	Relative bioavailability via soil ingestion (unitless)	Relative bioavailability via dust inhalation (unitless)
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Environment Agency

		Soil-to-water partition coefficient ($cm^3\ g^{-1}$)	Vapour pressure (Pa)	Water solubility ($mg\ L^{-1}$)	Soil-to-plant concentration factor for green vegetables (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for root vegetables (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for tuber vegetables (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for herbaceous fruit (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for shrub fruit (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for tree fruit (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)
1	Prochloraz	6.23E+00	7.60E-08	5.50E+00	model	model	model	model	model	model
2	2,6-bis(1,1-dimethyl)-4-(1-meth	7.51E+01	2.80E-03	2.48E-01	model	model	model	model	model	model
3	2,4-Dichloro-o-cresol	2.68E+00	7.24E-01	2.99E+02	model	model	model	model	model	model
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Environment Agency

	Soil-to-water partition coefficient ($cm^3 g^{-1}$)	Vapour pressure (Pa)	Water solubility ($mg L^{-1}$)	Soil-to-plant concentration factor for green vegetables (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for root vegetables (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for tuber vegetables (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for herbaceous fruit (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for shrub fruit (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)	Soil-to-plant concentration factor for tree fruit (mg g^{-1} plant DW or FW basis over mg g^{-1} DW soil)
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Annex 4: Derivation of Generic Assessment Criteira for the Protection of Human Health

Introduction

Laboratory analysis from soil characterisation at the site have identified a number of compounds not previously identified (CNPIs). Following a review of the available toxicity data for these compounds, three were considered in more detail, with generic assessment criteria (GACs) derived for each. These three compounds were:

- Prochloraz (CAS No. 67747-09-5)
- 2,4-dichloro-o-cresol (CAS No. 1570-65-6)
- 2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol (CAS No. 17540-75-9)

Five compounds were identified for which surrogates were adopted as detailed in Annex 1. These compounds and their surrogates are:

- 2,6-bis(1-methylpropyl)-phenol; surrogate -2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol
- Bis(2-ethylhexyl) maleate; surrogate - Benzene
- 1,2-bis(2,4,6-trichlorophenoxy)ethane; surrogate - Vinyl chloride
- 2,3,6-Trichlorotoluene; surrogate - Vinyl chloride
- 1-(2-Chloroethoxy)-2-(o-Tolyloxy)-ethane; surrogate - Vinyl chloride

Methodology

The derivation of any GACs involves a number of steps including a toxicological assessment and the collation of physical and chemical data for each contaminant. In the derivation of such criteria the Environment Agency has released two guidance documents, namely Science Report (SR)2 – Human Health toxicological assessment of contaminants in soil and SR7 – Compilation of data for priority organic pollutants for derivation of soil guideline values.

Following the methodology outlined in both of these documents, Atkins has carried out a toxicological search and review of physical and chemical data for the compounds identified, with each discussed in further detail below.

Toxicology

In order to evaluate the CNPI compounds appropriately, a number of steps were taken to ensure that these compounds were suitably assessed. A preliminary limited chemical search was undertaken for all the listed chemicals identified, in order to ascertain whether there were readily available toxicology data which had been reviewed by authoritative sources[1]. A shortlist of three compounds was composed on the basis of data availability and toxicity. Prioritisation in relation to these chemicals is presented in Annex 1.

Health criteria values were then derived for the further assessment of these three compounds, based on the principles for toxicological evaluation as outlined in SR2 as further detailed in Annex 1. For the remaining six CNPI compounds, the substance was allocated a suitable surrogate compound for assessment by evaluation of the similarities in chemical structure, as

[1] Authoritative sources of data were limited to the World Health Organization International Programme on Chemical Safety (IPCS), Toxicology Excellence for Risk Assessment (TERA) and Health and Safety Executive Workplace Exposure levels (WEL).

well as the comparison of the available Health Criteria Values (HCVs) for each short-listed surrogate compound with the limited toxicological for the CNPI compounds, where available. The rationale for selection of surrogates in included in Annex 1.

