ATKINS

Atkins Limited
The Axis
10 Holliday Street
Birmingham
B1 1TF

Telephone +44 (0)121 483 5000
Fax +44 (0)121 483 5858

info@atkinsglobal.com
www.atkinsglobal.com

Ext No: 5861

Your Ref:
Our Ref: 5036759/23/MAS

18 August 2010

Ms S Walford
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; Grid Cells H10, I10, J10, J11, K10 NAPL, K11, K12, K13 sand & gravel, K13 chalk, L11, L12 and L13

Further characterisation sampling and analysis have identified four 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 (21.07.2010 and 22.07.2010).

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
1-methylnaphthalene, *CAS 90-12-0*	K10 NAPL	TB6, TB69, TB71, TB91, TB92
2-(1-methylpropyl)-4,6-dinitro- phenol (Dinoseb), *CAS 88-85-7*	K10 NAPL	TB6, TB69, TB71, TB91, TB92
	J11	TB88, TB93, TB95
Trichloro benzenamine, Isomer not identified *2,3,4- CAS 634-67-3; or* *2,3,5- CAS 18487-39-3; or* *2,3,6- CAS 88963-39-7; or* *2,4,5- CAS 636-30-6; or* *2,4,6- CAS 634-93-5; or* *3,4,5- CAS 634-91-3*	J10	TB76, TB77
2,3-Dichlorotoluene *CAS 32768-54-0*	J10	TB76, TB77
	H10	TB83
	K13 chalk	TB6, TB87, TB94, TB96
	J11	TB88, TB93, TB95

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The compounds presented in Table 2 are CNPIs that 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.

Six further compounds were identified, however these were encountered and assessed during the site investigation and were deemed not to be priority contaminants.

Table 2 – CNPIs Risk Assessed in previous CNPI reports

Contaminant	Grid squares	Treatment beds
2,4-Dichloro-o-cresol *CAS 1570-65-6*	K10 NAPL	TB6, TB69, TB71, TB91, TB92
	J10	TB76, TB77
	L11	TB80, TB85, TB86
	H10	TB83
	I10	TB84
	L12	TB85, TB86, TB87
	K12	TB6, TB85, TB86, TB87, TB94, TB96
	K13 chalk	TB6, TB87, TB94, TB96
	K11	TB6, TB80
	J11	TB88, TB93, TB95
1-(2-Chloroethoxy)-2-(o-Tolyloxy)-ethane *CAS 21120-80-9*	J10	TB76, TB77
	K13 chalk	TB6, TB87, TB94, TB96
Trichloro toluene Isomers not identified *2,3,4- CAS 30583-33-6 / 7359-72-0; or* *2,3,5- CAS 56961-86-5; or* *2,3,6- CAS 2077-46-5; or* *2,4,5- CAS 6639-30-1; or* *2,4,6- CAS 23749-65-7; or* *3,4,5- CAS 21472-86-6*	I9	TB59-60
	J10	TB76, TB77
	H10	TB83
	I10	TB84
	K13 chalk	TB6, TB87, TB94, TB96
	J11	TB88, TB93, TB95

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

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.

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Table 3 – Surrogates Used

Contaminant	Surrogates	
	Human Health	Controlled Waters
1-methylnaphthalene	Benzene	-
2-(1-methylpropyl)-4,6-dinitro-phenol (Dinoseb)	-	-
Trichloro benzenamine	Vinyl chloride	-
2,3-Dichlorotoluene	Vinyl chloride	-

The CNPIs, derived or surrogate 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 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, 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.

For some CNPIs the derived Remedial Targets may be below the lowest commercially achievable LOD. In these instances, as was done for the already established contaminant of concern, the Remedial Target will be set at the lowest commercially achievable LOD. As a result, some restrictions, such as not placing the treated soils within 1m of final site levels and/or not within 20m of Riddy Brook may be imposed.

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	
1-methylnaphthalene	1790	Do not place in Inner Zone	Do not place at <1m depth	Do not place in Inner Zone	100
2-(1-methylpropyl)-4,6-dinitro- phenol (Dinoseb)	330	Do not place in Inner Zone	Do not place at <1m depth	Do not place in Inner Zone	100
Trichloro benzenamine	200,000	Do not place in Inner Zone	Do not place at <1m depth	Do not place at <1m depth	100
2,3-Dichlorotoluene	100,000	Do not place in Inner Zone	Do not place at <1m depth	Do not place at <1m depth	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 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.

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Yours sincerely
For and on behalf of Atkins Limited

Mark Smith
Project Manager

Cc Eileen Young – Environment Agency
Nigel Blazeby - South Cambridgeshire District Council

Enc.

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

Introduction

Laboratory analysis 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:

- Dinoseb (CAS No. 88-85-7)
- 1-Methylnaphthalene (CAS No. 90-12-0)
- 2,3-Dichlorotoluene (CAS No. 32768-54-0)
- Trichlorobenzenamine (CAS No. unspecified – six isomers of this compound exist)

Surrogates were adopted for the evaluation of three of these compounds, as detailed in Annex 2. These compounds are 1-methylnaphthalene, 2,3-dichlorotoluene and trichlorobenzenamine. The selection of surrogates is discussed further in this Annex, and in Annex 2.

GACs were derived for the remaining CNPI, namely dinoseb.

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 both of these documents, Atkins have 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 dinoseb, 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 1-methylnaphthalene, data are available for the toxicological data via the oral route of exposure which has been obtained by the Environmental Industries Commission (EIC) in their *Soil Generic Assessment Criteria for Human Health Risk Assessment* report. However, there was insufficient data to agree a HCV for the inhalation route of exposure, and there is enough evidence to suggest that 1-methylnaphthalene is significantly more toxic when inhaled than when ingested. Therefore, due to the fact that the CLEA model predicts inhalation to be a significant route of exposure for this compound, route-to-route extrapolation was considered inappropriate for derivation of an inhalation HCV. The structurally similar compounds naphthalene and benzene were considered for use as surrogates. Benzene was selected since a comparison of oral toxicity shows that 1-methylnaphthalene is comparatively more toxic than naphthalene, but less so than benzene.

For both 2,3-dichlorotoluene and trimethylbenzenamine, 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 Appendix A.

Physical and Chemical Data

In the derivation of appropriate physical and chemical data 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. In addition, due to the limited available physical and chemical data available, converting the already estimated value to 10°C, using estimated values would introduce further 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 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 dinoseb a DAF value of 0.5 was utilised and considered as a suitably conservative value based on an experimental study on dermal absorption. 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
Dinoseb	2.12E-01	6.16E-02	4.77E-02

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
1-Methylnaphthalene	4.93E-02
Dinoseb	4.77E-02
2,3-Dichlorotoluene	5.00E-04
Trichlorobenzenamine (all isomers)	5.00 E-04

Annex 2: Toxicological Data

SOURCE DATA CHECK LIST

Chemical name: 2,3-DICHLOROTOLUENE

Common name:

CAS RN: 32768-54-0

Source	Checked? (Y/N)	Type of Data found
		UK Sources
Food Standards Agency	Y	NO DATA
Health Protection Agency	Y	" "
Health and Safety Executive	Y	" "
Health and Safety Laboratory	Y	" "
UK Drinking Water Inspectorate	Y	" "
Pesticide Safety Directorate	Y	" "
COC	Y	" "
COM	Y	" "
COT	Y	" "
COMEAP	Y	" "
Expert panel an Air Quality Standards	Y	" "
		EU Sources
European Chemicals Bureau	Y	VERY LITTLE DATE ONLY CHEM STRUCTURE AVAILABLE.
European Food Safety Authority	Y	NO DATA
ECETOC	Y	NO DATA
		International
IPCS INCHEM:	Y	NO DATA
IARC	Y	"
PIM	Y	"
EHC	Y	"
HSG	Y	"
PDS	Y	"
JECFA	Y	"
JMPR	Y	NO DATA
OECD SIDS	Y	" "
CICADS		
WHO:	Y	NO DATA

Guidelines for DW Quality	Y	NO DATA
Air Quality Guidelines for Europe	Y	NO DATA
Foreign National		
RIVM MPR	Y	NO DATA
Health Canada Tox Ref Values	Y	NO DATA. OSHA, CAS NO. FULL NAME + DICHLOROTOLUENE
US EPA:	Y	FOR SU/SU LIMIT FOR DETERMINAND.
AEGL	Y	NO DATA
Health Advisories	Y	SI + SU WERE FOR DETERMINAND NY
IRIS	Y	NO DATA
ATSDR	Y	YES FOR DICHLOROTOLUENE ONLY
Other		
TOXNET (including TERA)	Y	NO DATA
Pubmed	Y	NO DATA

Type of Data Found: This section should contain the following codes for easy classification of data found. Acronym should be separated with ';' or '/'

CID: Chemical Identification
TKn: Toxicokinetics (data on absorption, distribution, metabolism and excretion round the organism)
AT: Acute Toxicity
SaT: Subacute Toxicity (short term repeat dose studies)
ScT: Subchronic Toxicity (longer-term studies)
CT: Chronic Toxicity (long-term toxicity data)
RT: Reproductive Toxicity
DT: Developmental Toxicity (specific to developmental effects in offspring)
GT: Genotixicity
C: Carcinogenicity
O: Other

Originated By: ZA _____ **Date:** 28.07.10

Checked By: T.A. _____ **Date:** 29/07/2010

TOXICOLOGICAL DATA SUMMARY FOR 2,3-DICHLOROTOLUENE

Chemical name: __2,3-Dichlorotoluene_____

Common name/ synonyms: Benzene, 1,2-dichloro-3-methyl, Benzyl dichloride; Benzylene chloride; Benzylidine chloride; Chlorobenzal; (Dichloromethyl)benzene; Dichlorophenylmethane.

