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Ms C Sproats
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South Cambs Hall
Cambourne Business Park
Cambourne
Cambridge
CB3 6EA

30 November 2010

Dear Claire,

Former Bayer CropScience, Hauxton: Risk Assessment of Contaminants Not Previously Identified; Grid Cells G10-G11, G15, I6, L4-L5, M4-M9, N3-N6 (CNPI letter No. 7)

Further characterisation sampling and analysis have identified three contaminants not previously identified (CNPIs) requiring further assessment and derivation of Remedial Targets. These CNPIs were notified to South Cambridgeshire District Council by Harrow Estates (02.11.2010).

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 CNPIs will be added to the contaminants of concern verification list for both the respective grid cells in which the CNPIs were identified and the corresponding treatment beds. The grid squares are shown on the enclosed Site Survey Reference Grid plan.

Table 1 – CNPIs Requiring Further Assessment and Derivation of Remedial Targets

Contaminant	Grid squares	Treatment beds
Dibromo chloromethane	G10	TB119
Ethyl methyl phenol	G15	TB115, TB122, TB123
Dimethyl naphthalene	G15	TB115, TB122, TB123

The compounds presented in Table 2 are CNPIs identified within the recent grid squares which have been risk assessed previously and for which Remedial Targets have already been derived. The CNPIs will be added to the list of verification sampling priority contaminants for the relevant grid cell and corresponding treatment beds.

Twenty three further compounds were identified within the recent grid squares, however these were encountered and assessed during the site investigation and were deemed not to be priority contaminants.

Toxicological assessments and human health and controlled waters risk assessments have been carried out for the new CNPIs and, where sufficient toxicological, physical and chemical data is available, preliminary Remedial Targets have been derived. The preliminary Remedial Targets will be provided to Vertase, who currently intend to use these for the CNPIs.

Table 2 – Recent CNPIs Risk Assessed in Previous CNPI Reports

Contaminant	Grid squares	Treatment beds
Dichloromethylphenol *previously identified in:*	G10, G11, G15 *H7, H10, H13, I9, I10, I11, I15, J10, J11, J12, K10, K12, K13, L11, L12, G12*	TB115, TB119, TB122-123 *TB6, TB17-18, TB23, TB30-31, TB46-47, TB50-51, TB53, TB59-60, TB63, TB67, TB69, TB70a, TB70b, TB71, TB73, TB77-80, TB83-88, TB91-102, TB104-106, TB108-109, TB111-114, TB118-119, TB122-123*
Trichloro methyl benzene (trichloro toluene) *previously identified in:*	G11 *H10, H13, I9, I10, I11, I14 J10, J11, K13*	TB119 *TB6, TB46-47, TB59-60, TB63, TB77, TB83-84, TB87-88, TB93-100, TB102, TB104, TB106, TB108-109, TB111-114*
1-methylnaphthalene CAS 90-12-0 *previously identified in:*	G11, G15 *K10, I12, I13, G13*	TB115, TB119, TB122-123 *TB6, TB69, TB71, TB73, TB78, TB80, TB91-92, TB102, TB104. TB108-109, TB111, TB113, TB118-119*
1-ethyl-3-methyl benzene (ethyl toluene) *previously identified in:*	G15 *J14, H12*	TB115, TB122, TB123 *TB1, TB105, TB113*

Where there is insufficient toxicological, physical and chemical data available for assessment and modelling, suitable surrogate compounds for which Remedial Targets have already been derived for the Hauxton site have been identified and selected based on chemical structures and toxicity data, see Table 3. Where surrogates have been adopted and identified for a particular CNPI, the actual CNPI be measured and assessed against the Remedial Target for the surrogate.

Table 3 – Surrogates Used

Contaminant	Surrogates	
	Human Health	Controlled Waters
Dibromo chloromethane	-	
Ethyl methyl phenol	Benzene	
Dimethyl naphthalene	Naphthalene	

The CNPI Remedial Targets and required laboratory limits of detection (LODs) are summarised in Table 4. As for the previously identified contaminants of concern, four Remedial Targets have been derived for the 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, after levels have been raised to account for flood risk, (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 Remedial Targets will be added to the list of Contaminants of Concern for the relevant grid square and treatment bed validation suites.

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Table 4 – Preliminary Remedial Targets

Contaminant	Remedial Targets (µg/kg)				LOD (µg/kg)
	Greater than 1m depth		Less than1m depth		
	Outer Zone	Inner Zone	Outer Zone	Inner Zone	
Dibromo chloromethane	1460	Do not place in Inner Zone	Do not place at <1m depth	Do not place in Inner Zone	100
Ethyl methyl phenol	100,000	306	Do not place at <1m depth	Do not place at <1m depth	100
Dimethyl naphthalene	100,000	Do not place in Inner Zone	4400	Do not place in Inner Zone	100

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

The treatability of this compound has been reviewed by Vertase FLI and the remediation of the CNPI 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.

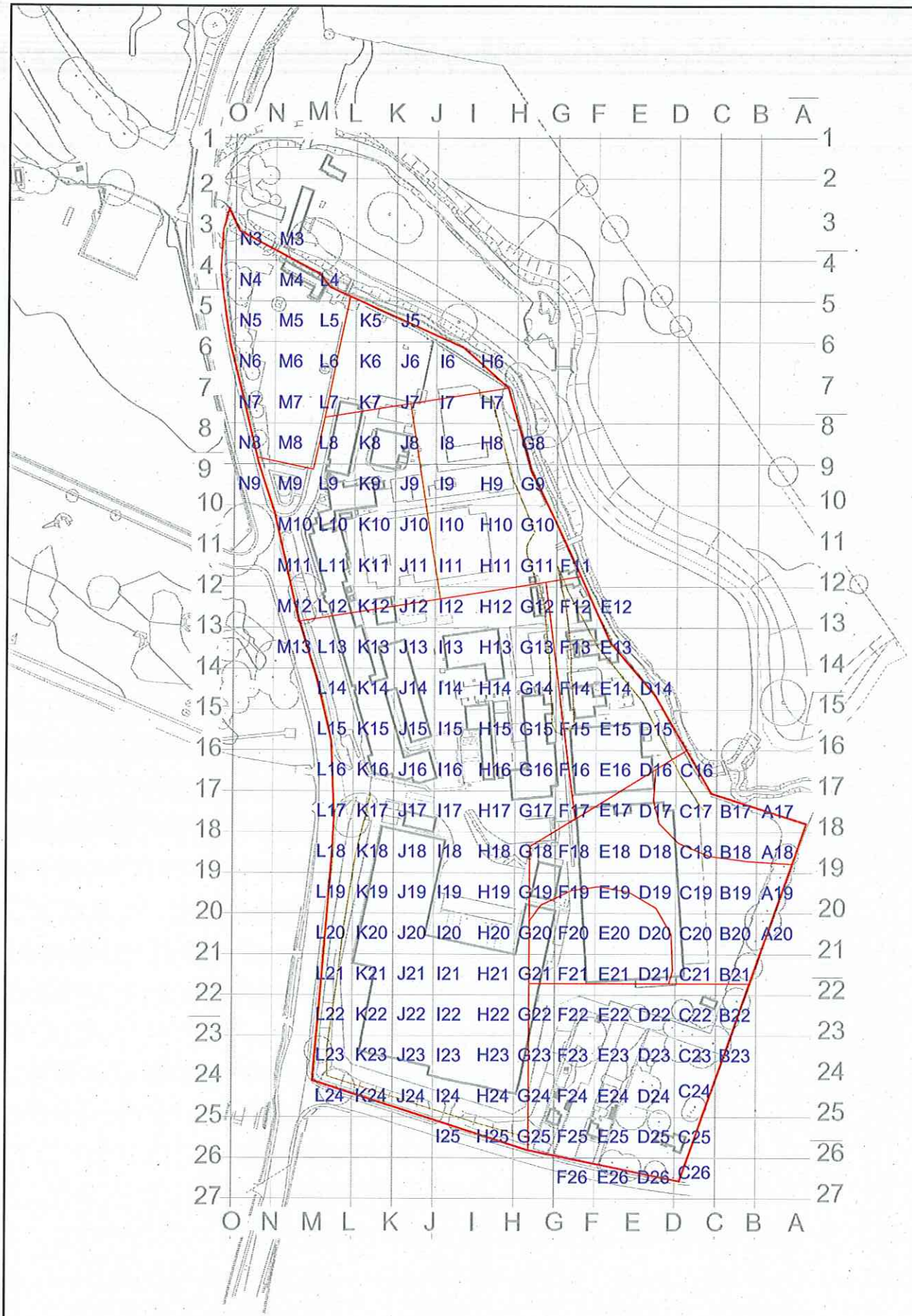
Yours sincerely
For and on behalf of Atkins Limited