Physical and Chemical Data

In the derivation of appropriate physical and chemical data the Environment Agency methodology presented in SR 7 was followed.

Each source was consulted and the available data collated as presented in Annex 2. As these chemicals are not well reported, data were limited. Where more than one result was recorded, the selection process as presented in SR2 for selection of a parameter was followed. A rationale for the use of each value is also presented in Annex 2. In the absence of data from any of the nine sources in SR7, the Estimation Programs Interface (EPI) Suite from the United States (US) Environmental Protection Agency (EPA) was consulted. Results of this are also presented in Annex 2.

Where a value was reported at 25 degrees celsius, Atkins has retained this value. This is consistent with the approach that was carried out in the previous SSVs. In addition, due to the limited available physical and chemical data available, converting the already estimated value to 10 degrees celsius, using estimated values would further introduce additional uncertainty.

Modelling

Modelling was undertaken using CLEA v1.06 selecting the standard residential with the consumption of homegrown produce land use. In order to retain consistency with previous work undertaken at the site a default sand soil type as defined in SR3 was selected. A soil organic matter of 1% was also selected.

A default soil to dust transport factor of 0.5 g/g was applied in the modelling.

The data available in relation to the compounds and their dermal toxicity was studied prior to selecting a dermal absorption factor (DAF). The DAF is used in the calculation of the assessment criteria for the dermal pathway. Limited data were available with regard to the dermal toxicity and therefore a decision was taken with regard to the DAF that would be applied. The structure of each compound was taken into account, along with the fact that the criteria being derived are being used at the generic stage of assessment.

SR3 presents as range of DAF for various compounds including common pesticides and herbicides. The DAF for pentachlorophenol, which has similarities in structure to the compounds considered herein is given as 0.25, therefore assuming that a quarter of all the substance that is in contact with the skin is available for uptake by the body. This DAF was selected for use herein. It should be noted, that refinement of the conceptual model could result in the removal of the dermal pathway, for example if suitable fill was placed on the site. In such a scenario, the DAF would therefore become irrelevant.

The modelling outputs are presented in Annex 3.

Results

The results of the modelling are presented in Table 4 below.

Table 4 – Summary of Modelling Results.

Compound	Oral Criteria mg/kg	Inhalation Criteria mg/kg	SSV mg/kg
Prochloraz	8.49	2.23E+4	8.49E+0
2,4-dichloro-o-cresol	3.13E+1	2.44E+3	3.11E+1
2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol	2.28E+1	2.38E+2	2.17E+1

Where a surrogate is suggested for a CNPI, the GAC is presented below in Table 5.

Conclusion

The remedial targets for the CNPIs identified are presented below.

Table 5 – Summary of Remedial Targets.

Compound	Remedial Target mg/kg
Prochloraz	8.49E+0
2,4-dichloro-o-cresol	3.11E+1
2,6-bis(1,1-dimethyl)-4-(1-methylpropyl)-phenol	2.17E+1
2,6-bis(1-methylpropyl)-phenol;	2.17E+1
Bis(2-ethylhexyl) maleate	4.93E-2
1,2-bis(2,4,6-trichlorophenoxy)ethane	5E-3*
2,3,6-Trichlorotoluene	5E-3*
1-(2-Chloroethoxy)-2-(o-Tolyloxy)-ethane	5E-3*

*based on Limit of detection

Annex 5: Derivation of Generic Assessment Criteria the Protection of Controlled Waters

This Annex provides an initial assessment of the substances detected at the Former Agrochemical works, Main Site at Hauxton, near Cambridge with respect to risk to controlled waters receptors.

The CNPIs are listed in the following table:

Table 5 – CNPIs for assessment.