CAS RN: __32768-54-0_____

Chemical Identification:
The density, melting point and boiling point of 2,3-dichlorotoluene are reported as1.228 g/mL at 25°C; 6°C; and 207-208°C, based on information collated from a number of literature sources within a secondary source (Lookchem, 2010).

Sources
No data are available in open literature.

Toxicokinetics
No data are available in open literature.

Acute Toxicity
There are no readily available data in open literature for 2,3-dichlorotoluene. However, data are available for 2,4-dichlorotoluene:

The LD_{50} in acute oral toxicity studies in rats were reported as >2,000 mg/kg or 2,790 mg/kg. Also, the LC_{50} in an acute inhalation toxicity study in rats was >2,669 mg/kg over 4 hours (OECD, 1994).

Repeat dose studies (Sub-acute and sub-chronic toxicity)
There are no readily available data in open literature for 2,3-dichlorotoluene. However, data are available for 2,4-dichlorotoluene and are discussed below.

Oral
There is only one key study on repeated dose toxicity of 2,4-dichlorotoluene. Male and female SD rats were orally administered (gavage) at doses of 0, 12.5, 79 and 500 mg/kg bw/day. In male rats, the administration period was two weeks prior to mating, 2 weeks of mating and 2 weeks after the completion of the mating period. In females, in addition to a maximum four weeks pre-mating and mating period, they were exposed through pregnancy until day 3 of post delivery (OECD, 1994).

Dose dependent salivation was noted immediately after administration in all treated groups. Decreases in body weight gain were noted in the females of the 500 mg/kg bw/day group at the gestation and lactation periods. In food consumption, decreases were noted in both sexes of the 500 mg/kg bw/day groups. In haematological and blood chemical examinations, decreases in platelet count, alfaglobulin fraction, triglyceride and blood urea nitrogen, and increase in cholinesterase were noted in the 500 mg/kg bw/day male group. In the 500 mg/kg bw/day group, increased relative liver weights in both sexes, and relative kidney weights in the males were noted. In autopsy, dark brown discoloration of the liver was noted in 500 mg/kg bw/day male group. In histopathological examination of the liver, centrilobular swelling of hepatocytes was noted in all males of the 500 mg/kg bw/day group and 2 males of the 79 mg/kg bw/day group. In kidneys, atrophy and regeneration of tubular epitherium, and dilation of tubules were noted in the 79 mg/kg bw/day groups and above. In addition, the number of the males with hyalin droplets and eosinophilic depositions in tubular epitherium increased progressively in the 79 mg/kg bw/day and 500 mg/kg bw/day groups. On the basis of above-described effects, the no observed effect level (NOEL) for this compound was indicated to be less than 12.5 mg/kg bw/day (OECD, 1994).

Subchronic Toxicity (longer-term/medium duration studies)
No data are available in open literature.

Chronic Toxicity (long-term toxicity data)
No data are available in open literature.

Reproductive Toxicity
There are no readily available data in open literature for 2,3-dichlorotoluene. However, data are available for 2,4-dichlorotoluene.

2,4-dichlorotoluene was studied for oral toxicity in rats at doses of 0, 12.5, 79, 500 mg/kg bw/day. Although this combined study was designed to investigate reproductive capability in parental generation as well as development in F1 (first generation) offspring, parameters to evaluate developmental toxicity were limited to only body weights at day 0 and day 4 after birth, and autopsy findings at day 4 (OECD, 1994).

Regarding reproductive ability, all pairs in the 12.5 and 79 mg/kg bw/day groups achieved pregnancy. In the 500 mg/kg bw/day group, 12 pairs showed evidence of copulation with a sperm positive vaginal smear. However, only five pairs out of these achieved pregnancy. Vaginal plugs (used as an indication of successful mating) were not noted in six non-pregnant pairs in the 500 mg/kg bw/day group. Comparatively few sperm were also found following examination of this test group in the vaginal smears. The report authors state that this result suggests that the male reproductive organs and secondary reproductive organs had functional disorders. Regarding body weight changes of pups, decreases in liver and body weights were noted in the 500 mg/kg bw/day group on day 1 of lactation. No adverse effects on delivery, lactating behaviour of dams, viability or general appearance on autopsy related to exposure to 2,4-dichlorotoluene were noted. On the basis of above-described effects, the NOEL for reproductive/ developmental toxicity for both sexes was considered to be 79 mg/kg bw/day (OECD, 1994).

Developmental Toxicity
No data are available in open literature.

Genotoxicity
There are no readily available data in open literature for 2,3-dichlorotoluene. However, data are available for 2,4-dichlorotoluene.

Although the International Agency for Research on Cancer (IARC) does not provide detailed study data, it states that benzal chloride (dichlorotoluene) is a bacterial mutagen (IARC, 1999). However, it has also been reported that 2,4-dichlorotoluene showed no genotoxic effects in bacteria or in a chromosomal aberration test *in vitro* (OECD, 1994).

Carcinogenicity
There are no readily available experimental or epidemiological data in open literature sources specific to for 2,3-dichlorotoluene or 2,4-dichlorotoluene. However, benzal chloride (dichlorotoluene) is included in a review by the International Agency for Research on Cancer (IARC), as detailed below.

Other Irritation and Sensitisation
There are no readily available data in open literature for 2,3-dichlorotoluene. However, data are available for 2,4-dichlorotoluene.

2,4-dichlorotoluene is reported to cause eye irritation and may cause chemical conjunctivitis and corneal damage. It also causes skin irritation and dermatitis and may cause cyanosis of the extremities. It also causes respiratory tract irritation (OECD, 1994).

Background exposure (food, drinking water, air)
No relevant data are available in open literature for 2,3-dichlorotoluene or 2,4-dichlorotoluene.

Regulatory guidelines/ advisories/ guideline values

International Agency for Research on Cancer
IARC states that '*there is limited evidence in experimental animals for the carcinogenicity of benzal chloride (dichlorotoluene). Combined exposures to alpha-chlorinated toluenes (*such as 2,3-dichlorotoluene*) are probably carcinogenic to humans (Group 2A)'* (IARC, 1999).

Selection of Health Criteria Value (HCV)

There are no readily available data in open literature for 2,3-dichlorotoluene. There is also insufficient data for derivation of an HCV, based on data for the isomer, 2,4-dichlorotoluene. In the light of this, and the potential for carcinogenic effects, Atkins considers that the toxicity data for other compounds should be considered for use as surrogates.

Based on the chemical structure, toluene, benzene and vinyl chloride are considered to be the most suitable surrogate compounds for evaluation of 2,3-dichlorotoluene. Although the structure of this compound (2,3-dichlorotoluene) has greater similarity to the structure of benzene and toluene, there is potential for comparatively increased toxicity due to the presence of halide substituents (such as chlorine) to the basic benzene or toluene structure. Therefore, since chlorine is present in both 2,3-dichlorotoluene and vinyl chloride, vinyl chloride has also been considered for adoption as a surrogate.

The toxicity data for vinyl chloride is more conservative than that of either benzene or toluene, and is considered to be more appropriate for the evaluation of the potential toxicity of 2,3-dichlorotoluene. This is likely to provide a suitable means of assessing the presence of additional chlorine substituents, which could result in toxic properties that exceed that of benzene or toluene. Therefore, **vinyl chloride is adopted as a surrogate compound for evaluation of 2,3-dichlorotoluene**.

Although there is physical and chemical data for 2,3-dichlorotoluene, due to the potential for genotoxic effects and a paucity of data for other endpoints, it is suggested that the physical and chemical data for vinyl chloride should also be retained for use. This is a conservative approach which takes into account a comparatively higher degree of volatility for vinyl chloride when assessing the behaviour of 2,3-dichlorotoluene in soil.

References

Chemcas, 2010. Summary Data on 2,3-dichlorotoluene
http://www.chemcas.com/material/cas/archive/32768-54-0.asp

IARC, 1999. Group evaluation for chlorinated toluenes and benzylchloride
http://www.inchem.org/documents/iarc/vol71/013-chltoluenes.html

Lookchem, 2010:
http://www.lookchem.com/2-3-DICHLOROTOLUENE/#Chemistry

OECD, 1994. SIDS for 2,4-dichlorotoluene.
http://www.inchem.org/documents/sids/sids/95738.pdf

Pubmed chemical database substance summary, 2010:
http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?sid=88810792&loc=es_rss#Subinfo

Saint Regis Mohawk Tribe Environmental Division, Water Quality Standards, August 2007:
http://www.epa.gov/waterscience/standards/wqslibrary/tribes/srmt_2_%20wqs.pdf

TOXICOLOGICAL DATA SUMMARY FOR DINOSEB

Chemical name: __2-sec-Butyl-4,6-dinitrophenol _____

Common name/ synonyms: __Dinoseb, DNBP, 2-sec-Butyl-4,6-dinitrophenol, 2-(1-Methylpropyl)-4,6-dinitrophenol 2,4-Dinitro-6-(1-methylpropyl)phenol and 2,4-Dinitro-6-sec-butylphenol, Chafer Dinosol, Farmon Desicoil, Haulmex, Haulmone, and Super Haulmone (other trade names of formulations with or without other active ingredients are also available)_____

CAS RN: __88-85-7 _____

Chemical Identification:

Pure dinoseb is a yellow or orange crystalline solid (Environment Agency, 2010). Dinoseb is combustible and explosive. Technical dinoseb has a melting point between 38 and 42°C and the pure compound is very soluble in water (52 g/L at 20°C) and in most organic solvents. Dinoseb has a vapour pressure of 10 Pa at 20°C (IPCS INCHEM, 1994).

