APPENDIX I

TOXICOLOGICAL INPUT PARAMETERS / GAC DERIVATION WORKSHEETS

CONTAMINANT	RESIDENTIAL WITHOUT PLANT UPTAKE HCV (mg/kg)			
	SGV	GAC	DERMAL ASC	COMBINED SGV/GAC
Arsenic	20		590	19.34
Cadmium	30		59000	29.98
Chromium (hexavalent)	200		17700	197.7
Chromium (total)	200		17700	197.7
Lead	450			450
Mercury	15		1770	14.87
Selenium	260		2950	238
Boron (water soluble)				
Copper				
Nickel	75			
Zinc				
Phenols (monohydric)	21900		413000	20797
Cyanide (free)		53		53
Cyanide (total)		53		53
Cyanide (complex)		53		53
Sulphate (water soluble) g/l				
SO_4				
Sulphide				
Sulphur (free)				
pH				
TPH				
PAH (total)				
Naphthalene		33.4	9076	33.3
Acenaphthylene		2030		1650
Acenaphthene		2030		1650
Fluorene		811	18514	776
Phenanthrene		2030		1650
Anthracene		6089	136153	5828
Fluoranthene		2550	136153	2503
Pyrene		255	13615	250
Benzo(a)anthracene		20.3		16.5
Chrysene		20.3		16.5
Benzo(b)fluoranthene		20.3		16.5
Benzo(k)fluoranthene		20.3		16.5
Benzo(a)pyrene		2.03	9.08	1.65
Indeno(1,2,3-cd)pyrene		20.3		16.5
Dibenz(a,h)anthracene		2.03		1.65
Benzo(g,h,i)perylene		20.3		16.5
Barium				
Beryllium				
Vanadium				
Nitrate				
Sulphate (total)				
Organic Matter				
TPH C10-C12				

CONTAMINANT	RESIDENTIAL WITHOUT PLANT UPTAKE HCV (mg/kg)			
	SGV	GAC	DERMAL ASC	COMBINED SGV/GAC
TPH C12-C16				
TPH C16-C21				
TPH C21-C35				
TPH C35-C40				
TPH Aromatic EC5-EC7		0.134	171	0.133
TPH Aromatic EC7-EC8	3		118000	2.9
TPH Aromatic EC8-EC10		15.99	24000	15.97
TPH Aromatic EC10-EC12		79.6	24000	77.0
TPH Aromatic EC12-EC16		291.7	24000	288.1
TPH Aromatic EC16-EC21		608	17700	587.8
TPH Aromatic EC21-EC35		608	17700	587.8
TPH Aliphatic EC5-EC6		24.07	>1000000	24.06
TPH Aliphatic EC6-EC8		52.79	>1000000	52.78
TPH Aliphatic EC8-EC10		9.96	59000	9.95
TPH Aliphatic EC10-EC12		45.28	59000	52.54
TPH Aliphatic EC12-EC16		198.54	59000	197.8
TPH Aliphatic EC16-EC34		40596	>1000000	3901
Benzene		0.134	171	0.133
Toluene	3		118000	3
Ethyl Benzene	16		59000	15.99
m+p-Xylene		22.91	105610	22.90
o-Xylene		22.91	105610	22.90

Derivation of ASC for the Dermal Pathway

Equation 3.1 from CLEA CLR 10

$$ADE = \frac{IR_{DERMAL} \times EF \times ED}{BW \times AT}$$

ADE – Average Daly Exposure (mg/kg bw/day)
IR_{DERMAL} – Chemical Exposure Rate via the Dermal Pathway
EF - Exposure Frequency (days/year)
ED – Exposure Duration (years)
BW – Body Weight (kg)
AT – Averaging Time (day)

Equation 6.6 from CLEA CLR 10

$$IR_{DERMAL} = (DA \times A_{SKIN})_{OUTDOOE} + (DA \times A_{SKIN} \times F_{DUST})_{INDOOR}$$

DA – Average Absorbed Contaminant dose per unit area of skin ($mg/cm^2/day$)
A_{skin} – Exposed Skin Area (cm^2)
F_{dust} – Fraction of locally derived soil in indoor dust

$$C_{soil} = \frac{BW \times AT \times HCV}{((AF \times ABS \times A_{AKIN})_{OUTDOOR} + (AF \times ABS \times A_{SKIN} \times F_{DUST})_{INDOOR}) \times EF \times ED \times 10^{-6}}$$