Chemical Name	CAS Number	Chemical Formula
2,6-bis(1-methylpropyl)-phenol	5510-99-6	$C_{14}H_{22}O$
2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol	17540-75-9	$C_{18}H_{30}O$
2,4-Dichloro-o-cresol	1570-65-6	$C_7H_6Cl_2O$
Bis(2-ethylhexyl) maleate	142-16-5	$C_{20}H_{36}O_4$
1,2-bis(2,4,6-trichlorophenoxy)ethane	1165-91-9	$C_{14}H_4C_{16}O_4$
Prochloraz	67747-09-5	$C_{15}H_{16}Cl_3N_3O_2$
2,3,6-Trichlorotoluene	2077-46-5	$C_7H_5Cl_3$
1-(2-Chloroethoxyl)-2-(o-Tolyloxy)-ethane	21120-80-9	$C_{11}H_{14}ClO_2$

This memo provides a summary of the physical and chemical properties of each of these substances and relevant information on their likely origin from the history of the Hauxton site. For each substance the relative risk is assessed with respect to the wide range of substances screened as part of the pre-planning risk assessment, and specifically the priority contaminants selected for the Atkins controlled waters risk assessment in 2007 (Ref 1).

Phenolic compounds

2,6-Bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol

This substance is similar to the substance discussed above in comprising a phenol molecule with branched alkane groups attached to the benzene ring. This substance is known as DTBSBP in the chemical industry and is apparently used as an antioxidant and liquid stabilizer in plastics such as polyvinyl chloride (PVC) and polyurethane, as well as in brake fluids, ink resins and mineral/vegetable oils used industrial applications. It is also used as an antioxidant in the petrochemical sector. This substance is not naturally produced in the environment.

It is also possible that 2(1-methylpropyl)-phenol and 2,6-bis(1-methylpropyl)-phenol (discussed below) could be breakdown products of bio-degradation of 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol through the loss of branched alkane group(s) from the benzene ring. This possibility is not suggested or confirmed by the literature sources investigated.

Table 6 – Physical and chemical properties of 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol

Properties	Units	Values	Reference
Henry's Law	atm-cu m/mol	$3.66x10^{-4}$	http://www.ec.gc.ca/substances/ese/eng/challenge/batch8/batch8_17540-75-9.cfm
Log K_{OC}	-	4.47	
Solubility	mg/l	2.47	
Half Life (Aerobic)	Days	182	

The physico-chemical properties in the table above are not directly referenced to peer reviewed literature.

The transport properties of 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol in groundwater are likely to be dominated by the large K_{OC} value (log K_{OC} of 4.47 equates to a K_{OC} value of 29,512). This would suggest its transport in groundwater would be highly retarded, and preferentially when compared to substances with lower K_{OC} values, such as those considered amongst the priority contaminants in the 2006 risk assessment (e.g. phenol, TCE etc). The half lives quoted in the web site source from Canada (see Table above) suggest that under suitable conditions this substance would be expected to degrade in aerobic conditions.

2,6-Bis(1-methylpropyl)-phenol

This substance is similar to 2(1-methylpropyl)-phenol however is has an additional methylpropyl group added on the 6th carbon on the benzene ring. The "bis" reference refers the orientation of the methylpropyl groups in the molecular structure.

Very little information on the physical or chemical properties of this substance have been found in searches other than its boiling point which is 530.7 Kelvin, which equates to 257.55 centigrade from the CRC Handbook of Data on Organic Compounds, 2nd Edition**,** Weast, R.C and Grasselli, J.G., ed(s)., CRC Press, Inc., Boca Raton, FL, 1989, 1.

It is probable that this substance will have properties between those of 2(1-methylpropyl)-phenol and 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol. These are similar types of molecules comprising a phenol molecule with methylpropyl groups attached to the benzene ring. 2(1-methylpropyl)-phenol and 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol are smaller and larger than 2,6-bis(1-methylpropyl)-phenol respectively.

Bis(2-ethylhexyl) maleate

A web search has identified that *'Bis(2-ethylhexyl) maleate is used as an intermediate for the reaction of hydrogenation or acetylation to produce organic synthesis especially for succinic acid and its derivatives. It is a dienophilen intermediate for cycloaddition reaction into olefinic solid bonds to form dienes. Its end applications include paints, vanishes, adhesives, copolymers and film'*. (http://chemicalland21.com/specialtychem/finechem/BIS(2-ETHYLHEXYL)%20MALEATE.htm).