Prior to it being withdrawn from use, it was rated by the World Health Organisation (WHO) as highly hazardous[1] (Environment Agency, 2010).

Occurrence and Use

Dinoseb was introduced as a contact herbicide in the 1950s. It has formerly been used on cereals, lucerne and peas, and as a pre-emergent herbicide (applied before the crop plants emerge from the ground) on beans, potatoes, hops, strawberries and raspberries. The Environment Agency states that dinoseb is banned in the UK and the rest of the EU and believe that it is no longer manufactured or marketed as a plant protection product. It has been banned from use in the UK since 1988 because of concerns over its toxicity (Environment Agency, 2010).

The main source of dinoseb release to the environment occurred through its former application to agricultural crops, but some may also escape during manufacture, transport or storage of the chemical. There are believed to be no natural sources of release to the environment. (Environment Agency, 2010).

Toxicokinetics

Dinoseb is absorbed through the skin, inhaled and can irritate eyes causing temporary blindness if it comes into contact with the eyes (INCHEM, 1994).

Dinoseb containing radioactively labelled carbon atoms was applied as either a solid, aqueous paste, suspension, or dissolved in the volatile vehicle ethanol. Dermal absorption of DNBP-derived radioactivity was approximately 50% of the recovered dose[2] after application in the four physical forms, and the major route of excretion was via the urine. Following this exposure, it is reported that twelve percent of the absorbed dose of DNBP was retained in the body 120 hrs (5 days) after exposure. The data indicate that the dinoseb can penetrate the skin as readily when applied either as a solid, aqueous paste, or suspension, as when applied in the volatile vehicle ethanol (Hughes et al, 1992)). Although data are limited, evidence in this study indicates that a significant amount of dermally exposed dinoseb is absorbed via the skin of rodents, and a conservative **dermal absorption fraction (DAF) of 0.5** would be appropriate as a conservative modelling parameter.

[1] The WHO pesticide classification scheme is based on a comparison of the acute toxicity of a substance, its form (solid, liquid or gas) as well as its concentration within the formulation that it is used in.

[2] During dermal exposure studies, the recovered dose can refer to the amount recovered via various methods of excretion, and within tissue samples. Although not explicitly stated in the readily available data, it can be assumed that this substance was extensively absorbed based on the proportion of the recovered dose that was assumed to be absorbed.

[2] During dermal exposure studies, the recovered dose can refer to the amount recovered via various methods of excretion, and within tissue samples. Although not explicitly stated in the readily available data, it can be assumed that this substance was extensively absorbed based on the proportion of the recovered dose that was assumed to be absorbed.

Acute Toxicity

The acute toxicity of dinoseb is high, with oral LD_{50}s of 37 to 58 mg/kg bw for rats and 25 mg/kg bw for guinea pigs. The acute percutaneous LD_{50} is 50 mg/kg for rats, 80 to 200 mg/kg for rabbits and 500 mg/kg for guinea pigs. Mild skin and eye irritations have also been observed in rabbits (Health Canada, 1991).

In other studies, the inhalation LC50 of 35-130 mg/m³ for 4-hr exposure in rats was reported, and laboured breathing and decreased activity were observed. The dermal LD50 is 40-146 mg/kg bw in rabbits, and decreased activity, salivation, nasal discharge, increased respiratory rate and ataxia were found. The oral LD50 is reported to be 5-50 mg/kg bw in rats, and prone position, bradypnea (slow breathing), diarrheal stool and decreased motor activity were noted (SIAM, 2007).

Irritation and sensitisation

It has been reported that dinoseb is highly irritating to the eye in rabbits (SIAM, 2007). Inhalation of dusts and sprays may be irritating to the lungs and eyes, and may cause serious illness (ATSDR, 2003).

Repeat dose studies (subacute and subchronic toxicity data)

In a 90-day dog study conducted in 1967 in which dinoseb was administered in the diet at 0, 50, 100 or 200 ppm, effects on the heart (endocarditis) were noted at the highest dose level; the no-observed-adverse-effect level (NOAEL) was 100 ppm, or approximately 3.8 mg/kg bw/day (Health Canada, 1991).

In male rats given dinoseb (99% purity) at dietary concentrations of 0, 1.35, 2.7, 5.4 or 13.5 mg/kg per day in food for six months, increased liver weight was observed at 5.4 mg/kg per day, as was increased mortality at the highest dose level (Health Canada, 1991).

It has been reported that dietary levels of about 25 mg/kg/day in food caused marked food refusal and some deaths after five or more doses, although the the study duration has not been reported. Lower doses (5 to 20 mg/kg/day in food) were also reported to cause statistically significant decreases in growth (EXTOXNET, 2010)

Chronic Toxicity (long-term toxicity data)

In an unpublished report from Dow Chemical Company (1981) male and female mice were fed diets containing dinoseb at 0, 1, 3, and 10 mg/kg/day for 100 weeks. Survival was not affected by exposure to the chemical. However, body weight gain was significantly reduced in the mid- and high-dose females. At the end of the study, the body weight gain was 10 and 13% less than the controls of the mid- and the high-dose females, respectively, and no differences were found in the food consumption in the treated group against controls. (US EPA IRIS, 2003).

Reproductive Toxicity

In a three-generation (later extended to five generations) rat reproduction study, four groups (25 per sex per group) rats were exposed to dinoseb in the diet at doses of 0, 1, 3 or 10 mg/kg bw per day for 29 weeks. The study authors report a consistent, compound-related depression in parental body weight gain at the high dose in both sexes in the pre-mating period in all three generations, which persisted into later study periods. No reproductive effects were observed other than a slight non-significant reduction in the number of progeny in the F_1 (first) generation, although a statistically significant decrease in pup weight was observed 21 days post-partum at the highest dose level (US EPA IRIS, 2003).

Based this study, Health Canada determined that the no observed adverse effect level (NOAEL) for male reproductive toxicity in this study was 10 mg/kg bw per day. The NOAEL based on decreased body weight gain in parents and offspring was 3 mg/kg bw per day (Health Canada, 1991).The subsequently depressed pup weight gains during the lactation period was taken as a reproductive effect, and a reproductive lowest effect level (LEL) of 1 mg/kg/day was determined (US EPA IRIS, 2003).

In a two-generation reproduction study (continued from the three-generation study above) in rats, a reproduction lowest effect level (LEL) of 1 mg/kg bw/day was reported based on consistent decreases in gonadal weights and gonadal weights/body weight ratios in the fourth generation at all dose levels. A systemic LEL of 1 mg/kg bw/day was also reported, based on treatment-related or dose-related reductions in relative parental body weights with significant decreases at low and high doses in third generation males (US EPA IRIS, 2003).

Diets of 225 or 300 ppm dinoseb resulted in marked oligospermia (reduction in the number of spermatozoa in the semen), extensive damage to the seminiferous tissues of surviving rats and irreversible reproductive failure. In rats fed 150 ppm, decreased epididymal sperm counts, abnormal epididymal spermatozoa and histologic changes in the testes were observed; reproduction was unaffected, and the anomalies appeared to be reversible in the 16 weeks following treatment. There were no detectable effects in rats fed 75 ppm. Mating behaviour and libido appeared to be unaffected at all concentrations. The NOAEL observed for this study was 75 ppm (3.8 mg/kg bw per day). Health Canadas state that adverse effects on testes, spermatozoa and sperm motility have also been reported in other experiments on rats, at dose levels of 7.5 mg/kg bw and higher (Health Canada, 1991).

In an unpublished report from Dow Chemical Company (1981) reported above, male and female mice were fed diets containing dinoseb at 0, 1, 3, and 10 mg/kg/day for 100 weeks. In addition to other effects, reproductive organs in males and females were also affected. Adverse effects on the lining of the womb (cystic endometrial hyperplasia) and atrophy were observed in females, and hypospermatogenesis (reduction in sperm production) and degeneration were seen in the testes of all the treated males (US EPA IRIS, 2003).

A primary study has been obtained from data available in the open literature, which has not been assessed by authoritative bodies. This study reports that gavage and feeding doses of dinoseb resulted in testicular toxicity. Consecutive doses of dinoseb by gavage seemed to induce spermatotoxicity by disturbing spermiogenesis or the maturation process of sperm in the epididymis, and the most probable target cells of spermatotoxicity were thought to be testicular spermatids in rats. Prolonged exposure to dinoseb in the diet also induced testicular toxicity in rats. However, the feeding dose of dinoseb irreversibly affected the early stage of spermatogenesis and produced infertility in rats. The study authors report that further studies in laboratory animals are required for clarification of their testicular toxicity and for risk assessment in humans (Matsumoto et al, 2008a).