C_{soil} is equivalent to ASC_{dermal}

The SSAC including the dermal pathway is:

$$\frac{1}{SSAC_{TOTAL}} = \frac{1}{SSAC_{SNIFFER}} + \frac{1}{ASC_{CDERMAL}}$$

For residential scenarios (both Residential With and Without Plant Uptake) the following input parameters are used:

BW	= 11.15kg	- Taken from SNIFFER
AT	= 2190 days	- Taken from SNIFFER
$AF_{outdoor}$	=1mg/cm^2	- Taken from CLEA Briefing Note 1
AF_{indoor}	=0.06mg/cm^2	- Taken from CLEA Briefing Note 1
ABS	= CONTAMINANT SPECIFIC	
$A_{skin\text{-}outdoor}$	=544cm^2	- Time Averaged exposed skin based on data from CLEA Briefing Note 1
$A_{skin\text{-}indoor}$	= 685cm^2	- Time Averaged exposed skin based on data from CLEA Briefing Note 1
ED	= 120 days	- Taken from CLEA CLR 10
ED	= 6 years	- Taken from CLEA CLR 10
10^{-6}	= conversion factor for kg to mg	
HCV	= CONTAMINANT SPECIFIC	

For Residential scenarios ASC_{DERMAL} is:

$$ASC_{DERMAL} = \frac{11.15 \times 2190 \times HCV}{((1 \times ABS \times 544) + (0.06 \times ABS \times 685 \times 0.75)) \times 120 \times 6 \times 10^{-6}}$$

$$ASC_{DERMAL} = \frac{24418.5}{((544 \times ABS) + (30.825 \times ABS)) \times 0.00072} = \frac{33914583.33}{574.825} \frac{HCV}{ABS} = 58999.98 \bullet \frac{HCV}{ABS}$$

CONTAMINANT	ABS	HCV	ASC_{DERMAL}
Arsenic	0.03	0.0003	590.00
Cadmium	0.001	0.001	59,000
Chromium (hexavalent)	0.01	0.003	17,700
Chromium (total)	0.01	0.003	17,700
Lead			
Mercury	0.01	0.0003	1,770
Selenium	0.01	0.005	2,950
Nickel	0.01	0.005	29,500
Phenols (monohydric)	0.1	0.7	413,000
Naphthalene	0.13	0.02	9076.92
Fluorene	0.13	0.04	18,514
Anthracene	0.13	0.3	136,153
Fluoranthene	0.13	0.3	136,153
Pyrene	0.13	0.03	13,615
Benzo(a)pyrene	0.13	0.00002	9.08
TPH Aromatic EC5-EC7	0.1	0.00029	171
TPH Aromatic EC7-EC8	0.1	0.2	118,000
TPH Aromatic EC8-EC10	0.1	0.04	24,000
TPH Aromatic EC10-EC12	0.1	0.04	24,000
TPH Aromatic EC12-EC16	0.1	0.04	24,000
TPH Aromatic EC16-EC21	0.1	0.03	17,700
TPH Aromatic EC21-EC35	0.1	0.03	17,700
TPH Aliphatic EC5-EC6	0.1	5	>1,000,000
TPH Aliphatic EC6-EC8	0.1	5	>1,000,000
TPH Aliphatic EC8-EC10	0.1	0.1	59,000
TPH Aliphatic EC10-EC12	0.1	0.1	59,000
TPH Aliphatic EC12-EC16	0.1	0.1	59,000
TPH Aliphatic EC16-EC34	0.1	2.0	>1,000,000
Benzene	0.1	0.00029	171
Toluene	0.1	0.2	118,000
Ethyl Benzene	0.1	0.1	59,000
M+p-Xylene	0.1	0.179	105,610
o-Xylene	0.1	0.179	105,610

References:

Draft Human Health and Ecological Risk Assessment for the Georgia-Pacific California Wood Products Manufacturing Facility

Basis and Background of the Soil Remediation Standards for the Combined Ingestion and Dermal Absorption Pathway