The structure of this substance is roughly symmetrical with the maleate group in the centre, and open carboxylic ring structure with oxygens linking the maleate group to branched alkane (ethylhexyl) groups. The molecule contains no benzene rings or chloride groups therefore it is unlikely to degrade to produce a benzene or phenolic substance, or any chlorinated hydrocarbons. The kinds of degradation products that might be generated by the breakdown of Bis(2-ethylhexyl) maleate would include carboxylic acids and esters.

Internet searches have yielded the following parameters on the contaminant transport properties of Bis(2-ethylhexyl) maleate.

Properties	Units	Values	Reference
Henry's Law	atm-m3/mole	$7.32x10^{-6}$	http://www.epa.gov/chemrtk/hpvis/rbp/Butenedioic%20Acid%20Dialkyl%20Esters_HBP_March%202009.pdf
K_{OC}	l/kg	11000	
Aerobic biodegradation	Days	72% in 28 days	

In the absence of a suitable surrogate for this substance the properties have been used to generate conservative target concentrations for Bis(2-ethylhexyl) maleate using the risk assessment methodology presented in reference 1. The target concentrations were established using a conservative compliance concentration at the receptor of 0.1µg/l and assuming no effective (anaerobic) degradation in groundwater.

2,4-Dichloro-o-cresol

This substance is a synonym of 2,4-dichloro-6-methylphenol, which was detected at Hauxton in previous water analysis at the Main Site. No information was obtained on the contaminant transport properties of this substance in 2007 (Ref 1) and none has been found in searches carried out for this assessment.

This substance consists of a phenol molecule with two chloride ions attached and a methyl group. It is broadly similar to a wide range of other chlorinated, methylated phenols such as 4-chloro 2-methyl phenol which was considered as a priority contaminant in the 2006 risk assessment. 4-chloro 2-methyl phenol is a known biodegradation product of a number of acid herbicides including Mecoprop and MCPA which are prevalent in groundwater at Hauxton in high concentrations.

The properties of 2,4-dichloro-6-methylphenol could be assumed to be similar to other similar phenolic substances such as 4-chloro 2-methyl phenol, 4-chloro-3-methylphenol, pentachlorophenol, 2,4,5-trichlorophenol, 2,4-dimethylphenol. Of these substances 4-chloro 2-methyl phenol was considered to represent the higher risk of these phenolic substances identified at Hauxton by virtue of its high solubility (4000 mg/l at 20^{o}C) and low to moderate range of K_{OC} values in the literature (124 – 645). This resulted in a high risk score in the qualitative screening for priority contaminants (Ref 1). The additional factor in favour of assessing 4-chloro 2-methyl phenol as a substance for a remedial target is that it is likely to be produced as a result of degradation of Mecoprop and MCPA. 4-chloro 2-methyl phenol is therefore considered to act as a suitable surrogate in the remedial criteria for a wide range of similar substances, including 2,4-dichloro-6-methylphenol (i.e. 2,4-Dichloro-o-cresol).

1,2-Bis(2,4,6-trichlorophenoxy)ethane

This substances is a synonym of Bis(2,4,6-trichlorophenyl)ethanedioate. It has not been identified in previous analyses of groundwater at Hauxton. No information was obtained on the contaminant transport properties of this substance in searches carried out for this report.

The structure of this molecule consists of two trichlorinated phenol molecules linked by an ethanoate group, which is an ethane molecule bonded to two oxygens, one via a double bond.

A purely qualitative view of the molecule suggests it is not likely to be highly stable in the environment given presence of double bonds in the structure.

Internet searches revealed a single reference quoting a high K_{OC} value for 1,2-bis(2,4,6-trichlorophenoxy)ethane of 266325.7. This value has been used in conjunction with conservative assumptions of its other properties, i.e. no degradation or volatilisation and a low compliance criteria at the receptor (0.1µg/l (drinking water standard for pesticides/detection limit in water)) to generate a target concentration using the risk assessment methodology applied in 2007 (Ref 1).