Mark Smith
Project Manager

cc Eileen Young – Environment Agency

cc from Harrow Estates Nigel Blazeby - South Cambridgeshire District Council

Enc.



Legend

Site Boundary

A1

Rev.	Description	Checked By	Date
B	Text Updated	JWH	21-04-10
A	Text added to Grid Squares FIRST ISSUE	JWH	01-04-10
			19-02-10

Vertase F.L.I.

Bristol Head Office: Tel: 01275 337937 Fax: 01275 337951

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Site Address:
Dwyer Site
Fulbourn
Cambridge

Sheet: B

Title: 3ds Survey Reference Grid

Client: Hermor Estates

Drawn: JWH	Checked: JWH	Approved: GL
Dwg:D0972_04	Comment:997.BW	Scale: 1:1250

Annex 1: Derivation of Generic Assessment Criteria for the Protection of Human Health

Introduction

Laboratory analyses from soil characterisation at the site have identified a number of compounds not previously identified (CNPI). These compounds did not have available generic assessment criteria (GAC). The CNPIs were:

- Dibromochloromethane (CAS No. 124-48-1);
- Ethylmethylphenol (CAS No. 30230-52-5, mixed isomers); and
- Dimethylnaphthalene (CAS No. 28804-88-8, mixed isomers).

Surrogates were adopted for the evaluation of two of these compounds, as detailed in Annex 2. These compounds are ethylmethylphenol and dimethylnaphthalene. The selection of surrogates is discussed further in this Annex, and in Annex 2.

A GAC was derived for the remaining CNPI, namely dibromochloromethane.

Methodology

The derivation of any GAC 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 three guidance documents, namely:

- Science Report (SR)2 – Human Health toxicological assessment of contaminants in soil;
- SR3 – Updated technical background to the CLEA model; and
- SR7 – Compilation of Data for Priority Organic Pollutants for Derivation of Soil Guideline Values.

Following the methodology outlined in 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. The search was conducted as described in SR2, particularly an evaluation of the available data from all 33 sources listed, as advised. An example checklist of the toxicological sources used for this research has been included in Annex 2.

For dibromochloromethane, sufficient toxicity information was gathered and taken forward for the derivation of a suitable health criteria value (HCV). HCVs were then derived for oral and inhalation exposures, also based on the principles for toxicological evaluation as outlined in SR2. A detailed summary of the data collated and the HCV obtained is included in Annex 2.

For both ethylmethylphenol and dimethylnaphthalene, there was insufficient information available in order to derive a suitable HCV for use in the further assessment. For these compounds a suitable surrogate was identified using the information available based on similarities in structure, toxicity and physical and chemical data, as detailed in Annex 2.

Dibromochloromethane

Physical and Chemical Data

In the derivation of appropriate physical and chemical data for dibromochloromethane, the methodology that the Environment Agency presented in SR7 was followed. Each source was consulted and the available data collated as presented in Annex 3. Where more than one result was recorded, the selection process as presented in SR2 was followed for each parameter. A rationale for the use of each value is also presented in Annex 3.

Where a value was reported at 25°C, Atkins has retained this value. This is consistent with the approach that was carried out in the previous GACs.

Modelling

Modelling was undertaken for dibromochloromethane 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 exposure 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 and available data on dermal absorption from toxicokinetic evaluations of each compound was taken into account, along with the fact that the criteria derived are being used at the generic stage of assessment. SR3 presents a range of DAF for various compounds including common pesticides and herbicides.

For dibromochloromethane a DAF value of 0.25 was utilised and considered as a suitably conservative value based on an experimental study on dermal absorption, and comparison with other compounds that were expected to behave in a similar manner. These decisions are documented in the substance specific toxicological data summaries available in Annex 2.

The modelling outputs are presented in Annex 4.

Results

The results of the modelling are presented in Table 1 below.

Table 2 - Summary of Modelling Results

Compound	Oral Criteria mg/kg	Inhalation Criteria mg/kg	GAC mg/kg
Dibromochloromethane	6.21E-01	6.58E-02	6.23E-02

Ethylmethylphenol and dimethylnaphthalene

In order to evaluate ethylmethylphenol and dimethylnaphthalene appropriately, a search for toxicological data was undertaken. The search was conducted on similar principles to those described in the Environment Agency's *Human Health toxicological assessment of contaminants in soil – Science Report SC050021/SR2*, particularly an evaluation of the available data from the majority of the 33 sources listed, as advised. The checklist showing the toxicological sources used for this research has been included in Annex 2.

There was insufficient information available in order to derive suitable Health Criteria Values (HCVs) for use in a further assessment of these compounds. Therefore, a suitable surrogate was identified using the information available based on similarities in structure, toxicity and physical and chemical data.

Surrogate Allocation

The comparison of structures included evaluation of all compounds previously assessed at the site during earlier phases of the project, as well as chemicals evaluated at other sites and the available soil screening value (SSV) suite of chemicals. The most suitable were then selected on the basis of basic structure, as well as similarity of additional chemical groups and substituent groups such as nitro, halogen, hydroxyl and alkyl groups. Those deemed most suitable were then compared initially on the basis of relative toxicity. Following on from the comparison of structure and relative toxicity, specific chemical and physical parameters were evaluated to make sure that estimated exposure to the surrogate would not be significantly lower than that of the chemical of concern (CoC).

Physical and Chemical Data

Following the preliminary search for toxicological data, it was decided that a surrogate compound would be assigned. Therefore, the Henry's Law Constant (HLC) and log octanol-water coefficient (log Kow) were chosen as the most relevant physical and chemical parameters for surrogate selection. These parameters would aid in an evaluation of potential exposure to the receptor, in the absence of detailed exposure modelling. There was a paucity of data within the seven data sources that the Environment Agency presented in SR7, Indicative values for these two parameters were therefore obtained from the Estimation Programs Interface (EPI) Suite from the United States (US) Environmental Protection Agency (EPA).

The HLC was used as an indication of a chemical's tendency to partition between soil air and soil water, and therefore its tendency to be present in ambient and indoor air. A chemical of concern (CoC) with a higher HLC than its chosen surrogate will, under the same atmospheric conditions, usually be present in higher concentrations in soil vapour. Therefore, the comparison of HLC was done in order to ensure that the CoC would not be more likely to partition to soil air than its chosen surrogate.

In a similar manner, the log Kow was used to determine the potential for a compound to partition to lipid phase, and therefore to be present within home grown produce.

Further information on the surrogate selection is presented in Annex 2.

Results

The result of surrogate selection is presented in Table 2 below. Benzene and naphthalene have been chosen as surrogates for the assessment of ethylmethylphenol and dimethylnaphthalene, respectively. The presented GAC is based on the GAC derived for the allocated surrogate.