INPUT DATA FOR GAC'S

Assumptions made in the derivation of GAC's:

The following assumptions have been made in the derivation of GAC's:

- The soil is a sand matrix
- The Soil Organic Matter Content is 1%

The input parameters used in the derivation worksheets are presented hereunder:

Parameter	Value	Justification
Childhood Ingestion Factor	0.485	Taken from Table 3.6 LQ01
Time Averaged Body Weight	11.15kg	Table 3-2 of LQ01
Childhood Inhalation Factor	0.362	Taken from Table 3-6 of LQ01
Time Averaged Body Height	0.93m	Table 3-4 of LQ01
Soil Density	1.6 g dry weight/cm^3	CLEA Briefing Note 2
Soil-Water content by volume (Water filled porosity)	0.15 cm^3/cm^3	CLEA Briefing Note 2
Soil-Air content by volume (Air filled porosity)	0.31 cm^3/cm^3	CLEA Briefing Note 2
Dilution Ratio	20,000	Taken from LQ01 (page 63)
Temperature	12°C	Taken from 6.99 of CLEA CLR 10
Ambient air velocity in the mixing zone	3m/s	Taken from LQ01
Source Zone Width Parallel to Wind Direction	15m	LQ01
Depth to Subsurface Contamination	1m	LQ01

Receptor Data Used in the Derivation of GAC's:

The critical receptor for the 'Residential Without Plant Uptake' scenario is a female child. The selection of an Exposure Duration and averaging period of 0-6 years is considered appropriate; hence the averaging time is 2190 days, a Time Averaged Body Weight (TABW) of 11.15kg and a Time Averaged Body Height (TABH) of10.93m.

ARSENIC

Arsenic occurs naturally in many soils. A survey of 2691 uncontaminated sites is (Berrow and Reaves, 1984) indicates that the mean concentration of arsenic in 'uncontaminated' soils to be 10 mg/kg. Urban surveys of soils in Wolverhampton and Stoke has reported arsenic concentrations in the range of 2-167mg kg^{-1} (EA, in preparation).

The data collated from literature review of the toxicological properties of arsenic are summarised below:

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 1 – March 2002
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties are presented below:

		Description effects	Source
Acute Oral Toxicity	70mg – Lethal Dose	Severe gastroinintestional damage and heamorrhaging, vomiting and diarrhea, cramps and cardiac abnormalities	CLEA CLR TOX 1
Repeated oral toxicity	Index Dose is 0.3μg/kg bw/day	Skin cancer, thickening the walls blood vessels	CLEA CLR TOX 1
Inhalation Toxicity	Index Dose is 0.002μg/kg bw/day	Lung cancer	CLEA CLR SGV 1

Epidermological studies indicate that skin lesions are the most sensitive indicator of chronic toxicity.

The ingestion Index Dose is based on WHO drinking water guidance of 10μg/l, which has an associated lifetime excess cancer risk of $6x10^{-4}$.

The dermal and inhalation pathways account for less that 1% of the overall exposure (CLEA CLR SGV 1), hence they have not been taken into account.

CADMIUM

Cadmium occurs naturally in soils, but is normally expected to be less than 1mg/kg (Alloway,1995).

The data collated from literature review of the toxicological properties cadmium are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 3
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/a		

A summary of the toxicological properties are presented below;

		Description effects	Source
Acute Effects	Lethal Dose 25mg/kg bw	Hemorrhages in the gastrointestinal tract, odema, severe liver and kidney damage	CLEA CLR TOX 3
Ingestion and inhalation chronic exposure	TDI_{ing} 1μg/kg bw/day	Damage to the kidneys	CLEA CLR TOX 3 - JECFA
Inhalation Toxicity	ID_{inh} 0.001μg/kg bw/day	Nasal itching, runny nose, nose bleeding, nasal mucosal atrophy, bronchitis, pneumonia and lung cancer	CLEA CLR TOX 3

The background exposure data for cadmium is presented below:

	Value	Source
$MDI_{ingestion}$	16ug/kg bw/day	CLEA CLR TOX 3

The empirical relationship between plant uptake and pH of the soil should not be used where the pH is less than 6.5, and the soil to plant concentration factor should be determined on a site specific basis.