In another study obtained from data available in the open literature, which has not been assessed by authoritative bodies, the study authors describe a combined repeated dose toxicity study with reproduction/developmental toxicity screening test. Rats were dosed with dinoseb, by gavage at 0 (vehicle only), 0.78, 2.33, or 7.0 mg/kg bw/day. Six males per group were dosed for a total of 42 days beginning 14 days before mating. Twelve females per group were dosed for a total of 44-48 days beginning 14 days before mating to day 6 of lactation throughout the mating and gestation period. Recovery groups of six males per group and nonpregnant six females per group were dosed for 42 days followed by a 14-day recovery period (Matsumoto et al, 2008b).

No deaths were observed in males of any dose group or in females of the recovery groups. At 7.0 mg/kg bw/day, eight females died and two animals were moribund during late pregnancy, and a significant decrease in body weight gain was found in both sexes. Adverse effects to blood parameters were reported at 0.78 mg/kg bw/day and above in the main group males at the end of administration period. Reduction in extramedullary haematopoiesis (production of red blood cells) in the spleen was significant at 2.33 mg/kg bw/day in the main group females. Sperm analysis revealed a decrease in sperm motility and an increase in the rates of abnormal sperm, abnormal tail, and abnormal head at 7.0 mg/kg bw/day. A number of dams delivered their pups and the number of dams with live pups at delivery was significantly lowered in the 7.0 mg/kg bw/day group (Matsumoto et al, 2008b).

The study authors report that the lowest observed adverse effect (LOAEL) for males was 0.78 mg/kg bw/day, based on the adverse effects on blood parameters. A NOAEL could not be

established for this effect due to the absence of a lower dosing concentration in this study. The NOAEL for effects on females was 0.78 mg/kg bw/day based on a reduction in extramedullary haematopoiesis. The NOAEL for reproductive toxicity was considered to be 2.33 mg/kg bw/day based on decrease in sperm motility and an increase in the rates of abnormal sperm, as well as reduced number of total and live deliveries (Matsumoto et al, 2008b).

Developmental Toxicity

In a developmental toxicity study, four groups of 25 rats were administered dinoseb (96.1% purity) orally by gavage at levels of 0, 1, 3 or 10 mg/kg bw per day on days 6 through 15 of gestation. Food consumption and body weight gain of highest-dose females were slightly depressed during the dosing interval but were comparable to those of other groups at the end of the experiment. No other effects were observed in females. Foetuses at the highest dose showed a slight decrease in body weight, increased incidence of skeletal ossification at a number of sites and an increase in the number of supernumerary ribs and absence of thoracic vertebrae; the latter were also absent at 3 mg/kg bw per day. A NOAEL of 1 mg/kg bw per day was identified for foetal effects, based on absence of thoracic vertebrae at the next highest dose of 3 mg/kg bw per day (Health Canada, 1991).

In an oral rabbit teratology study, four groups of 16 Chinchilla rabbits were exposed by oral gavage to dinoseb (98% purity) at levels of 0, 1, 3 or 10 mg/kg bw per day on days 6 through 18 of gestation. In the highest dose group, statistically significant increases in malformations and anomalies were observed in 11 of 16 litters examined. The major developmental toxic effects were neural tube defects, and adverse effects on the skeletal system. The NOAEL for foetal effects was 3 mg/kg bw per day based on the occurrence of neural tube defects at the highest dose level of 10 mg/kg bw per day (Health Canada, 1991).

In a third study obtained from data available in the open literature, pregnant rats were given dinoseb by gavage at 0, 8.0 or 10 mg/kg bw/day on days 6-15 of gestation, or in the diet at 0, 120 or 200 ppm (0, 6.52 or 8.50 mg/kg bw/day) on days 6-16 of gestation, and litters were evaluated on day 20 of gestation. Maternal toxicity was observed as evidenced by significantly decreased body weight gain and reduced food consumption during the administration period in all the dinoseb-treated groups, and two dams died at 10 mg/kg bw/day. Significantly lower foetal weights and delayed skeletal ossification were observed in the dinoseb-treated groups except for the group fed dinoseb at 120 ppm. The teratogenic potential of the gavage dose of dinoseb was confirmed as evidenced by increased incidences of foetuses with external and skeletal malformations at 10 mg/kg bw/day. The incidence of foetuses with microphthalmia (comparatively reduced eye size) was significantly increased at this dose. On the other hand, study authors report that feeding doses of dinoseb up to 200 ppm did not induce teratogenicity in this study and that these data indicate that dinoseb is teratogenic at maternally toxic doses, but the exposure range of dinoseb at which malformations occur seems to be narrow (Matsumoto et al, 2010)

Genotoxicity

It is reported that dinoseb (2-sec-Butyl-4,6-dinitrophenol) was not mutagenic in bacteria [OECD TG 471 and 472] and did not induce chromosomal aberrations in mammalian cells in vitro [OECD TG 473] either with or without metabolic activation (SIAM, 2007). It did not induce gene mutations either in S. typhimurium TA100, TA1535, TA98 or TA1537 or in E. coli WP2 uvrA strains with or without S9 mix. Health Canada also report that based on the available studies, there is no strong evidence of the mutagenic potential of dinoseb (Health Canada, 1991).

Carcinogenicity

In an oncogenicity study conducted in CD-1 mice (50 per sex per dose) administered doses of 0, 1, 3 or 10 mg/kg bw per day in the diet for 100 weeks, a NOAEL of 1 mg/kg bw per day was observed in mice based on cataractogenesis in both sexes at 3 and 10 mg/kg bw per day (Health Canada, 1991).

In an unpublished report from Dow Chemical Company (1981) male and female CD-1 mice (70/sex/group) were fed diets containing dinoseb at 0, 1, 3, and 10 mg/kg/day for 100 weeks. Dinoseb induced statistically significant increases in liver adenomas in female mice at the 3 and 10 mg/kg/day doses. The incidence was 0/57, 4/59, 7/60, and 5/58 for control through 10 mg/kg/day doses, respectively. Only one carcinoma was observed (in a low-dose female). There were no decreases in latency period, no dose-response and no hepatocytic change commonly associated with carcinogens. The tumours were late-appearing (the first tumour appeared after 78 weeks, and the remaining ones after 100 weeks) (US EPA, 2003).

Two strains of mice were exposed to dinoseb for 18 months. The animals were first exposed via gavage at 2.15 mg/kg/day for three weeks beginning at one week of age, then they were fed a diet containing 7 ppm dinoseb (1.05 mg/kg/day) throughout the observation period of approximately 18 months. Equal numbers of mice served as controls. After 18 months of treatment, dinoseb did not cause any significant increase in tumours in mice (US EPA, 2003).

Based on research undertaken by Health Canada, there is no strong evidence of the carcinogenic potential of dinoseb. However, Health Canada considers that additional two-year chronic feeding and oncogenicity studies in rats are required to clarify its status (Health Canada, 1991).

Dinoseb induced statistically significant increases in liver adenomas in female mice at the 3 and 10 mg/kg/day doses. The incidence was 0/57, 4/59, 7/60, and 5/58 for control through 10 mg/kg/day doses, respectively. Only one carcinoma was observed (in a low-dose female). There were no decreases in latency, no dose-response and no hepatocytic change commonly associated with carcinogens. The tumors were late-appearing (the first tumor appeared after 78 weeks, and the remaining ones after 100 weeks) (US EPA IRIS, 2003).

Other

It is reported that dinoseb interferes with cellular conversion of food molecules (such as glucose) into useable energy for the body. Specifically, it disturbs the production of adenosine triphosphate (ATP) in the mitochondria of the cells, ATP being the molecule that provides energy for all cellular activities. This may account for many of the toxic effects caused by dinoseb (EXTOXNET, 2010).

Background exposure

Dinoseb was detected in 14 of 406 samples taken from municipal and private water supplies in Canada between 1978 and 1987 and the highest concentration recorded was 16.2 mg/L, However, none of the 900 samples of 115 municipal drinking water supplies in had detectable levels of dinoseb (during 1984 to 1990). In the United States, dinoseb was found in one of 79 surface water samples at a maximum concentration of 1 mg/L (Health Canada, 2003). Health Canada also reports that few data are available pertaining to residues of dinoseb in consumer food products, but crops treated with dinoseb showed no detectable residues.