Conclusion

The GAC for the CNPIs identified are presented below. Where a surrogate is suggested for a CNPI, the soil screening value (SSV) is presented below in Table 2 as the GAC. It should be noted that as benzene was not previously identified on the site, the current Atkins SSV (from 2009) is presented as a GAC for this constituent.

Table 3 - Summary of Generic Assessment Criteria

Compound	GAC mg/kg
Dibromochloromethane	6.23E-02
Ethylmethylphenol	4.93E-02
Dimethylnaphthalene	4.4

References

Environment Agency, 2008. Compilation of Data for Priority Organic Pollutants for Derivation of Soil Guideline Values Science Report Final SC050021/ SR7.

Environment Agency, 2009a. Human Health toxicological assessment of contaminants in soil. Science Report Final SC050021/SR2.

Environment Agency, 2009b. Updated technical background to the CLEA model Science Report Final SC050021/SR3.

Annex 2: Derivation of Generic Assessment Criteria the Protection of Controlled Waters

TOXICOLOGICAL DATA TEMPLATE

Chemical name: Dibromochloromethane___

Common name: DBCM _____

CAS RN: 124-48-1_____

Chemical Identification
Synonyms: Chlorodibromomethane,
Dibromochloromethane, Monochlorodibromomethane, Methane, chlorodibromo-; Methane, dibromochloro-

Occurrence and uses
DBCM can be formed as a chlorination disinfection by product. This occurs in a reaction between chlorine and natural organic matter (NOM) (COT, 2008). In drinking-water, each of these chlorination byproducts (CBPs) is typically present at a concentration below 1 part per billion (1 µg/l). Some, however, such as the trihalomethanes (THMs), i.e. chloroform, bromodichloromethane, chlorodibromomethane and bromoform, are often present at concentrations between 10 and 100 µg/l (COC, 2007).

DBCM is a colourless to yellow, heavy, non-flammable, liquid with a sweet odour. Small amounts are formed naturally by plants in the ocean. It is somewhat soluble in water and readily evaporates into the air. Most of the dibromochloromethane that enters the environment is formed as a by product when chlorine is added to drinking water to kill bacteria. It was used in the past as a solvent and flame retardant, or to make other chemicals, but now it is used mainly as a laboratory reagent (ATSDR, 2010).

Toxicokinetics
The THMs are absorbed, metabolised and eliminated rapidly by mammals after oral or inhalation exposure. Following absorption, the highest tissue concentrations are attained in the fat, liver and kidneys. Half-lives generally range from 0.5 to 3 h, and the primary route of elimination is via metabolism to carbon dioxide. Metabolic activation to reactive intermediates is required for THM toxicity, and the three brominated species are all metabolised more rapidly and to a greater extent than chloroform (WHO, 2005).

Available studies indicate that gastrointestinal absorption is high for all THMs and they accumulate in tissues like the liver, fat and kidneys due to their high lipophilicity. They are metabolised to trihalomethanols, which can then decompose to yield highly reactive dihalocarbonyls which may be responsible for their toxicity or carcinogenicity. There is a species-dependent difference in metabolic activation and decomposition to trihalomethanols is higher in mice than in rats (WHO, 2005). A dermal permeability constant (PC, the rate of absorption through a given area of skin per unit of time, usually from water) for trihalomethanes, of 0.0020 cm/h (2.0E-3 cm/h) has been reported (Semerjian and Dennis, 2007). This value is used in conjunction with molecular weight and other physical and chemical parameters to determine the absorbed dose after dermal exposure. For comparison, values in the range of 1.4 E-1 to 6.8E-3 cm/h have been reported for chloroform (0.14 to 0.0068 cm/h) and 3.9E-1 cm/h (0.39 cm/h) for pentachlorophenol, respectively (USEPA, 2004).

A dermal absorption fraction (ABS_d) of 0.1 is the default value suggested in current guidance for risk assessment of soil for organic compounds (Environment Agency, 2009). The value of 0.1 is considered suitable for an organic compound such as chloroform, where there are no additional data. It has been reported that brominated substitution would be expected to confer greater lipophilicity on DBCM compared with chloroform (Health Canada, 2009), which would affect both absorption and tissue solubility In the light of this information, it is considered unsuitable to adopt a dermal absorption fraction of 0.1 for DBCM, It is therefore assumed that DBCM is more likely to have an absorption rate similar to pentachlorophenol, for which a ABS_d of 0.25 has been adopted. **Therefore, as a conservative measure an ABS_d of 0.25 is adopted for DBCM**.

Mode of Action
The cytotoxicity of the DBCM observed in the liver and kidneys of exposed animals has been proposed to result from covalent adducts formed between cellular proteins and lipids and dihalocarbonyls or dihalomethyl free radicals. The adducts presumably impair the function of these molecules and cause cell injury. Induction of lipid peroxidation by free radical metabolites of reductive metabolism has been proposed as another mechanism underlying their cytotoxicity (WHO, 2005).

Acute Toxicity
Acute oral LD50[1]s of 800 and 1200 mg of DBCM per kg of body weight were reported for male and female ICR Swiss mice, respectively, whereas LD50s of 1186 and 848 mg/kg of body weight were found for male and female Sprague-Dawley rats, respectively. A DBCM dose of 500 mg/kg of body weight produced ataxia, sedation and anaesthesia in mice. In a study in which male Sprague-Dawley rats were dosed with DBCM by corn oil gavage, a dose of 2450 mg/kg of body weight was found to be lethal but no clinical evidence for significant liver or kidney toxicity was found at sub-lethal doses (IPCS, 2000).

Subacute Toxicity (short term repeat dose studies)
Daily gavage of male and female CD-1 mice with DBCM in an aqueous vehicle for 14 days produced hepatotoxicity in both sexes at the highest dose of 250 mg/kg of body weight per day. Depressed immune function was also observed in both sexes at doses of 125 and 250 mg/kg of body weight per day, whereas the 50 mg/kg of body weight per day dose was without effect (IPCS, 2000).

Corn oil gavage of DBCM to male CD-1 mice for 14 days led to observations of kidney and liver toxicity at a lower dose (147 mg/kg of body weight per day) than had been observed with an aqueous vehicle. In another 14-day corn oil gavage study, National Toxicity Programme (NTP) (1985) found that a dose of 500 mg/kg of body weight per day was lethal to B6C3F1 mice, and doses of 500 and 1000 mg/kg of body weight per day were lethal to F344/N rats. Dietary administration of microencapsulated DBCM to Wistar rats for 1 month caused liver cell vacuolization, with a lowest observed adverse effect level (LOAEL) of 56 mg/kg of body weight per day and a no observed adverse effect level (NOAEL) of 18 mg/kg of body weight per day (IPCS, 2000).

Chronic Toxicity (long-term toxicity data)
The chronic oral toxicity of DBCM was studied by NTP (1985) in F344/N rats and B6C3F1 mice using corn oil gavage (5 days per week for 104 weeks) and doses of 0, 40 or 80 mg/kg of body weight per day for rats and 0, 50 or 100 mg/kg of body weight per day for mice (USEPA 1991).

Reproductive and Developmental Toxicity
In a two-generation reproductive study of DBCM conducted in ICR Swiss mice, male and female mice at 9 weeks of age were maintained on drinking-water containing 0, 0.1, 1.0 or 4.0 mg of DBCM per ml, leading to average doses of 0, 17, 171 or 685 mg/kg of body weight per day. Fertility and gestational index were reduced in the high-dose group for the first generation. Only fertility was decreased (high-dose) in the second generation. At the mid and high doses in both generations, litter size and the viability index were decreased. Other effects included decreased lactation index and reduced postnatal body weight. No dominant lethal or teratogenic effects were observed in the first or second generations (IPCS, 2000).