The dermal and inhalation pathways account for less that 1% of the overall exposure (CLEA CLR SGV 3), hence they have not been taken into account. This may not be the case on sites where:

- The majority of the site is bare for long periods and dry/windy conditions prevail
- Activities such as vehicle movements increase dust generation
- The contamination itself is in a dry and/or dusty form

HEXAVALENT CHROMIUM

Cadmium is a common element in rocks, and soils in England and Wales have a chromium content in the range of 0.2mg/kg to 838mg/kg, with a median of 39.2mg/kg (McGrath and Loveland, 1992)

The data collated from literature review of the toxicological properties of chromium are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 4 – March 2002
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties are presented below;

		Description effects	Source
Acute Effects	Lethal Dose – 300mg	Hemorrhaging in the gastrointestinal tract, odema, severe kidney and liver damage	CLEA CLR TOX 4
Ingestion and inhalation chronic exposure	TDI_{ing} 3µg/kg bw/day	Affects on gastrointestinal tract (oral ulcer, diarrhea, vomiting, abdominal pain and indigestion) and the blood	CLEA CLR TOX 4
Inhalation Toxicity	ID_{ing} 0.0013µg/kg bw/day	Lung cancer	CLEA CLR TOX 4

The background exposure data for hexavalent chromium is presented below:

	Value	Source
$MDI_{ingestion}$	13ug/kg bw/day	CLEA CLR TOX 4

The SGV for hexavalent chromium is also used for total chromium as it is assumed that all other forms of chromium in the soil can be transformed to the hexavalent form.

The dermal and inhalation pathways account for less that 1% of the overall exposure (CLEA CLR SGV 3), hence they have not been taken into account. This may not be the case on sites where:

- The majority of the site is bare for long periods and dry/windy conditions prevail
- Activities such as vehicle movements increase dust generation

- The contamination itself is in a dry and/or dusty form

INORGANIC FREE CYANIDE

The GAC for free cyanide for the 'Residential With Plant Uptake' scenario is 53mg/kg.

The data collated from literature review of the toxicological properties chromium are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 5 – March 2002
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties are presented below;

		Description effects	Source
Acute Effects	Fatal oral dose 0.56mg kg-1 bw Fatal dermal dose 100mg kg-1 bw	Death	CLEA CLR TOX 5

The GAC for free cyanide is based on acute effects and is derived using the following algorithm:

$$SSAC = \frac{(LDL_0/UF) \times BW}{OTSIR}$$

where LDL_0 is the lowest lethal dose, UF is the safety factor, BW is body weight, and OTSIR is time soil ingestion rate.

Based on a LDL_0 of 0.56mg/kg bw/day, an UF 50, a BW 11.15kg and an OTSIR 2g, the GAC is 53mg/kg.

The dermal and inhalation pathways account for less that 1% of the overall exposure (CLEA CLR SGV 3), hence they have not been taken into account.

Soil parameters are based on a sandy soil and have been taken from CLEA CLR 10 and/or the CLEA Briefing Notes

MERCURY

The data collated from literature review of the toxicological properties of mercury are summarised below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 7 – March 2002
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties for elemental mercury are presented below;

		Description effects	Source
Acute Effects from inhalation	1mg/m^3	Damage to major organs, particularly the lungs	CLEA CLR TOX 7
Inhalation chronic exposure	TDI_{ing} 0.3µg/kg bw/day	Damage to the kidneys	CLEA CLR TOX 7

A summary of the toxicological properties for inorganic mercury are presented below;

		Description effects	Source
Acute Effects	Lethal Dose – 0.7g	Severe gastrointestinal damage, cardiovascular collapse, renal failure.	CLEA CLR TOX 7
Ingestion and inhalation chronic exposure	TDI_{ing} 0.3µg/kg bw/day	Damage to the kidneys	CLEA CLR TOX 7
Inhalation Toxicity	ID_{ing} 0.3µg/kg bw/day		CLEA CLR TOX 7

The background exposure data for inorganic mercury is presented below:

	Value	Source
$MDI_{ingestion}$	2.5ug/kg bw/day	CLEA CLR TOX 7

The dermal and inhalation pathways account for less that 1% of the overall exposure (CLEA CLR SGV 5), hence they have not been taken into account. This may not be the case on sites where:

- The majority of the site is bare for long periods and dry/windy conditions prevail
- Activities such as vehicle movements increase dust generation

- The contamination itself is in a dry and/or dusty form

NICKEL

The SGV published for nickel by the Environment Agency for the 'Residential With Plant Uptake' scenario is 50mg/kg.