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

Regulatory guidelines/ advisories/ guideline values

Health Canada

Health Canada states that the principal toxic effects of dinoseb that are of concern are its teratogenic and foetotoxic effects at doses below those that cause maternal toxicity and its potential as a cataract-inducing agent. In a recent rat study in which dinoseb was administered by gavage, skeletal anomalies were observed at 3 mg/kg bw per day and higher; the NOAEL was 1 mg/kg bw per day This finding was supported by an oral teratology study in rabbits in which the NOAEL for neural tube defects was 3 mg/kg bw per day; a dermal teratology study in rabbits with a NOAEL of 1 mg/kg bw per day; and a 100-week dietary study in mice in which the NOAEL for cataract formation was 1 mg/kg bw per day. They derived an acceptable daily intake (ADI) as follows:

$$\text{ADI} = \frac{1 \text{ mg/kg bw per day}}{1000} = 0.001 \text{ mg/kg bw per day}$$

where:

1 mg/kg bw per day is the NOAEL for the rat reproduction study
1000 is the uncertainty factor (x10 for intraspecies variation; x10 for interspecies variation; and x10 for teratogenicity, considered to be a serious effect; in addition, there are limitations in the toxicity data base--i.e., other toxicological studies are needed).(Health Canada, 1991)

United States Environmental Protection Agency
The US EPA has derived an oral Reference dose of 0.001 mg/kg bw/day, based on a reproductive LEL of 1 mg/kg/day. An uncertainty factor of 1000 was applied to account for uncertainties in the extrapolation from laboratory animals to humans (factor of 100), as well as concern for the lack of a no observed effect level (NOEL) in the reproduction study (factor of 10) (US EPA IRIS, 2003).

Selection of Health Criteria Value (HCV)

Oral Health Criteria Value (HCV)
The oral RfD derived by the US EPA (US EPA IRIS, 2003) and Health Canada (2003) of 1 µg/kg bw/day (0.001 mg/kg bw/day) has been selected for use as a point of departure by Atkins. An additional safety factor of 5 has been applied to this, to account for more recent studies (Matsumoto et al, 2008b) in which a LOAEL 0.78 mg/kg/day was obtained, based on adverse effects on the blood of male rats. This effect was observed at the lowest test dose, and a NOAEL was not identified for this effect. However, a factor of 5 is considered to be appropriate to account for the effect observed in male rats, which differs in severity from the reproductive and developmental effects previously identified as the critical effect of exposure to dinoseb by the US EPA and Health Canada. Atkins considers that the resultant TDI would be protective of the critical effect for which a number of studies have been identified with effects occurring at similar levels, as well as the potential effect identified in a single study in male rats.
Therefore, the TDI_{oral} is 0.2 µg/kg bw/day (0.0002 mg/kg bw/day).

Oral Mean Daily Intake (**MDI)**

Food
There are no readily available data on exposure to dinoseb via food. However, as it is no longer licensed for use in food products in the UK or Europe, exposure via dietary sources is assumed to be negligible.

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 dinoseb per day, assuming that all 'other' pesticide is made up of dinoseb, for an adult consumer. This is equivalent to a dose of 0.00286 µg/kg bw/day (0.00000286 mg/kg bw/day). This is a conservative approach accounting for the fact that it may still be present in water abstracted for drinking water supply, due to previous use.

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

Therefore:
MDI_{oral} for 70 kg adult = 0.2 µg/day
= 0.00286 µg/kg bw/day
= 0.00000286 mg/kg bw/day.

Therefore, the Tolerable Daily Soil Intake (TDSI)$_{oral}$ for an adult is:
TDI – MDI = (0.2-0.00286) µg/kg bw/day
= 0.197 µg/kg bw/day
= 0.000197 mg/kg bw/day

This HCV compares favourably with the acute oral exposure value.

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 0.2 µg/kg bw/day** (0.0002 mg/kg bw/day). Assuming the 70kg adult inhales 20m³ air per day, this is also equivalent to 0.0007 mg/m³ per day.

There are no readily available data on ambient air concentrations of dinoseb. However, as it is no longer approved for use in the UK, exposures to dinoseb in ambient air are assumed to be negligible. Therefore, no MDI inhalation is applied.

In the absence of other inhalation data, this HCV compares favourably with the acute inhalation exposure value.

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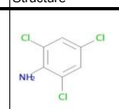
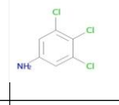
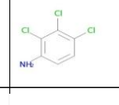
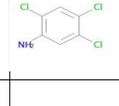
Determinand	Cas Number	Formulae	Structure	Ref No.	LD50 Rat Oral	Units	LD50 Mouse oral	Units	Koc	Henry's law constant (Unitless)	Log Kow	Solubilities	Units	Vapour Pressure	Units	Boiling Point	Units	Melting Point	Units	pKa/pKb	HLC	
2,4,6-Trichlorobenzenamine	634-93-5	C6H4Cl3N		1 3	2400	mg/kg	1180	mg/kg	2400 198	0.00000134 0.000055 0.0000317	3.69 3.52	40	mg/l in water @ 25 deg C	0.000000147 0.02	mm Hg at 25 deg C hPa at 25oC	262	deg C @ 746 mm Hg	78.5	deg C	14.03	0.0000013	
3,4,5-Trichlorobenzenamine	634-91-3	C6H4Cl3N			n/a	-	n/a		n/a	0.0000317 5.50E-005	3.01	n/a	-	n/a	-	n/a	-	n/a	-	n/a	n/a	
2,3,4-Trichlorobenzenamine	634-67-3	C6H4Cl3N		2	n/a	-	n/a		398	0.0000317 5.50E-005	3.01	n/a	-	n/a	-	n/a	-	n/a	-	n/a	n/a	
2,4,5-Trichlorobenzenamine	636-30-6	C6H4Cl3N		3	n/a	-	n/a		198	0.0000317 5.50E-005	3.45 3.01	25	mg/l	0.01	hPa at 25oC	n/a	-	n/a	-	12.91	0.0000013	

1 http://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@rn+@rel+634-93-5
2 http://esc.syrres.com/scripts/CHFcgi.exe Chemfate
3 http://www.epa.gov/hpvis/rbp/Chloroanilines_HC-HBP_September_2008.pdf

SELECTION OF HEALTH CRITERIA VALUE

There are very limited toxicity data for any of the isomers of trichlorobenzeneamine and benzene and vinylchloride are considered to be suitable for consideration as surrogate compounds. Although this compound is more similar to the structure of benzene, there is potential for comparatively increased toxicity due to the presence of halide substituents (such as chlorine) to the basic benzene structure. Therefore, since chlorine is present in both trichlorobenzeneamine and vinyl chloride, vinyl chloride has also been considered for adoption as a surrogate. Thethe toxicity data for vinyl chloride is more conservative than that of benzene, and is considered to be more appropriate for the evaluation of the potential toxicity of trichlorobenzeamine. This is a conservative approach which takes into account a comparatively higher degree of volatility when assessing the behaviour of trichlorobenzeamines in soil. This is likely to provide an assessment criteria conservative enough to account for the fact that the additional chlorine substituents (when compared to benzene) could result in toxic properties that exceed that of benzene. Although there is physical and chemical data for 2,3-dichlorotoluene, due the paucity of data for other endpoints, it is suggested that the physical and chemical data for vinyl chloride should also be retained for use. Therefore, vinyl chloride is adopted as a surrogate compound for evaluation of the listed trichlorobenzeneamine isomers.

Annex 3: Physical and Chemical Data

Physchem Parameters Identified for: DINOSEB

Physchem Parameters	A			B			C			D			E			F			G			H		
	HOWARD, 1990			LIDE, 2008			MACKAY et al, 2006			MERCK, 2006			MONTGOMERY, 1997			OECD, 2000 (INCHEM)			OECD, 2000 (HPV)			OECD, 2000 (HSDB)		
	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**	**Units**	**Temp if present**
Relative Molecular Mass	240.20			240.21			240.21			240.22			240.22			240.20								
Henry's Law Constant (HLC)	5.04 x 10^{-4}	atm-m^3/mole	20°C				51.1	Pa-m^3/mol	20°C				5.0 x 10^{-4}	atm-m^3/mole	20°C				4.43 x 10^{-6}	atm-m^3/mole	20°C	5.04 x 10^{-4}	atm-m^3/mol	
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	52	mg/L	25°C				50 52 50 52 100 52 52	g/m^3 or mg/L g/m3 or mg/L g/m3 or mg/L g/m3 or mg/L g/m3 or mg/L g/m3 or mg/L g/m3 or mg/L	25°C 25°C 25°C 25°C rm temp 20°C 20 - 25°C				52	mg/L	20°C	<0.1	g/100ml	20°C	34.5	mg/L	20°C	0.0052 48 27 Miscible in ethyl ether, toluene and xylene	g/100g water g/100g ethanol g/100g N-Heptane	
Chemical Boiling Point (ambient pressure)							362	°C											>300	°C				
Chemical Melting Point (ambient pressure)	38-42	°C		40	°C		40	°C		38-42	°C		38-42	°C		38-42	°C		40.6	°C		38-42	°C	
Log Octanol - Water Coefficient (Kow)	3.69						3.59 3.69 3.69 4.10 3.14 3.0(pH 7) 3.57(pH 2) 3.69 3.56						2.29											
Molar Volume (Le Bas method)							218	cm^3/mol																
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)	124	(unlogged)					2.85 2.09 2.71 3.82 2.68 2.70 2.09 1.80,2.04,2.08 1.48		Soil lit values 20-25°C				2.09 2.70									124	(unlogged)	
Vapour Pressure	8.5 x 10^{-2} 7.5 x 10^{-2}	mm Hg mm Hg	20°C 20°C				130 133 0.0008 0.0067 0.0067 0.0023 10 0.183 0.0067	Pa	151.5°C 151.1°C supercooled liquid 25°C 30°C 20°C 60°C 20-25°C				1	mm Hg	151°c	0.007	Pa	20°C	9.77 x10^{-3}	Pa	25°C	1	mm Hg	151.1°C
Air-water partition coefficient (Kaw)																								
Density				1.265	g cm^{-3}		1.265	g cm^3	45°C				1.2647		45/4°C	1.3	Water=1	30°C				1.2647		45°C
Critical Temp																								