In a developmental study in rats, gavage doses of DBCM (0, 50, 100, or 200 mg/kg of body weight per day) on gestational days 6-15 caused a depression of maternal weight gain, but no foetal malformations (IPCS, 2000).

Genotoxicity
Although the UK Committee On Mutagenicity Of Chemicals In Food, Consumer. Products And The Environment (COM) concluded DBCM is not genotoxic in a review in 1995, further

[1] Dose that results in death in 50% of the animals within the test group.

work was required to verify the results from additional studies showing positive results for genotoxicity in the liver of both mice and rats, (COM, 2007).

The International Agency for Research on cancer (IARC) have classified DBCM in Group 3 (not classifiable as to its carcinogenicity to humans) (WHO, 2005). This is based on evidence that DBCM was mutagenic to bacteria and resulted in chromosomal aberrations in cultured mammalian cells. Some mutagenic effects were also observed in in rodents treated in vivo (IARC, 1991).

Carcinogenicity

The available data for exposure to humans are for trihalomethanes (THMs) as a group, from exposure to drinking water sources. Interviews were conducted and exposure was estimated over 40 years. Among males, colon cancer risk was associated with cumulative exposure to THMs, duration of exposure to chlorinated surface water, and duration of exposure to THM levels of at least 50 µg/L and of at least 75 µg/L. Males exposed to chlorinated surface water for 35–40 years had an increased risk of colon cancer compared with those exposed for less than 10 years. Males exposed to an estimated THM level of 75 µg/L or more for at least 35 years had double the risk of those exposed for less than 10 years (COC, 2007).

Increased risk of chronic myelocytic leukaemia was associated with increasing years of exposure to several chlorination by products (such as DBCM) indices, with an adjusted occurrence rate (OR) of 1.72 for the highest exposure duration to total THMs of more than 40 µg/L. In contrast, the risk of the other studied leukaemia subtypes was found to decrease with increasing years of exposure. This can be shown by the statistically significantly low occurrence rates which were noted for chronic lymphocytic leukaemia (OR 0.60) associated with the highest exposure duration to total THMs of more than 40 µg/L, and for hairy cell leukaemia (OR 0.31) in subjects a sub-analysis of subjects exposed only to chlorinated water sources during the 40-year exposure period (COC, 2007).

In a NTP carcinogenesis bioassay, DBCM was administered in doses of 0, 40, or 80 mg/kg body weight by gavage in corn oil 5 times per week for 104 weeks to groups of 50 male and female F344/N rats. In addition, 0, 50, or 100 mg/kg bw per day was administered in similar fashion to groups of 50 male and female B6C3F1 mice 5 days per week for 105 weeks (Health Canada, 2009).

Body weight gain in the high-dose group of male rats was decreased, and there was a dose-related increase in adverse effects to the liver. There was, however, no evidence of carcinogenicity in rats (Health Canada, 2009).

In male mice, survival was significantly lower in both dose groups. In both sexes, the incidences of adverse liver and kidney effects (in females) was increased. There was equivocal evidence of carcinogenicity in male B6C3F1 mice based on an increased incidence of hepatocellular carcinomas, but only a marginal increase in hepatocellular adenomas or carcinomas (combined). There was also some evidence of carcinogenicity in female mice, based on an increased incidence of hepatocellular adenomas and hepatocellular adenomas or carcinomas (combined) (Health Canada, 2009).

In summary, a recent review by Health Canada concludes that even though recent studies suggest that some association exists between colon, rectal, and brain cancer and exposure to THMs in drinking water, the data presented in the studies are not sufficient to reliably confirm a dose–response or causal relationship (Health Canada, 2009). This is a similar conclusion to the World Health Organization (WHO) during the derivation of a drinking water guideline value, as shown in following sections of this summary.

Background exposure (food, drinking water, air)

Food

There is little data regarding the content of DBCM in food sources. An analysis of 12 samples of various German milk products (ice cream, yogurt, curds, buttermilk) found DBCM levels ranging from not detectable to 0.3 ug/kg with an overall mean concentration of 0.1 ug/kg.

DBCM concentrations in food samples ranged from not detected to 0.6 ppb (0.6 µg/kg) for 24 hour duplicate portion diet in Japanese housewives (HSDB, 2010). Considering its presence in drinking water sources Atkins considers that it is likely to be present in a variety of food sources, as it would enter it during food processing.

Drinking Water
The UK Water Supply (Water Quality) regulations state that the maximum concentration of trihalomethanes, of which DBCM is listed, should be 100 µg/L (HMSO, 2000).

Air
Ambient air concentrations at several urban locations in the USA averaged 32 ng/m³ for DBCM and the highest value reported was 0.23 µg/m³ (WHO, 2005). In separate monitoring studies in the USA, mean DBCM levels of 0.0, 0.48, 14, 14 and 19 parts per trillion (0, 0.0044, 0.128, 0.128 and 0.174 µg/m³) have been detected in the ambient air of Magnolia, El Dorado, Chapel Hill , Beaumont, and Lake Charles, respectively.

In data for Europe, an analysis of ambient air of several German cities found lower concentrations of DBCM generally ranging from not detectable to 0.1 ug/m³, although one industrial city had a level of 0.9 ug/m³ (HSDB, 2010).

Atmospheric DBCM levels ranging from 0.06-10 parts per trillion (0.00055 – 0.0917 µg/m³), with a median of about 0.4 parts per trillion (0.00367 µg/m³) were found in ambient air samples collected from the north and south Atlantic Ocean, the beaches of the Azore Islands and Bermuda, and southern Germany between 1982-1985 (HSDB, 2010).

Reviews by authoritative bodes

WHO Drinking Water Guideline Values
WHO have a limit of 0.1mg/l for the presence of DBCM in drinking water. This is based on a tolerable daily intake (TDI) of 21.4 µg/kg of body weight, based on the adverse effects in the liver in a well conducted and well documented 90-day study in rats conducted by the NTP, discussed above. They applied an uncertainty factor of 1000 (100 for intra- and interspecies variation and 10 for the short duration of the study) to a NOAEL of 30 mg/kg of body weight per day, and adjusted the value for continuous exposure from the 5-day a week regime used in the experimental study. An additional uncertainty factor for potential carcinogenicity was not applied because of the questions regarding mouse liver tumours from corn oil vehicles and inconclusive evidence of genotoxicity (WHO, 2005). It is noted that they limit drinking water exposures to 20%[2] of the TDI during the derivation of the guideline value. Although this is standard procedure that is intended to account for potential for exposure from other (non-drinking water) sources, the allocation means that the 'safe' drinking water exposure is still assumed to be only a fraction of the TDI.

US EPA
The US EPA have evaluated the non-cancer oral toxicity data for DBCM. They chose to use a sub-chronic NOAEL of 30 mg/kg bw/day from the same study as that selected by the WHO (conducted by the NTP) as the basis of their RfD and adjusted this value in a similar manner to the WHO to account for continuous exposures. They also applied uncertainty factors (UFs) of 100 to account for inter- and intra-species variability, as well as an additional factor of 10 to extrapolate from a sub-chronic study. An oral RfD of 0.02 mg/kg bw/day was derived.

EPA classified this chemical as C - possible human carcinogen. The cancer weight-of-evidence classification is based on all routes of exposure. The Toxicology Excellence for Risk Assessment (TERA) converted the EPA slope factor to a dose at the 1 in 100,000 (E-5) risk level by dividing 1E-5 by the slope factor of 8.4E-2 per (mg/kg)/day to determine a risk specific dose (RSD) of 1.2E-4 mg/kg-day.

[2] Only 20% of the TDI is expected to be obtained from drinking water sources. Therefore, the GV is based on a value of 4.28 µg/kg of body weight (20% of the TDI of 21.4 µg/kg body weight). The WHO states that the final guideline value has been rounded.