The data collated from literature review of the toxicological properties of nickel are summarised below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 8 – March 2002
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties for nickel is presented below:

		Description effects	Source
Acute Effects	Lethal Dose – 382mg/m^3	Headache, nausea, vomiting, insomnia, irritability and pulmonary lesions	CLEA CLR TOX 8
Ingestion chronic exposure	TDI_{ing} 5µg/kg bw/day	Damage to the kidneys	CLEA CLR TOX 8
Inhalation Toxicity	TDI_{inh} / ID_{ing} 0.006µg/kg bw/day	Reduction body weight	CLEA CLR TOX 8

The background exposure data for nickel is presented below:

	Value	Source
$MDI_{ingestion}$	160ug/kg bw/day	CLEA CLR TOX 8
$MDI_{inhalation}$	0.3ug/kg bw/day	CLEA CLR TOX 8

The dermal and inhalation pathways account for less that 1% of the overall exposure (CLEA CLR SGV 7), hence they have not been taken into account. This may not be the case on sites where:

- The majority of the site is bare for long periods and dry/windy conditions prevail
- Activities such as vehicle movements increase dust generation
- The contamination itself is in a dry and/or dusty form

SELENIUM

The data collated from literature review of the toxicological properties of selenium are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 10 – March 2002
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties for selenium is presented below;

		Description of effects	Source
Acute Effects	Lethal dose 250mg	Fever, dermatitis, anorexia and death	CLEA CLR TOX 8
Ingestion chronic exposure	TDI_{ing} 5µg/kg bw/day	Damage to the kidneys	CLEA CLR TOX 8
Inhalation Toxicity	TDI_{inh} / ID_{ing} 0.006µg/kg bw/day	Reduction body weight	CLEA CLR TOX 8

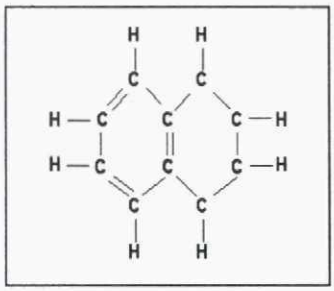
The background exposure data for selenium is presented below:

	Value	Source
$MDI_{ingestion}$	13ug/kg bw/day	CLEA CLR TOX 10

The dermal and inhalation pathways account for less that 1% of the overall exposure (CLEA CLR SGV 9), hence they have not been taken into account. This may not be the case on sites where:

- The majority of the site is bare for long periods and dry/windy conditions prevail
- Activities such as vehicle movements increase dust generation
- The contamination itself is in a dry and/or dusty form

NAPHTHALENE



Structure naphthalene

The data collated from literature review of the toxicological properties of naphthalene are summarised below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 20 – April 2002
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties for naphthalene is presented below;

		Description effects	Source
Acute Effects	LD 2000mg	In humans, the deliberate ingestion of naphthalene mothballs has caused nausea, vomiting, lethargy, ataxia, convulsions, abdominal pain, hemolytic anemia (resulting from red cell breakdown), liver toxicity, renal failure, coma and death (ATSDR, 1995; EC-JRC, 2003; IPCS, 1998).	CLEA CLR TOX 20
Ingestion chronic exposure	20ug/kg bw/day	Oral toxicity was moderate in mice (LD50 400 to 700 mg kg–1 bw (milligrams per kilogram body weight)) and moderate to low in rats (LD50 about 500 to 9400 mg kg–1 bw) (EC-JRC, 2003; IPCS, 1998). An 8-hour LC50 value greater than 0.5 mg L–1 (500 mg m-3) air for inhalation has been reported for rats (IPCS, 1998). Bronchiolar necrosis was seen in mice exposed for 4 hours at 0.1 mg L–1 (100 mg m–3) (Buckpitt and Franklin, 1989). Acute dermal toxicity in rats was low (LD50 > 2500 g kg–1 bw; probably 24/48-hour covered contact) (EC-JRC, 2003; IPCS, 1998). Rodents do not appear to be sensitive to the blood effects naphthalene, and this should be considered when using rodent data to derive tolerable naphthalene exposure levels for humans. Naphthalene induced hemolytic anemia has been reported in dogs (Zuelzer and Apt, 1949).	CLEA CLR TOX 20