Reference List	
A	Handbook of Environmental Fate and Exposure Data for Organic Chemicals, Philip H. Howard, Lewis Publishers.
B	Handbook of Chemistry and Physics-88th Edition 2007-2008, David R. Lide.
C	Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, MacKay et al, 2006.
D	The Merck Index, Twelfth Edition.
E	Agrochemicals Desk Reference Environmental Data. John H. Montgomery, Lewis Publishers 1993.
F	Organisation for Economic Co-operation and Development, Chemical Summary from the International Programme on Chemical Safety - http://www.inchem.org/documents/icsc/icsc/eics0149.htm
G	Organisation for Economic Co-operation and Development, Screening Information Data Set (SIDS) for High Production Volume - http://webnet.oecd.org/Hpv/UI/handler.axd?id=bc26a1c2-5c7d-403a-8deb-d6fa3a3dfa10
H	Organisation for Economic Co-operation and Development, Hazardous Substances Data Bank. - http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~ZlpXNu:2

Decision Making for Physchem Parameters for Dinoseb

Physchem Properties	Unit														Min	Max	Mean	Median	Chosen Value	Justification
Relative Molecular Mass		240.20	240.21	240.21	240.22	240.22	240.20								240.20	240.22	240.21	240.21	240.21	The value is from a consistent range.
Henry's Law Constant (HLC)	atm-m^3/mole	5.04E-04	5.04E-04	5.04E-04	4.43E-06	5.04E-04									4.43E-06	5.04E-04	4.04E-04	5.04E-04	5.04E-04	The most common value has been selected from a consistent range.
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/l at 20-25oC	52	50	52	50	52	52	52	52		34.5	52			34.50	52.00	4.99E+01	5.20E+01	5.20E+01	The most common value has been selected from a consistent range.
Chemical Boiling Point (ambient pressure)	oC	362													362.00	362.00	3.62E+02	3.62E+02	3.62E+02	Only one value identified.
Chemical Melting Point (ambient pressure)	oC	38	42	40	40	38	42	38	42	38	42	40.6	38	42	38.00	42.00	4.00E+01	4.00E+01	4.00E+01	The central value was taken from a consistent range.
Log Octanol - Water Coefficient (Kow)	unitless	3.69	3.59	3.69	4.1	3.14	3	3.69	3.56	2.29					2.29	4.10	3.42E+00	3.59E+00	3.59E+00	The values range from 2.29 - 4.10, the majority lay above 3.57 therefore the central value is selected.
Molar Volume (Le Bas method)	cm^3/mol	218													218.00	218.00	2.18E+02	2.18E+02	2.18E+02	Only one value was identified for this determinand.
Vapour Pressure	Pa	11.33	9.99	0.0067	0.0023	10	0.0067	0.007	9.77E-03						2.30E-03	11.33	3.92E+00	8.39E-03	1.00E+01	There were two ranges of values identified. Therefore, the vapour pressure was correlated to the Henry's Law Constant, molecular weight and solubility using equations within Environment Agency report P5-079/TR1. The higher range correlated best with the Henry's Law Constant. As such, the mid point from the higher range has been selected.
Density	g cm^{-3}	1.265	1.265	1.2647	1.3	1.2647									1.26	1.30	1.27E+00	1.27E+00	1.265E+00	The most common value has been selected from a consistent range.

Physchem Parameters Identified for: Trichloromethylbenzene

Physchem Parameters	A			B			C			D			E			F			G		
	HOWARD, 1990			LIDE, 2008			MACKAY et al, 2006			MERCK, 2006			OECD INCHEM			OECD HSDB			OECD ESIS		
	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**
Relative Molecular Mass	195.48			195.474			195.474			195.47						195.48					
Henry's Law Constant (HLC)																2.6×10^{-4}	atm-cu m/mole		2.81×10^{-4}	atm-cu m/mole	
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	Hydrolyzes rapidly in water						5.3	g/m^3 or mg/L	25°C				0.1	g/l	20°C	53	mg/L	5°C	0.1	g/l	20°C
Chemical Boiling Point (ambient pressure)	220.8	°C	760 mm Hg	221	°C		221	°C		220.8 129 105 89	@760mmHg @60mmHg @25mmHg @10mmHg	°C	220.7	°C		220.8 129 105	@760 mm Hg @60 mm Hg @25 mm Hg	°C	219-223 220.7	°C	
Chemical Melting Point (ambient pressure)	-5	°C		-4.42	°C		-4.42	°C		-5	°C		-4.8	°C		-5	°C		-7.5 -5 -4.8 -4.6	°C	
Log Octanol - Water Coefficient (Kow)	2.92						2.92						2.92			2.92	log kow				
Molar Volume (Le Bas method)							180.9	cm^3/mol	20°C							0.142809	m^3/kmol	(not Le Bas)			
Enthalpy of Vaporisation at normal boiling point (EVNBP)																12168.6	Gcal/Gmole				
Chemical Critical Point temperature (ambient pressure)																					
Critical Pressure																					
Diffusion Coefficient in Air																					
Diffusion Coefficient in Water																					
Log (organic carbon-water partition coefficient)(Koc)																1200					
Vapour Pressure	0.23	mm Hg	20°C				133.3 666.6 1333 2666 5333 7999 13332 26664 53329 101325	Pa	45.8°C 73.7°C 87.6°C 102.7°C 119.8°C 130.0°C 144.3°C 165.6°C 189.2°C 213.5°C				0.2	hPa	20°C	0.4137 1.35 5.4	mm Hg	25°C 50°C 75°C	0.16 0.2 0.3 0.49 1.46 1.8	hPa	20°C 20°C 20°C 30°C 50°C 50°C
Air-water partition coefficient (Kaw)																					
Density				1.3723	g/cm^{-3}		1.3723	g/cm^3	20°C	1.3756	d_4^{20}		1.37	g/cm^3	20°C	1.3756		20°C/ 4°C	1.38 1.373 1.3723 1.394	g/cm^3	15.5°C 20°C
Critical Temp																					

A	Handbook of Environmental Fate and Exposure Data for Organic Chemicals, Philip H. Howard, Lewis Publishers.
B	Handbook of Chemistry and Physics-88th Edition 2007-2008, David R. Lide.
C	Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, MacKay et al, 2006.
D	The Merck Index, Twelfth Edition.
E	Organisation for Economic Co-operation and Development, Chemical Summary from the International Programme on Chemical Safety - http://www.inchem.org/documents/sids/sids/98077.pdf
F	Organisation for Economic Co-operation and Development, Screening Information Data Set (SIDS) for High Production Volume - http://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@na+BENZOTRICHLORIDE
G	Organisation for Economic Co-operation and Development, Hazardous Substances Data Bank. - http://ecb.jrc.ec.europa.eu/esis/index.php?GENRE=CASNO&ENTREE=98-07-7

Decision Making for Physchem Parameters for Dinoseb

Physchem Properties	Unit											Min	Max	Mean	Median	Mode	Chosen Value	Justification
Relative Molecular Mass		195.48	195.474	195.474	195.47	195.48						195.47	195.48	195.48	195.47	195.48	195.47	The values are consistent therefore the most common was chosen.
Henry's Law Constant (HLC)	atm-m^3/mole	2.60E-04	2.81E-04									2.60E-04	2.81E-04	2.71E-04	2.71E-04	#N/A	2.81E-04	There were only two values identified. The highest value was selected as a conservative measure for inhalation pathways.
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L @ 20-25oC	5.3	100	100								5.30	100.00	6.84E+01	1.00E+02	100	1.00E+02	The most common value was chosen.
Chemical Boiling Point (ambient pressure)	oC	220.8	221	221	220.8	220.7	220.8	220.7				220.70	221.00	2.21E+02	2.21E+02	220.8	2.21E+02	The central value was taken from a consistent range.
Chemical Melting Point (ambient pressure)	oC	-5	-4.42	-4.42	-5	-4.8	-5	-7.5	-5	-4.8	-4.6	-7.50	-4.42	-5.05E+00	-4.90E+00	-5	-4.90E+00	The central value was selected.
Log Octanol - Water Coefficient (Kow)	unitless	2.92	2.92	2.92	2.92							2.92	2.92	2.92E+00	2.92E+00	2.92	2.92E+00	All values are the same.
Molar Volume (Le Bas method)	cm^3/mol	180.9										180.90	180.90	180.9	180.9		180.9	Only one value from the calculated Las Bas method
Enthalpy of Vaporisation at normal boiling point (EVNBP)	Gcal/Gmole	12168.6										12168.60	12168.60	1.22E+04	1.22E+04		1.22E+04	Only one value.
Vapour Pressure	Pa	30.66	20	55.2	16	20	30					16.00	55.20	2.86E+01	2.50E+01	20	2.00E+01	The most common value was chosen.
Density	g/cm^{-3}	1.3723	1.3723	1.3756	1.37	1.3756	1.373					1.37	1.38	1.37E+00	1.37E+00	1.3723	1.37E+00	All of the values identified are the same within 3 significant figures.