Agency for Toxic Substances and Disease Registry (ATSDR)
The ATSDR has not derived inhalation minimal risk levels (MRLs) for acute-, intermediate-, or chronic-duration inhalation exposure to dibromochloromethane because quantitative data were not available to determine NOAELs or LOAELs. They have derived MRLs of 0.1 mg/kg/day and 0.09 mg/kg/day for acute and chronic duration oral exposure. The NTP study, in which rats received gavage doses of 0, 40, or 80 mg/kg of DBCM in corn oil, 5 days/week, for 104 weeks, was selected as the basis for the chronic-duration oral MRL, and applying an uncertainty factor of 300 (3 for use of a minimal LOAEL[3], 10 for extrapolation from animals to humans, and 10 for human variability) to the LOAEL of 28 mg/kg/day (ATSDR, 2005).

Internation Agency for Research on Cancer (IARC)
IARC classifies DBCM as not classifiable as to its carcinogenicity to humans (Group 3), based on limited evidence for carcinogenicity in experimental animals. No epidemiological data relevant to the carcinogenicity of DCBM were available at the time of their review. The IARC evaluation considers the evidence of carcinogenicity in humans and experimental animals, as well as other data relevant to the evaluation of carcinogenicity and its mechanisms. Although ATSDR discusses the carcinogenicity data in its Toxicological Profiles, it does not currently assess cancer potency or perform cancer risk assessments.

Health Criteria Values (HCV)
Oral exposure
The TDI of 21.4 µg/kg bw/day (adjusted for continuous exposure) derived by the WHO is selected as a point of departure for derivation of a health criteria value (HCV). This TDI was based on a NOAEL of 30 mg/kg bw/day for the absence of adverse (histopathological) effects, and 1000 (100 for intra- and inter-species variation and 10 for the short duration of the study) (WHO, 2005). This value is similar to the value of 0.02 mg/kg bw/day (20 µg/kg bw/day) derived by the USEPA.

Atkins has applied an additional safety factor of 10 to account for the potential carcinogenic effects. Therefore, a TDI oral of 0.002 mg/kg bw/day is derived (2 µg/kg bw/day)

Mean Daily Intake (MDI)
Drinking water
The UK Water Supply (Water Quality) regulations state that the maximum concentration of trihalomethanes, of which DBCM is listed, should be 100 µg/L (HMSO, 2000). Assuming a 70 kg adult has a daily water intake of 2L, this is equal to a daily MDI of 200 µg/day (2.86 µg/kg bw/day) using the relatively conservative assumption that all the trihalomethane present is DBCM. This value is considered to be reasonable, based on the fact that the WHO report that THMs such as bromodichloromethane are often present at concentrations between 10 and 100 µg/l (COC, 2007). This value exceeds the TDI.

Dietary sources
There is currently no quantitative estimate of intake from all dietary estimates.

However, in light of the data available for drinking water exposures, the dietary sources can be assessed within the total MDI allocation. The MDI will be equal to 50% of the TDI, based on current guidance for risk assessment of soils (Environment Agency, 2009).

MDI_{oral} = 0.5 x 2 µg/kg bw/day
= 1 µg/kg bw/day(70 µg/ day)

Tolerable daily soil intake (TDSI)
= TDI – MDI
= (2 - 1) µg/kg bw/day
= 1 µg/kg bw/day (0.001 mg/kg bw/day).

[3] The ATSDR defines a minimal LOAEL as an experimental exposure level in which there was some minimal effect that would reduce the ability of an organ, or system to function normally, but would not result in the inability of the whole organ, organ system or organism from functioning normally (Abadin *et al*, 1998).

Inhalation Exposure

In the absence of route-specific data, the TDI for oral exposures will be extrapolated for inhalation exposures. Although there are no data for inhalation exposures, Atkins considers that this is a suitably conservative value for potential inhalation effects, considering available UK Guidance (Environment Agency, 2009). There is adequate data on systemic effects and metabolism, as well as the added conservatism within the oral HCV for potential carcinogenic effects.

Mean Daily Intake (MDI)

An analysis of ambient air of several German cities found DBCM concentration generally ranging from not detectable to 0.1 ug/m³. A single value in one industrial city had a level of up to 0.9 ug/m³. The values reported in German cities (excluding the maximum value of 0.9 µg/m³ reported in a single location) are assumed to be the most likely to be similar to UK sources. Therefore, the upper limit of the range (**0.1 µg/m³) will be a adopted as the MDI $_{inhalation}$.** Assuming a 70kg adult inhales 20m³ air per day, this is equivalent to 2 µg/day (0.0286 µg/kg bw/day).

$MDI_{inhalation}$ = 0.0286 µg/kg bw/day

Tolerable daily soil intake (TDSI)

= TDI – MDI

= (2 – 0.0286) µg/kg bw/day

= 1.97 µg/kg bw/day (0.00197 mg/kg bw/day).

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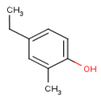
SURROGATE SELECTION SUMMARY

Chemical name	CAS Number	Structure	Available tox data	Henry's law Constant (HLC)	Log Kow	Suggested Surrogate(s)	HCV(oral) (µg/kg/bw/day)	HCV(inh) (µg/kg/bw/day)	Surrogate Inhalation HCV (mg/m^3)	Surrogate selected	Justification
Ethylmethylphenol	30230-52-5 (mixed isomers)		None available	1.17E-6 atm m^3/mol (0.0000478)	3.0985	Ethylbenzene Benzene Toluene (methyl benzene) Phenol Cresols	100 0.29 223 695 100 (EIC, 2010)	213 1.4 1372 7.845 100 (EIC, 2010)	393 2.58 2530 14.5 -	 **Benzene (HLC dimensionless 0.116; Log Kow 2.13. Ref: EA, 2008)),**	There are no available toxicological data for ethylmethylphenol. Data for oral exposure to structurally similar cresols (methylphenols) indicate that they may have a similar toxicity to ethylbenzene. However, in the absence of any other data, benzene is considered to provide a more suitable degree of conservatism for the assessment of ethylmethylbenzene. Benzene is therefore selected as a surrogate, since its toxicity is considered likely to be conservative enough to compensate for any potential differences in toxicity, as well as any differences in physical and chemical charcteristics.

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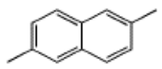
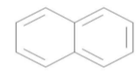
ANNEX 2 - SURROGATE SELECTION SUMMARY

Chemical name	CAS Number	Structure	Available tox data	Henry's law Constant (HLC)	Log Kow	Suggested Surrogate(s)	Surrogate Inhalation HCV (mg/m³)	Surrogate Oral HCV (µg/kg bw/day)	Surrogate selected
Dimethyl naphthalene	28804-88-8 (mixed isomers)	(2.6-dimethylnaphthalene shown, several isomers possible) 	No chemical specific data	4.25E-4 atm m³/mol (0.0174)	4.26	Naphthalene; Benzo(a)pyrene; Benzene; Aromatic TPH 10-12	0.00248; 0.000245; 0.005; 0.0998	20; 0.02; 0.29; 20	**Naphthalene (HLC dimensionless 0.116; Log Kow 2.13. Ref: EA, 2008),** 

JUSTIFICATION

There are no readily available toxicity data for any of the isomers of dimethylnaphthalene in the open literature. On the basis of the structure, naphthalene and benzo(a)pyrene are considered to be the most suitable for consideration as surrogate compounds. Although the structure of this compound is more similar to the structure of naphthalene, there is potential for comparatively increased toxicity due to the presence of methyl substituents to the basic naphthalene structure, such as can be found when comparing the oral toxicity of naphthalene to that of 1-methylnaphthalene and 2-methylnaphthalene for which oral toxicity HCVs of 2.3 and 4 µg/kg bw/day respectively, have been reported (CL:AIRE, 2010). Therefore, benzo(a)pyrene has also been considered for adoption as a conservative surrogate on the basis of toxicity, due to its comparatively low HCVs. However, its physical and chemical properties make it vastly different to dimethylnaphthalene.