Chronic Inhalation Toxicity	0.86 mg/kg bw/day	Individuals living in houses where large numbers mothballs were distributed have suffered anemia and kidney effects (ATSDR, 1995; EC-JRC, 2003; IPCS, 1998). There is limited evidence linking occupational inhalation naphthalene with cataracts in humans, but the studies are old and typically involved co-exposure to other substances (ATSDR, 1995; EC-JRC, 2003; IPCS, 1998). No reports lung damage to humans exposed to naphthalene by the inhalation (or any other) route were found during this review. A woman who ingested 400 mg naphthalene per day for 7 days (for medicinal purposes) suffered numb extremities and enlarged liver and spleen, while hemoglobin and albumin were detected in the urine (MacGregor, 1954).	CLEA CLR TOX 20

The background exposure data for naphthalene is presented below:

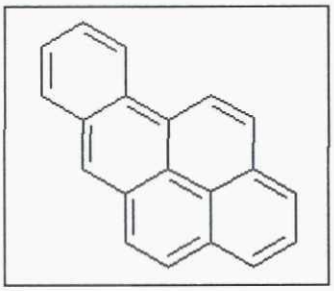
	Value	Source
$MDI_{ingestion}$	7ug/kg bw/day	CLEA CLR TOX 20
$MDI_{inhalation}$	2.8ug/kg bw/day	CLEA CLR TOX 20

The USEPA classes naphthalene as a "possibly carcinogenic to humans".

The physical properties of naphthalene used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	2511 l water per l octanol	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	2000 cm^3/g	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.0198	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$7.5x10^{-10}$ m^2/s	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$5.9x10^{-6}$ m^2/s	BP RISC V4.03 DATABASE
Molecular weight	128.2 g/mole	BP RISC V4.03 DATABASE
Saturated vapour pressure	0.085 mmHg	BP RISC V4.03 DATABASE

BENZO(a)PYRENE



Structure benzo(a)pyrene

The data collated from literature review of the toxicological properties of benzo(a)pyrene are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 2 – April 2002
European Commission *Committees*	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties for benzo(a)pyrene is presented below;

		Description effects	Source
Acute Effects	Lethal dose for mice *1,600mg*	Death	CLEA CLR TOX 2
Ingestion chronic exposure	ID_{ing} 0.02µg/kg bw/day	Dermatitis, breathing problems, chest pains, skin and lung cancer, depressed immune system	CLEA CLR TOX 2
Chronic Inhalation Toxicity	ID_{inh} 7ng/kg bw/day	Lung cancer	CLEA CLR TOX 2
Chronic Dermal Toxicity	N/A	Skin cancer	CLEA CLR TOX 2

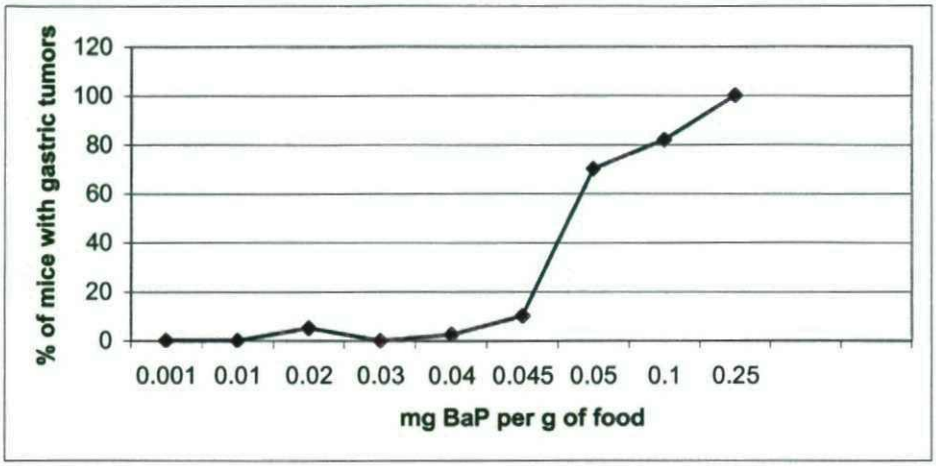
The USEPA classes benzo(a)pyrene as a "probable human carcinogen".