Prochloraz

Prochloraz has the chemical name N-propyl-N-[2-(2,4,6-trichlorophenoxy)ethyl]imidazole-1-carboxamide. It is a fungicide and was produced at Hauxton over an unknown period. There was a plant named the Procloraz plant in the northern part of the Main site which was reportedly

constructed in 1982. A large leak of toluene into the shallow groundwater was attributed to a sump in the Procloraz plant during the 1980's. The substance Procloraz has not previously been identified in analysis of groundwater at the Hauxton Main site.

Some published information on the contaminant transport properties of this substances have been sourced from the internet (http://sitem.herts.ac.uk/aeru/iupac/Reports/536.htm).

Properties	Units	Values	nce
Henry's Law	dimensionless	6.74x10^{-}	sitem.herts.ac.uk/aeru/iupac/Reports/536.htm
K_{OC}	l/kg	2225	
Half Life (Aerobic)	days	120 - 45	

Web site articles (http://www.fwi.co.uk/Articles/2008/03/08/109561/Crops-feature-Is-cereal-fungicide-prochloraz-worth-the.htm) suggest that Prochloraz is a currently used fungicide and may be more widely used in future cereal production.

The information in the fate and transport properties of this substance have been used to generate target concentrations using the methodology applied in the 2007 risk assessment using a compliance criteria at the receptor of 0.1µg/l (drinking water standard for pesticides/detection limit in water).

2,3,6-Trichlorotoluene

This substances is a synonym of 1,2,4-Trichloro-3-methylbenzene. This is a relatively simple molecule, similar to many contaminants prevalent at Hauxton comprising a chlorinated benzene ring and a methyl group. The substance has not previously been identified in analysis of groundwater at the Hauxton Main site. No published information on the contaminant transport properties of 2,3,6-Trichlorotoluene has been found in searches carried out for this report.

Other chlorinated toluene type contaminants have been detected at the Hauxton Main site in the past, including 2-chlorotoluene and 4-chlorotoluene. The properties of these two substances should most closely approach those of 2,3,6-trichlorotoluene, of those assessed in the risk screening in 2007 (Ref 1). The most similar molecule to 2,3,6-trichlorotoluene for which a K_{OC} value could be obtained from literature was for 2,4-dichlorotoluene. The log K_{OC} values for all these substance are presented in the table below for comparison.

Table 9 – log K_{OC} values

Substances	K_{OC}	Reference
2-chlorotoluene	346 - 397	Bannerjee, P., Piwoni, M.D. & Ebeid, K., (1985). Sorption of Organic Contaminants to a low Carbon Subsurface Core. Chemosphere 14, 1057 - 1067.
4-chlorotoluene	327 - 512	OECD SIDS Initial Assessment Report for SIAM 20. Paris, France 19th-22nd April 2005. p-CHLOROTOLUENE UNEP PUBLICATIONS
2,4-dichlorotoluene	4786	Howard, P.H., Ed. (1997) Handbook of Fate and Exposure Data for Organic Chemicals. Vol. V, Solvents 3. Lewis Publishers, Inc., Chelsea,

Substances	K_{OC}	Reference
		Michigan.

The values for K_{OC} for chlorinated toluene molecules appears from the properties shown in the table rises with the number of chloride ions attached the benzene ring. This suggests that an increase in the number of chloride ions attached the benzene ring makes the molecule preferentially sorb to organic carbon. 2,3,6-Trichlorotoluene would therefore be anticipated to have a K_{OC} value higher than 2,4-dichlorotoluene which would make it a moderate to highly retarded substance, unlikely to pose a higher risk to controlled waters receptors than the priority contaminants which include toluene, 1,2-dichlorobenzene and 4-chloro 2-methyl phenol which should be suitable surrogates given their higher risk to controlled waters.

1-(2-Chloroethoxyl)-2-(o-Tolyloxy)-ethane

1-(2-Chloroethoxyl)-2-(o-Tolyloxy)-ethane has a superficial resemblance in its molecular structure to certain acid herbicides, such as Mecoprop and MCPA, which historically were synthesised at Hauxton. It comprises a toluene molecule (a benzene ring with a methyl group attached) at one end, and then a long chain attached to it from the second carbon in the benzene ring, comprising oxygen ions separating ethane length carbon chains. The chain is completed by a chloride ion.