It has also been found that a number of dimethylnaphthalene isomers are present within the aromatic TPH C10-12 fraction, as listed within the Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG) Series Composition of Petroleum Mixtures - Volume 2 (API, 1998). It is assumed that since this compound contributes to the toxicological effect of this group of compounds and was considered during the derivation of GAC for this fraction, the toxicology data and physical and chemical data for the fraction-specific TPH mixture used to derive a GAC for the aromatic TPH C10-12 fraction will give a suitable indication of the toxicity of this compound. However, it was noted that there were no toxicity data available for dimethylnaphthalenes in particular during the toxicity evaluation undertaken by the TPHCWG. Therefore, since a lack toxicity data for these compounds prevented their evaluation during the derivation of an HCV for the aromatic TPH C10-12 fraction, naphthalene is chosen as a more conservative means of assessing their potential toxicity. It is assumed that the uncertainty in selecting a surrogate on the basis of toxicity (in particular the toxicity associated with the dimethyl substituents) will be compensated for by potential differences in physical and chemical characteristics. Therefore, in the absence of chemical specific toxicity data for dimethylnaphthalenes, rather than assume that they should be assessed within the TPH C10-12 fraction, naphthalene is chosen as a comparatively conservative surrogate compound for the assessment of dimethylnaphthalenes.

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Annex 3: Physical and Chemical Data

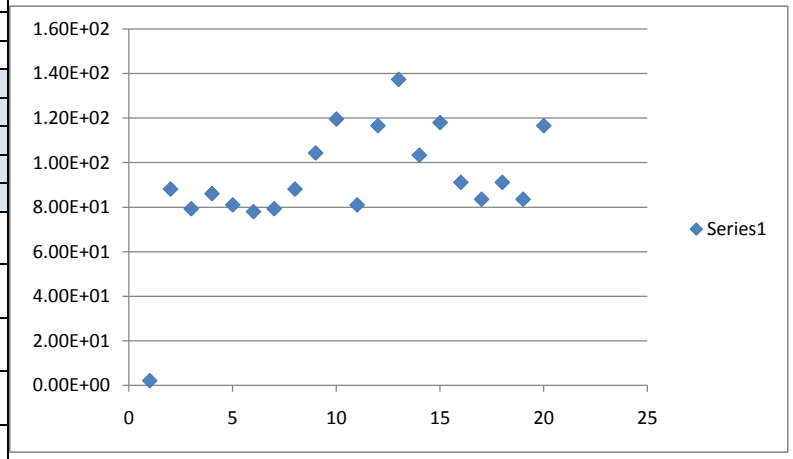
Dibromochloromethane **CHBr2Cl** **CAS: 124-48-1**							http://webbook.nist.gov/chemistry/ http://srdata.nist.gov/solubility/			http://srdata.nist.gov/solubility/			http://toxnet.nlm.nih.gov/			http://www.inchem.org/documents/icsc/icsc/eics0519.htm			Montgomery					
	B			**D**									**OTHER SOURCES**			**OTHER SOURCES**			**OTHER SOURCES**			**Decision**		
	HAYNES, 2010-2011 (replaced LIDE, 2008)			MERCK, 2006			NIST, 2005			Srdata			HSDB			INCHEM (ICSC)			Montgomery (2007)					
	Value	**Units**	**Temp if present**	**Value**	**Units**	**Temp if present**	**Value**	**Units**	**Temp if present**	**Value**	**Units**	**Temp if present**	**Value**	**Units**	**Temp if present**	**Value**	**Units**	**Temp if present**	**Value**	**Units**	**Temp if present**	**Value Selected**	**Units**	**Justification**
Relative Molecular Mass	208.28			208.28			208.28						208.28						208.28			208.28		All values are the same.
Henry's Law Constant (HLC)							0.86 0.73 0.97 0.85 1.1 1.2 1.1 1.2 0.86	 all mol/kg*bar 		3.5E-2 8.7E-4 7.83E-4 8.5E-4 8.0E-4 7.7E-4	(1st is dimensionless) rest are atm-m3/mol	25 deg C 20 deg C 24.85 deg C 20 deg C 20 deg C 20 deg C	7.83E-04	atm-m3/mole	20 deg C				7.83E-04 8.7E-04 3.8E-04 4.5E-04 10.3E-04 (sic) 11.8E-04 (sic) 15.2E-04 (sic) 8E-04 14E-4 (sic) 22E-04 (sic)	 atm-m3/mol	25 deg C 20 deg C 10 deg C, 15 deg C, 20 deg C, 25 deg C, 30 deg C 20 deg C, 30 deg C, 40 deg C	1.1 (91.2)	mol/kg*bar (Pa m3/mol)	Central value selected from medium consistency range.
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	2.51	g/kg H2O											2700	mg/L	20 deg C				2509 1049.9 3040 2375 3182	mg/L mg/L mg/kg (same as mg/L) mg/kg mg/kg	30 deg C 30 deg C 10 deg C 20 deg C 30 deg C	2.51 (2510)	g/kg (mg/L)	The data from the most recent source has been selected. This is also the central value of the data available at 20 degrees C.
Chemical Boiling Point (ambient pressure)	120	deg C		121.3-121.8 123-125	deg C deg C								121.3-121.8 123-125 120	deg C deg C deg C					115-120	deg C		120	deg C	The data from the most recent source has been selected. This also falls within the range of the boiling points quoted in Montgomery.
Chemical Melting Point (ambient pressure)	-20	deg C											-20	deg C					-23 to -21	deg C		-20	deg C	The data from the most recent source has been selected, which is not inconsistent with the third source.
Log Octanol - Water Coefficient (Kow)													2.16 2.16	log P log Kow					2.24 2.08			2.16		The central value from a low consistency range of data has been selected.
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																						8.25E-06		Calculated using SR7 calculations.
Diffusion Coefficient in Water																			9.70E-06	cm2/sec	20 deg C	7.14E-10		Calculated using SR7 calculations.
Log (organic carbon-water partition coefficient)(Koc)																			1.92			2.14		Calculated using SR7 calculations.
Vapour Pressure													5.54	mmHg	25 deg C				76	mmHg	20 deg C	76	mmHg	The value from the most recent source has been selected. As literature values have been selected for Henry's Law Constant, vapour pressure is not a critical parameter as it is only used in the calculation for vapour saturation limits.
Air-water partition coefficient (Kaw)																								Calculated using the Henry's Law Constant
Density	2.451	g/cm3		2.445															2.451	g/cm3	20 deg C	2.451	g/cm3	The data from the most recent source has been selected. Two of the three sources quote this same value. The value is from a consistent range.
Melting point																								
Critical Temp																								

Vapour Pressure

5.54	mmHg	convert to Pascals, multiply by	133.3224	738.61	Pa
76	mmHg	convert to Pascals, multiply by	133.3224	10132.50	Pa