The ingestion Index Dose is based on WHO guidelines 0.7µg/L, which is based on an excess lifetime cancer risk 10^{-5} (WHO 1996).

The inhalation Index Dose is based on the air quality standard 0.25ng/m^3.

No toxicological data is available for the dermal pathway.

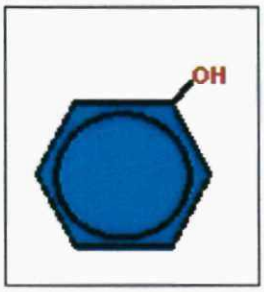
A review of the primary literature (Neal 1967) indicates that benzo(a)pyrene may be a non-threshold substance. A plot of dose versus reaction is presented below:



The physical properties of benzo(a)pyrene used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	1258925 l water per l octanol	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	1000000 cm^3/g	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.0000463	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$9x10^{-10}$ m^2/s	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$4.3x10^{-6}$ m^2/s	BP RISC V4.03 DATABASE
Molecular weight	252.3	BP RISC V4.03 DATABASE
Saturated vapor pressure	$5.5x10^{-9}$ mmHg	BP RISC V4.03 DATABASE

PHENOL



The data collated from literature review of the toxicological properties of phenol are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 9 – April 2002
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties for phenol is presented below;

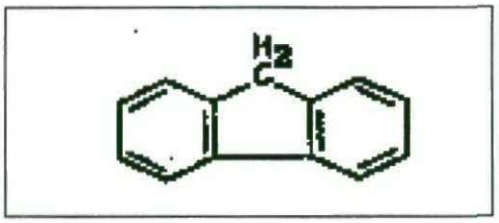
		Description effects	Source
Acute Effects	LD 140mg/kg bw	Nercosis, cardiovascular effects, cardiovascular effects, metabolic acidosis and cyanosis	CLEA CLR TOX 9
Ingestion chronic exposure	TDI_{ing}=0.7mg/kg bw/day	Mouth sores, diarrhea and dark urine	CLEA CLR TOX 9

The physical properties of phenol used in the derivation of the SGV are presented below:

Property	Value	Source
Log Kow (octanol/water partition coefficient)	1.47	CLEA SGV 8
Log Koc (organic carbon-water partition coefficient)	1.46 cm^3/g	CLEA SGV 8
Dimensionless Henry's constant	$3.97x10^{-7}$ $atm.m^3.mol^{-1}$	CLEA SGV 8
Diffusion coefficient in water	$9.1x10^{-10}m^2/s$	CLEA SGV 8
Diffusion coefficient in soil air	$8.2x10^{-6}m^2/s$	CLEA SGV 8

Saturated vapor pressure	48 Pa	CLEA SGV 8
Molecular Weight	94.11 g/mol	CLEA SGV 8

FLUORENE



Structure of Fluorere

The data collated from literature review of the toxicological properties of fluorene are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	IRIS	www.epa.gov/iris
Authoritative organisations	N/A		

The selected Relevant Health Criteria value for ingestion for fluorene as a threshold substance was the Oral Reference Dose, which is equivalent to the TDI.

The Oral TDI is 0.04mg/kg bw/day. No information on the MDI has been found during the literature search, hence the TDSI is assumed to be 20% of the TDI.

The data is based on Mouse oral subchronic toxicity study. Prepared by Toxicity Research Laboratories, LTD., Muskegon, MI for the fice Solid Waste, Washington, DC.

The USEPA have a low confidence in the RfD (TDI).