The molecule does not appear to be of a structure likely to be stable in the environment, including the electronegative oxygen and chloride ions within the main structure of the molecule.

The likely fate and transport properties of this substance in groundwater cannot be confirmed, however it is considered likely to be of lower risk than the majority of the existing priority contaminants for controlled waters, as the priority contaminants were selected on the basis of their high toxicity, mobility in groundwater and presence as large source bodies on the Hauxton Main Site. Its toxicity may be similar to other acid herbicides or priority compounds identified at the site, however its apparent instability inferred from its molecular structure and lack of identification previously would suggest that it is of lower priority than other more prevalent compounds that could be used as surrogates. 4-chloro 2-methyl phenol is considered to be the most suitable surrogate for 1-(2-Chloroethoxyl)-2-(o-Tolyloxy)-ethane.

Summary

In summary the following recommendations are made as a result of screening the potential risks associated to controlled waters with regard to the substances detected by the TIC GCMS screening during initial remediation activities at the Hauxton Main Site:

- The two phenolic substances (2,6-bis(1-methylpropyl)-phenol and 2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol) are considered to pose a relatively low risk to the water environment when compared to similar substances which were assessed as priority contaminants in the 2006 risk assessment. The remedial targets for the priority contaminants are therefore considered to include suitable surrogates for these three substances in the remediation criteria.
- 2,4-Dichloro-o-cresol (2,4-dichloro-6-methylphenol) was assessed in the risk screening in 2007 (Ref 1) and was not considered as representing a high risk, therefore was not included among the list of priority contaminants. The similar substance, 4-chloro 2-methyl phenol is considered to act as a suitable surrogate in the remedial criteria for 2,4-dichloro-6-methylphenol.

- 2,3,6-Trichlorotoluene is considered likely to be highly retarded in groundwater if the properties of similar chlorinated toluene molecules are considered. This is likely to render it a low risk to controlled waters receptors, certainly lower than the priority contaminants which include 4-chloro 2-methyl phenol.
- The lack of literature values on the chemical and physical properties of 1-(2-Chloroethoxyl)-2-(o-Tolyloxy)-ethane make specific assessment of its risk to controlled waters problematic. In the absence of literature values on its properties, a surrogate (4-chloro 2-methyl phenol) has been selected for setting target concentrations.
- Sufficient data on the contaminant transport properties of Prochloraz, 1,2-bis(2,4,6-trichlorophenoxy)ethane and Bis(2-ethylhexyl) maleate have been sourced to permit calculation of target concentrations for these substances on a conservative basis. The methodology used to calculate the targets was the same as used in the 2007 risk assessment (Ref 1).

The table below lists the CNPIs and the surrogates considered to represent them in the remedial targets. Not all substance types are fully represented in the priority contaminants by substances with similar structural or chemical components. Newly derived target concentrations have been calculated for three of the newly identified substances.

Table 10 – Priority Contaminants Surrogates

Substances	Priority Contaminant Surrogates	Target Concentration (µg/kg)	
		Inner Zone	Outer Zone
2,6-bis(1-methylpropyl)-phenol	4-chloro 2-methyl phenol	2.25	3170
2,6-bis(1,1-dimethylethyl)-4-(1-methylpropyl)-phenol	4-chloro 2-methyl phenol	2.25	3170
2,4-Dichloro-o-cresol	4-chloro 2-methyl phenol,	2.25	3170
Bis(2-ethylhexyl) maleate	No specific surrogates of related chemical structure.	1.8	2.71
1,2-bis(2,4,6-trichlorophenoxy)ethane	No specific surrogates of related chemical structure.	5100	>500,000
Prochloraz	No specific surrogates of related chemical structure	1.1	5230
2,3,6-Trichlorotoluene	4-chloro 2-methyl phenol	2.25	3170
1-(2-Chloroethoxyl)-2-(o-Tolyloxy)-ethane	No specific surrogates of related chemical structure. 4-chloro 2-methyl phenol, used as surrogate	2.25	3170

References

1 Atkins Ltd; Groundwater Modelling Report; Remediation of Former Bayer Site, Hauxton; February 2007