Henry's Law Constant

8.70E-04	dimensionles	convert to Pa m^3/mol, multiply by	2471.341	2.15E+00	Pa m3/mol
8.70E-04	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	8.82E+01	Pa m3/mol
7.83E-04	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	7.93E+01	Pa m3/mol
8.50E-04	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	8.61E+01	Pa m3/mol
8.00E-04	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	8.11E+01	Pa m3/mol
7.70E-04	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	7.80E+01	Pa m3/mol
7.83E-04	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	7.93E+01	Pa m3/mol
8.70E-04	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	8.82E+01	Pa m3/mol
1.03E-03	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	1.04E+02	Pa m3/mol
1.18E-03	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	1.20E+02	Pa m3/mol
8.00E-04	atm m^3/mol	convert to Pa m^3/mol, multiply by	101325	8.11E+01	Pa m3/mol
8.60E-01	mol/kg*bar	convert to Pa m^3/mol, divide by 100,000, multiply by 997 and take reciprocal	0.00997	1.17E+02	Pa m3/mol
7.30E-01	mol/kg*bar	convert to Pa m^3/mol, divide by 100,000, multiply by 997 and take reciprocal	0.00997	1.37E+02	Pa m3/mol
9.70E-01	mol/kg*bar	convert to Pa m^3/mol, divide by 100,000, multiply by 997 and take reciprocal	0.00997	1.03E+02	Pa m3/mol
8.50E-01	mol/kg*bar	convert to Pa m^3/mol, divide by 100,000, multiply by 997 and take reciprocal	0.00997	1.18E+02	Pa m3/mol
1.10E+00	mol/kg*bar	convert to Pa m^3/mol, divide by 100,000, multiply by 997 and take reciprocal	0.00997	9.12E+01	Pa m3/mol
1.20E+00	mol/kg*bar	convert to Pa m^3/mol, divide by 100,000, multiply by 997 and take reciprocal	0.00997	8.36E+01	Pa m3/mol
1.10E+00	mol/kg*bar	convert to Pa m^3/mol, divide by 100,000, multiply by 997 and take reciprocal	0.00997	9.12E+01	Pa m3/mol
1.20E+00	mol/kg*bar	convert to Pa m^3/mol, divide by 100,000, multiply by 997 and take reciprocal	0.00997	8.36E+01	Pa m3/mol
8.60E-01	mol/kg*bar	convert to Pa m^3/mol, divide by 100,000, multiply by 997 and take reciprocal	0.00997	1.17E+02	Pa m3/mol



Solubility

2.51	g/kg	convert to mg/L, multiply by	1000	2510	mg/L

Diffusion Coefficient in Air

Dibromochloromethane

Based on SR7 Section 2.4

	Answer	Units	Calcs		Parameter
Eqn 2-13	0.039319696	mol g-1	0.039319696		Mr
Eqn 2.15	0.002070854	Unitless	0.002070854		B'
Eqn 2.17	1.502025247	Unitless	1.502025247		T*
eqn 2.16	1.198630696	Unitless	1.198630696		Ω
eqn 2.14	**8.24557E-06**	**m2 s-1**	**8.25E-06**		**Da**
eqn 2.18	4.449247961	Å	4.449247961		δAB
	84.9625	$cm^3\ mol^{-1}$	84.9625		Vb

Parameters

	Units		
Mole Weight	g mol-1	208.28	
Boiling point	Kelvin	393.15	120 oC
Density	g cm3	2.451	
tamb	Kelvin	283.15	10 oC
Molcular weight of air	g mol-1	28.97	
Vb	$cm^3\ mol^{-1}$	85	

CHBr2Cl

C	14.8
H	3.7
Br	27
Cl	24.6

Vb calculation source: Fuller, E.N., Schettler, P.D., and Giddings, J.C., A New Method for Prediction of Binary Gas-Phase Diffusion Coefficients, Ind. Eng. Chem., 58, 19-27 (1966). Cited in Lyman, W. J., Reehl, W.F., Rosenblatt, D, H., Handbook for Chemical Property Estimation Methods: Enviornemental Behaviour of Organic Compounds. American Chemical Society, Washington DC., 1990.

Diffusion Coefficient in Water

Based on equation in SR7 Section 2.5 EQN 2.20

Eqn 2.20

Dibromochloromethane	7.14E-10	m2/s

Koc Value Calculated from Kow Value

	Non-hydrophobics	
	Eqn. 2	
Compound	**log Koc**	**log Kow**
Dibromochlorometha	2.14	2.16

Henry's Law Constant

Contaminant	H' (H'=H/RT)	H
	(dimensionless)	(Pa m3 mol-1)
Dibromochloromethane	3.68E-02	9.12E+01

Annex 4: Modelling

CLEA Software Version 1.06

Report generated 19/11/2010

Report title Hauxton Dibromochloromethane

Created by LM at Atkins

Environment Agency

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

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 Average	Homegrown fraction High	Soil loading factor	Preparation correction factor
	$g\ DW\ g^{-1}\ FW$	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	19-Nov-10
Report title	Hauxton Dibromochloromethane
Created by	LM at Atkins

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	Dibromochloromethane	6.21E-01	6.58E-02	6.23E-02	0.05	0.95	1.00	2.54E+03 (sol)	Yes	No
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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	Dibromochloromethane	79.0	20.1	0.9	100.0	6.23E-02	2.26E+00	3.12E-02	2.65E-11	0.00E+00	1.92E-03	3.16E-07	0.00E+00	8.37E-02	1.45E-01	6.07E-02	0.00E+00	0.00E+00	1.42E-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	Dibromochloromethane	4.62E-07	9.93E-05	5.93E-07	1.47E-09	1.78E-03	3.94E-03	1.21E-04	0.02	4.73	0.03	0.00	84.67	0.00	4.78	5.77
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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	Dibromochloromethane	TDI	2	TDI	2	70	2.002	3.68E-02	8.25E-06	7.14E-10	2.14	2.16	0.25	0.5	1	1	1
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Environment Agency

	Oral Health Criteria Value ($\mu g\ kg^{-1}\ BW\ day^{-1}$)		Inhalation Health Criteria Value ($\mu g\ kg^{-1}\ BW\ day^{-1}$)		Oral Mean Daily Intake ($\mu g\ day^{-1}$)	Inhalation Mean Daily Intake ($\mu g\ day^{-1}$)	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	Dibromochloromethane	8.01E-01	1.01E+04	2.51E+03	model	model	model	model	model	model
2										
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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 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 CNPI are listed in the following table:

Chemical Name	CAS Number	Chemical Formula
Dibromochloromethane	124-48-1	$CHClBr_2$
Ethylmethylphenol (isomers)	Inc. 2219-73-0, 6161-67-7, 3855-26-3, 1687-64-5 & 698-71-5	$C_9H_{12}O$
Dimethylnaphthalene (isomers)	Inc. 581-42-0, 581-40-8, 571-61-9, 571-58-4 & 575-41-7	$C_{12}H_{12}$

This annex provides a summary of the physical and chemical properties of each substance, and an assessment of its potential risk to controlled waters using a qualitative or quantitative risk assessment method as appropriate. Either a surrogate substance is selected from amongst the existing priority contaminants for controlled waters (qualitative) if appropriate to the CNPI; or a specific remedial target for the substance has been calculated (quantitative) using the methodology developed in 2007 (Ref 1).

Dibromochloromethane

Synonyms: Chlorodibromomethane; Dibromochloromethane; chlorodibromo; Cdbm; NCI-C55254; Monochlorodibromomethane; Dibromomonochloromethane; Chlorobromoform; DBCM

Dibromochloromethane is a small organic molecule consisting of a single carbon atom bonded to one hydrogen, one chloride and two bromide atoms. It is similar in shape to methane itself however is probably distorted by the presence of the halogens atoms in place of hydrogen atoms in methane.