Diffusion Coefficient in Air

Dinoseb
Based on SR7 Section 2.4

	Answer	Units	Calcs	Parameter
Eqn 2-13	0.038681491	mol g-1	0.038681491	Mr
Eqn2.15	0.002071662	Unitless	0.002071662	B'
Eqn 2.17	1.181729893	Unitless	1.181729893	T*
eqn 2.16	1.33057165	Unitless	1.33057165	Ω
eqn 2.14	**4.99163E-06**	**m2 s-1**	4.99E-06	**Da**
eqn 2.18	5.406392376	Å	5.406392376	δAB
	218	$cm^3\ mol^{-1}$	218	Vb

Parameters

	Units			
Mole Weight	g mol-1	240.21		
Boiling point	Kelvin	635.15	362	oC
Density	g cm3	1.27		
tamb	Kelvin	283.15	10	oC
Molcular weight of air	g mol-1	28.97		
Vb	$cm^3\ mol^{-1}$	218		

Trichloromethylbenzene

	Answer	Units	Calcs	Parameter
Eqn 2-13	0.039634342	mol g-1	0.039634342	Mr
Eqn2.15	0.002070458	Unitless	0.002070458	B'
Eqn 2.17	1.339759894	Unitless	1.339759894	T*
eqn 2.16	1.257937918	Unitless	1.257937918	Ω
eqn 2.14	**5.79091E-06**	**m2 s-1**	5.79E-06	**Da**
eqn 2.18	5.192310427	Å	5.192310427	δAB
	180.9	$cm^3\ mol^{-1}$	180.9	Vb

Parameters

Mole Weight	g mol-1	195.47		
Boiling point	Kelvin	494.15	221	
Density	g cm3	1.37	g/m3	
tamb	Kelvin	283.15		
Molcular weight of air	g mol-1	28.97		
Vb	$cm^3\ mol^{-1}$	180.9		

Koc Value Calculated from Kow Value

	Pesticides	Predominantly Hydrophobics	Phenols, anilines, benzonitriles, nitrobenzenes	
	Eqn. 4	Eqn. 1	Eqn.3	
Compound	**log Koc**	**log Koc**	**log Koc**	**log Kow**
Dinoseb	2.7773		3.1617	3.59
Trichloromethylbenzene		2.4652		2.92

SR7
From Table 2.12
Eqn. 1 logkoc=0.81*logkow+0.10
Eqn. 3 logkoc=0.63*logkow+0.90
Eqn. 4 logkoc=0.47*logkow+1.09

Diffusion Coefficient in Water

Based on equation in SR7 Section 2.5 EQN 2.20

Eqn 2.20

Dinoseb	4.10E-10
Trichloromethylbenzene	4.57E-10

Henry's Law Constant

Contaminant	H' (H'=H/RT) (dimensionless)	H (Pa m3 mol-1)	H (atm m3 mol-1)	
Dinoseb	2.08E-02	5.11E+01	5.04E-04	
Trichloromethylbenzene	1.16E-02	2.85E+01	2.81E-04	

R (gas constant) =	8.3144	Pa m3 mol-1 K-1
Temp of HLC (K)	295	
1atm=	101325	Pa

Annex 4: Modelling

CLEA Software Version 1.06

Report generated 03/08/2010

Report title Hauxton Criteria for Pesticides

Created by Zara Rostance 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

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

Environment Agency

Building Small terraced house

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 (µg m^{-3})	5.00E+01

Soil Sand

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	03-Aug-10
Report title	Hauxton Criteria for Pesticides
Created by	Zara Rostance 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	Dinoseb	2.12E-01	6.16E-02	4.77E-02	0.23	0.77	1.00	1.82E+02 (vap)	No	No
2	Trichloromethylbenzene	6.41E-04	2.07E-04	1.57E-04	0.24	0.76	1.00	1.92E+02 (sol)	No	No
3										
4										
5										
6										
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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
21									
22									
23									
24									
25									
26									
27									
28									
29									
30									

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	Dinoseb	94.4	5.5	0.1	100.0	4.77E-02	2.68E-01	2.38E-02	2.03E-11	0.00E+00	1.68E-04	7.40E-08	0.00E+00	6.28E-02	8.88E-02	2.02E-02	0.00E+00	0.00E+00	1.96E-02
2	Trichloromethylbenzene	89.2	10.6	0.2	100.0	1.57E-04	9.47E-04	7.83E-05	6.67E-14	0.00E+00	6.54E-07	2.72E-10	0.00E+00	2.30E-04	3.54E-04	8.82E-05	0.00E+00	0.00E+00	1.84E-04
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	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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		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	Dinoseb	3.54E-07	4.13E-05	9.08E-07	1.12E-09	1.55E-04	1.13E-05	0.00E+00	0.17	19.77	0.44	0.00	74.23	0.00	5.39	0.00
2	Trichloromethylbenzene	1.16E-09	1.93E-07	1.49E-09	3.69E-12	6.05E-07	0.00E+00	0.00E+00	0.15	24.09	0.19	0.00	75.57	0.00	0.00	0.00
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	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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		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	Dinoseb	TDI	0.2	TDI	0.2	0.2	0	2.08E-02	4.99E-06	4.10E-10	2.78	3.59	0.5	0.5	1	1	1
2	Trichloromethylbenzene	ID	0.0008	ID	0.0008	NR	NR	1.16E-02	5.79E-06	4.57E-10	2.47	2.92	0.25	0.5	1	1	1
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	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	Dinoseb	3.49E+00	1.00E+01	5.20E+01	model	model	model	model	model	model
2	Trichloromethylbenzene	1.71E+00	2.00E+01	1.00E+02	model	model	model	model	model	model
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	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 CNPIs are listed in the following table:

Chemical Name	CAS Number	Chemical Formula
Dinoseb	88-85-7	$C_{10}H_{12}N_2O_5$
1-methylnaphthalene	90-12-0	$C_{11}H_{10}$
2,3,4- Trichloro benzenamine, or 2,3,5- Trichloro benzenamine, or 2,3,6- Trichloro benzenamine, or 2,4,5- Trichloro benzenamine, or 2,4,6- Trichloro benzenamine., or 3,4,5- Trichloro benzenamine, or	634-67-3 18487-39-3 88963-39-7 636-30-6 634-93-5 634-91-3	$C_6H_4NCl_3$
2,3-Dichlorotoluene	32768-54-0	$C_7H_6Cl_2$

This annex provides a summary of the physical and chemical properties of each of these substances.

For each substance either a surrogate substance is selected from amongst the existing priority contaminants for controlled waters, and the remedial targets for this surrogate are applied to the CNPI; or a specific remedial target for the substance has been calculated using the methodology developed in 2007 (Ref 1).

Dinoseb

Chemical Name: 2-sec-butyl-4,6-dinitrophenol

Dinoseb was detected in NAPL from grid square K10 at the Main Site, Hauxton at a concentration of 68,000 mg/kg.

This substance is a phenol molecule with two nitrous groups (NO_2) and a branched alkane group attached. Dinoseb is an herbicide/insecticide organic substance.

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

Properties	Units	Values	Reference
Henry's Law	Pa m^3/mol	51.1	Suntio, L.R., Shiu, W.Y., Mackay, D., Seiber, J.N., Glotfelty, D. (1988) Critical review of Henry's law constants. Rev. Environ.
K_{OC}	-	65 - 708	Mackay D., Shiu W.Y., Lee S.C. & Ma K. Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Second Edition Aug 2006 (CD-ROM)
Half Life (Anaerobic)	days	4 – 246	Howard, P.H., Editor (1991) Handbook of Environmental Fate and Exposure Data for Organic Chemicals. Volume III. Pesticides. Lewis Publishers, Chelsea, Michigan.

This substance was not previously identified at Hauxton Main Site and was not known from available records to have been manufactured at Hauxton however a very wide range of substances were synthesised at the site over its history.

The parameters available for Dinoseb and their wide ranges for Koc and half lives make it desirable to calculate a specific remedial target rather than rely on a surrogate. However Dinoseb is superficially similar in structure and arrangement of groups around the benzene ring to 4,6-dinitro-o-cresol which was a priority contaminant taken forward from the risk screening in 2007 (Ref 1) for derivation of remedial targets.

As there are sufficient published data on the properties of Dinoseb, and it appears to have properties which might make it mobile in groundwater (a low K_{OC} value), a remedial target has been calculated for it using a conservative compliance concentration at the receptor of 0.1µg/l, as has been considered for all pesticide/herbicide substances at Hauxton. The methodology used to calculate the target was the same as used in the 2007 risk assessment (Ref 1).

1-methylnaphthalene

1-Methylnaphthalene was detected in NAPL from grid square K10 at the Main Site, Hauxton at a concentration of 2,400 mg/kg.

This substance is similar to 2-methylnaphthalene which was detected at the Hauxton Main Site historically. However 2-methylnaphthalene was only detected in relatively low concentrations in groundwater (up to 290µg/l). 2-methylnaphthalene was found to be of low risk in the risk screening carried out in 2007 (Ref 1) and therefore was not selected as a priority contaminant.

1-Methylnaphthalene was detected in a sample of NAPL from square K10 at a concentration of 2.4 g/kg.