The physical and chemical properties of dibromochloromethane pertaining to contaminant transport in groundwater, from literature sources, are as follows:

Properties	Units	Values	Reference
Henry's Law	Atm m^3/mol	$7.83x10^{-4}$	Warner HP et al, Determination of Henry's Law Constants of Selected Priority Pollutants. USEPA/600/D-87/229, NTIS PB87-212684 (1987)
K_{OC}	-	84	Swann RL et al; Res Rev 85: 17-28 (1983) Chu W, Chan KH; Sci Total Environ 248: 1-10 (2000)
Half Life (Anaerobic)	days	14 – 56 (i.e. 2 - 8 weeks)	Bouwer EJ et al; Environ Sci Technol 15: 596-9 (1981) Bouwer EJ, McCarty PL; Appl Environ Microbiol 45: 1295-1299 (1983)

There is considered to be sufficient published data on the properties of dibromochloromethane, to generate a conservative remedial target. The risk assessment to calculate the remedial target assumed a conservative compliance concentration at the receptor of 1 µg/l based on dibromochloromethane being a halogenated hydrocarbon. Other halogenated hydrocarbons; including chloroform, carbon tetrachloride, dichloromethane, 1,2-dichloroethane, trichloroethene and tetrachloroethene; have water quality standards (DWS and/or freshwater EQS) in the range 10 to 20 µg/l.

The methodology used to calculate the target was the same as used in the 2007 risk assessment (Ref 1).

Ethylmethylphenol (Non-specific isomer)

Selected Isomers: 4-ethyl-2-methylphenol (2219-73-0), 3-ethyl-5-methylphenol (698-71-5), 2-ethyl-6-methylphenol (1687-64-5), 2-ethyl-4-methylphenol (3855-26-3), 3-ethyl-4-methylphenol (6161-67-7).

Ethylmethylphenol consists of a phenol molecule (i.e. benzene with a hydroxyl group [OH] attached) with an ethyl group [C_2H_5] and a methyl group [CH_3] attached to different carbons on the benzene ring. The various potential positions of the ethyl and methyl groups around the benzene ring mean this substance can exist as several different isomers.

The physical and chemical properties of ethylmethylphenol isomers pertaining to contaminant transport in groundwater have been estimated using EPIWIN software in the absence of published literature on the properties. The EPIWIN predictions of the properties of 3-ethyl-2-methylphenol are as follows:

Properties	Units	Values	Reference
Henry's Law	Atm m^3/mol	$9.06x10^{-7}$ – $1.17x10^{-6}$	EPIWIN Model predictions http://www.chemspider.com/RecordView.aspx?rid=60a1f0e4-1899-4004-b052-ed6b7a053b7b
Log K_{OW}	-	3.1	EPIWIN Model predictions http://www.chemspider.com/RecordView.aspx?rid=60a1f0e4-1899-4004-b052-ed6b7a053b7b
Log K_{OC}	-	3.05	Converted from K_{OW} using equation 70 from Ref 2.
Log K_{OC}	-	3.151	EPIWIN Model predictions http://www.chemspider.com/RecordView.aspx?rid=60a1f0e4-1899-4004-b052-ed6b7a053b7b
K_{OC}	-	1116 – 1416	Converted from Log K_{OC} values (3.05 and 3.151)

Properties	Units	Values	Reference
Half Life	days	15 (water) 30 (soil)	EPIWIN Model predictions http://www.chemspider.com/RecordView.aspx?rid=60a1f0e4-1899-4004-b052-ed6b7a053b7b

There is considered to be some uncertainty that the range of values predicted for 3-ethyl-2-methylphenol will fully represent the risk to controlled waters for all the isomers therefore a margin of safety has been added to the biodegradation rate as the most uncertain property to estimate. A range of biodegradation rate between 30 days and 183 days (i.e. 1 to 6 months) has been applied in the remedial target calculations to account for this uncertainty. The risk assessment to calculate the remedial target assumed a compliance concentration at the receptor of 7.7 µg/l based on current freshwater EQS for phenol.

The methodology used to calculate the target was the same as used in the 2007 risk assessment (Ref 1).

Dimethylnaphthalene (Non-specific isomer)

Selected Isomers: 1,3 dimethylnaphthalene (575-41-7), 1,4 dimethylnaphthalene (571-58-4), 1,5 dimethylnaphthalene (571-61-9), 2,3 dimethylnaphthalene (581-40-8), 2,6 dimethylnaphthalene (581-42-0).

Dimethylnaphthalene is a PAH (polyaromatic hydrocarbon) consisting of a naphthalene molecule of two 6 carbon aromatic rings sharing two carbons, and two methyl groups attached. The substance identified from the Hauxton main site is not specifically one isomer of dimethylnaphthalene and there are many potential isomers.

The physical and chemical properties of a range of isomers of dimethylnaphthalene are summarised from literature sources, are as follows:

Properties	Units	Values	Reference
Henry's Law	Pa m^3/mol	35.5 – 121	Yaws, C.L., Yang, J.C., Pan, X. (1991) Henry's law constants for 362 organic compounds in water. Chem. Eng. November, 179–185.
Log K_{OW}	-	4.31 – 4.42	Yalkowsky, S.H., Valvani, S.C. (1979) Solubilities and partitioning relationships between aqueous solubilities, partition coefficients, and molecular surface areas of rigid aromatic hydrocarbons. J. Chem. Eng. Data 24, 127–129. Yalkowsky, S.H., Valvani, S.C. (1980) Solubility and Partitioning. Solubility of nonelectrolytes in water. J. Pharm. Sci. 69, 912–922
Log K_{OC}	-	4.24 – 4.35	Converted from K_{OW} using equation 70 from Ref 2.
K_{OC}	-	17,259 – 22,138	Converted from log K_{OC}

The reviewed literature did not provide information on the environmental biodegradation half lives of isomers of dimethylnaphthalene specifically.

Half lives in groundwater of PAHs with similar structures and functional groups have been reviewed to establish a conservative half life to apply to dimethylnaphthalene. These are listed in the following table.

Substance	Units	Values	Reference
1-methylnaphthalene	days	1611	Aronson, D. and Howard, P. H. (1997) Anaerobic Biodegradation of Organic Chemicals in Groundwater: American Petroleum Institute
Naphthalene	days	1 – 258	Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., Michalenco, E.M., Editors (1991) Handbook of Environmental Degradation Rates. Lewis Publishers, Inc., Chelsea, Michigan.
Phenanthrene	days	32 - 400	Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., Michalenco, E.M., Editors (1991) Handbook of Environmental Degradation Rates. Lewis Publishers, Inc., Chelsea, Michigan.

The half life of 1-methylnaphthalene (1611 days) is the most conservative value sourced likely to be applicable to the properties of dimethylnaphthalene. 1-Methylnaphthalene is similar in structure and functional groups to dimethylnaphthalene. Utilising this biodegradation rate a remedial target for dimethylnaphthalene has been calculated using the methodology developed in the 2007 risk assessment (Ref 1).

The risk assessment to calculate the remedial target assumed a compliance concentration at the receptor of 0.1 µg/l based on the drinking water standard for PAHs. A compliance concentration of 0.1 µg/l was used in relation to methylnaphthalene, a similar substance, previously assessed as a CNPI at Hauxton.

Summary

In summary, the following recommendations are made as a result of screening the potential risks associated to controlled waters with regard to dibromochloromethane, ethylmethylphenol and dimethylnaphthalene at the Hauxton Main Site.

Sufficient data on the contaminant transport properties of each of these substances were available for a species specific remedial target to be derived for each.

The table overleaf lists the CNPIs calculated remedial targets.

Substances	Priority Contaminant Surrogates	Target Concentration (µg/kg)	
		Inner Zone	Outer Zone
Dibromochloromethane	-	10*	1460
Ethylmethylphenol (all isomers)	-	306	100,000^
Dimethylnaphthalene (all isomers)	-	75.8	100,000#

* Calculated target concentration of 0.12 µg/kg. A limit of 10 µg/kg has been applied as a limit of detection that can be reliably achieved by a commercial laboratory.

^Calculated Target Concentration 3.24×10^9 µg/kg

#Calculated Target Concentration 1.55×10^9 µg/kg

References

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

2 US EPA Document: EPA/540/R-95/128 (July 1996). Soil Screening Guidance: Technical Background Document.