The physical and chemical properties of 1-methylnaphthalene are as follows:

Properties	Units	Values	Reference
Henry's Law	Pa m^3/mol	26.3	Mackay, D., Shiu, W.Y., Bobra, A., Billington, J., Chau, E., Yeun, A., Ng, C., Szeto, F. (1982) Volatilization of Organic Pollutants
K_{OC}	-	915 – 6764.7	Stauffer, T.B., MacIntyre, W.G., Wickman, D.C. (1989) Sorption of nonpolar organic chemicals on low-carbon-content aquifer materials. Environ. Toxicol. Chem. 8, 845–852.
Half Life (Anaerobic)	days	1611	Aronson, D. and Howard, P. H. (1997) Anaerobic Biodegradation of Organic Chemicals in Groundwater: American Petroleum Institute

The properties of 1-methylnaphthalene include relatively large K_{OC} values therefore transport of this substance in groundwater is likely to be slow. This has to be weighed against the relatively low half life for this substance. There is no obvious surrogate for this substance amongst the existing priority contaminants for controlled waters. PAHs were not found in highly elevated concentrations at Hauxton compared to other more highly mobile organic contaminants, and therefore were not considered to be priority contaminants.

It was considered necessary to calculate remedial targets for 1-methylnaphthalene using the parameters summarised above as a screening value for remedial validation purposes. The methodology used to calculate the target was the same as used in the 2007 risk assessment (Ref 1).

Trichloro benzenamine isomer

Synonyms: Trichloroaniline

Trichloro benzamine was detected in grid square J10 at a concentration of 11 mg/kg.

These substances are very similar and have identical molecular mass. They consist of a benzene ring with three chloride groups attached and a single amine/aniline group (NH_2). A couple of contaminants with amine/aniline groups were detected at Hauxton previously including analine (C_6H_7N) and 4-chloroaniline (C_6H_6NCl). The risk screening carried out in 2007 (Ref 1) to select the priority contaminants for controlled waters assessed analine and 4-chloroaniline as being of low risk.

The following properties on the 2,4,6 trichloroaniline were sourced from literature, principally toxnet references.

Properties	Units	Values	Reference
Henry's Law	Atm m^3/mol	$1.34x10^{-6}$	Meylan WM, Howard PH; Environ Toxicol Chem 10: 1283-93 (1991)
K_{OC}	-	2,400	Swann RL et al; Res Rev 85: 17-28 (1983) Meylan WM et al; Environ Sci Technol 26: 1560-67 (1992)
Half Life (Anaerobic)	days	143	Peijnenburg WJGM et al; Environ Toxicol Chem 11: 289-300 (1992)
Solubility	mg/l	40	Chem Inspect Test Inst; Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan; Published by Japan Chemical Industry Ecology-Toxicology & Information Centre. ISBN 4-89074-101-1 p. 3-34 (1992)

The contaminant transport properties of 2,3,4 trichloroaniline were researched however very little information appears to be available on this form of the molecule. Some reference to it biodegrading under anaerobic conditions were sourced from Elmar et. al. 1990 (Ref 2). However no indication of the rate of biodegradation that could be expected for 2,3,4 trichloroaniline after the incubation period was available.

In the absence of parameters to risk assess the 2,3,4 trichloroaniline version of trichloroanaline, it is considered that 2,4,6 trichloroaniline should have a remediation target calculated and that this remedial target should apply to both forms of the molecule. Should the laboratory find it

possible to differentiate then by laboratory techniques in subsequent analyses then the remedial target for 2,3,4 trichloroaniline should be applicable to both substances. The methodology used to calculate the target was the same as used in the 2007 risk assessment (Ref 1).

2,3-Dichlorotoluene

2,3-Dichlorotoluene has been detected in grid square J10 on the Hauxton Main Site at a concentration of 290 mg/kg.

The 2,3-dichlorotoluene molecule consists of a benzene ring with a methyl group attached and then two chloride attached to the next two carbons in the benzene ring. There are a wide variety of forms that dichlorotoluene could take depending on the locations of the chloride ions on the benzene ring. No information on the contaminant transport properties of 2,3-dichlorotoluene have been found in literature surveys carried out for this assessment.

Other chlorinated toluene type contaminants have been detected at the Hauxton Main Site in the past, including 2-chlorotoluene and 4-chlorotoluene which were assessed in the 2007 risk screening (Ref 1), and 2,3,6-trichlorotoluene which was detected in grid square I9 (July 2010) during the remediation.

The contaminant transport properties of these substances and two forms of dichlorotoluene, which do have published literature on their environmental fate and transport, are listed in the tables below.

K_{OC}

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	4786.3	Howard, P.H., Ed. (1997) Handbook of Fate and Exposure Data for Organic Chemicals. Vol. V, Solvents 3. Lewis Publishers, Inc., Chelsea, Michigan.
2,6-dichlorotoluene	5128.6	Howard, P.H., Ed. (1997) Handbook of Fate and Exposure Data for Organic Chemicals. Vol. V, Solvents 3. Lewis Publishers, Inc., Chelsea, Michigan.

Henry's Law

Substances	Henry's Law	Units	Reference
2-chlorotoluene	295	Pa m^3/mole	Staudinger, J., Roberts, P.V. (1996) A critical review of Henry's law constants for environmental applications. Crit. Rev. Environ. Sci. Technol. 25, 205–297. Staudinger, J., Roberts, P.V. (2001) A critical compilation of Henry's law constant temperature dependence relations for organic compounds in dilute aqueous solutions. Chemosphere 44, 561–576.
4-chlorotoluene	412.4	Pa m^3/mole	Howard, P.H., Ed. (1993) Handbook of Fate and Exposure Data for Organic Chemicals. Vol. IV, Solvents 2. Lewis Publishers, Inc., Chelsea, Michigan.
2,4-dichlorotoluene	350.6	Pa m^3/mole	Hine, J., Mookerjee, P.K. (1975) The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. J. Org. Chem. 40, 292–298.
2,6-dichlorotoluene	350.6	Pa m^3/mole	Hine, J., Mookerjee, P.K. (1975) The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. J. Org. Chem. 40, 292–298.

Biodegradation Rates (Anaerobic)

Substances	Half Life (days)	Reference
2-chlorotoluene	70*	Chemicals Inspection and Testing Institute; Japan Chemical Industry Ecology-Toxicology and Information Center. ISBN 4-89074-101-1. (1992)
4-chlorotoluene	70*	Kawasaki M; Ecotox Environ Safet 4: 444-54 (1980)
2,4-dichlorotoluene	90	Ramanand K et al; Appl Environ Microbiol 59: 3266-3272 (1993)
2,6-dichlorotoluene	230**	Ramanand K et al; Appl Environ Microbiol 59: 3266-3272 (1993)

* calculated from 30% reduction after 14 days
** calculated from 30-35% reduction after 150 days

It has been assumed that 2,3-dichlorotoluene will have similar environmental fate properties to the other dichlorotoluene species and therefore could be conservatively risk assessed using the most conservative parameter values obtained for either 2,4-dichlorotoluene or 2,6-dichlorotoluene.

The assumed parameters for the derivation of a remedial target for 2,3-dichlorotoluene would therefore be as follows.

Properties	Units	Values	Reference
Henry's Law	Pa m^3/mole	350.6	Hine, J., Mookerjee, P.K. (1975) The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. J. Org. Chem. 40, 292–298.
K_{OC}	-	4786.3	Howard, P.H., Ed. (1997) Handbook of Fate and Exposure Data for Organic Chemicals. Vol. V, Solvents 3. Lewis Publishers, Inc., Chelsea, Michigan.
Half Life (Anaerobic)	days	230	Ramanand K et al; Appl Environ Microbiol 59: 3266-3272 (1993)

The remedial target calculated for 2,3-dichlorotoluene should also be applicable as a conservative surrogate target for the unspecified species of dichlorotoluene identified during the remediation. The solubility of dichlorotoluene molecules are described as insoluble in the literature (Ref. 2).

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 TIC GCMS screening at the Hauxton Main Site.

Sufficient data on the contaminant transport properties of Dinoseb, 1-methylnaphthalene and Trichloro benzenamine were available for species specific remedial targets to be derived. The methodology used to calculate the targets was the same as used in the 2007 risk assessment (Ref 1).

For the case of 2,3-dichlorotoluene it was possible to select conservative parameters for two other dichlorotoluene species which could then be used to derive a conservative dichlorotoluene remedial target that could be applied to 2,3-dichlorotoluene.

The table below lists the CNPIs calculated remedial targets.

Substances	Priority Contaminant Surrogates	Target Concentration (µg/kg)	
		Inner Zone	Outer Zone
Dinoseb	-	0.16	330
1-methylnaphthalene	-	1.71	1790
Trichloro benzenamine	-	14.3	>100,000*
2,3-dichlorotoluene	-	39.6	>100,000**

* Calculated Target Concentration 8.75×10^{9}. Number based on solubility.

** Calculated Target Concentration 1.15×10^{11}. No Solubility data on substance, conservative value assumed based on an insoluble substance (Ref. 2)

References

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

2 Ashford, R.D. Ashford's Dictionary of Industrial Chemicals. London, England: Wavelength Publications Ltd., 1994., p. 290