Soil parameters have been taken from CLEA CLR 10 and/or the CLEA Briefing Notes

The physical properties of fluorene used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	15848 l water per l octanol	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	14000 cm^3/g	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.0261	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$7.9x10^{-10}m^2/s$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$3.6x10^{-2}m^2/s$	BP RISC V4.03 DATABASE
Saturated Vapor Pressure	0.0084 mmHg	BP RISC V4.03 DATABASE
Molecular Weight	166.2 g/mole	BP RISC V4.03 DATABASE

ANTHRACENE

The data collated from literature review of the toxicological properties of anthracene are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	IRIS	www.epa.gov/iris
Authoritative organisations	N/A		

The selected Relevant Health Criteria value for ingestion for anthracene as a threshold substance was the Oral Reference Dose, which is equivalent to the TDI.

The Oral TDI is 0.3mg/kg bw/day. No information on the MDI has been found during the literature search; hence the TDSI is assumed to be 20% of the TDI.

The data is based on a Subchronic toxicity in mice with anthracene. Final Report. Hazelton Laboratories America, Inc. Prepared for the fice of Solid Waste, Washington, DC.

The USEPA have a low confidence in the RfD (TDI).

The physical properties of anthracene used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	39810 l water per l octanol	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	30000 cm^3/g	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.00267	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$7.7x10^{-10}m^2/s$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$3.2x10^{-6}m^2/s$	BP RISC V4.03 DATABASE
Saturated Vapor Pressure	0.0000027mmHg	BP RISC V4.03 DATABASE
Molecular Weight	178.2 g/mol	BP RISC V4.03 DATABASE

FLUORANTHENE

The data collated from literature review of the toxicological properties of fluoranthene are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	IRIS	www.epa.gov/iris
Authoritative organisations	N/A		

The Oral TDI is 0.3mg/kg bw/day. No information on the MDI has been found during the literature search, hence the TDSI is assumed to be 20% of the TDI.

The data is based on a 13-Week mouse oral subchronic toxicity study. Prepared by Toxicity Research Laboratories, Ltd., Muskegon, MI for the fice Solid Waste, Washington, DC.

The USEPA have a low confidence in the RfD (TDI).

The critical receptor for this scenario is a female adult. The selection of an Exposure Duration and averaging period 0-6 years is considered appropriate, as is the chosen receptor body weight.

Soil parameters have been taken from CLEA CLR 10 and/or the CLEA Briefing Notes

The physical properties of fluoranthene used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	125892 l water per l octanol	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	110000 cm^3/g	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.00066	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$6.4x10^{-10}$ m^2/s	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$3.0x10^{-6}m^2/s$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	$1.2x10^{-8}$mmHg	BP RISC V4.03 DATABASE
Molecular Weight	202.3 g/mol	BP RISC V4.03 DATABASE

PYRENE

The data collated from literature review of the toxicological properties of pyrene are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	IRIS	www.epa.gov/iris
Authoritative organisations	N/A		

The selected Relevant Health Criteria value for ingestion for pyrene as a threshold substance was the Oral Reference Dose, which is equivalent to the TDI.

The Oral TDI is 0.03mg/kg bw/day. No information on the MDI has been found during the literature search, hence the TDSI is assumed to be 20% of the TDI.

The data is based on a Mouse Oral Subchronic Toxicity Pyrene. Study conducted by Toxicity Research Laboratories, Muskegon, MI for the fice Solid Waste, Washington, DC.

The USEPA have a low confidence in the RfD (TDI).

Soil parameters have been taken from CLEA CLR 10 and/or the CLEA Briefing Notes

The physical properties of pyrene used in the derivation GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	125892 l water per l octanol	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	110000 cm^3/g	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.000137	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$7.2x10^{-10}m^2/s$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$2.7x10^{-6}m^2/s$	BP RISC V4.03 DATABASE
Saturated Vapor Pressure	$2.5x10^{-6}$ mmHg	BP RISC V4.03 DATABASE
Molecular Weight	202.3 g/mol	BP RISC V4.03 DATABASE

ACENAPHTHYLENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC benzo(a)pyrene.

The TEF for acenaphthylene is 0.001.

ACENAPHTHENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC benzo(a)pyrene.

The TEF for aecnaphthene is 0.001.

BENZO(A)ANTHRACENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC benzo(a)pyrene.

The TEF for benzo(a)anthracene is 0.1

PHENANTHRENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC benzo(a)pyrene.

The TEF for phenanthrene is 0.001.

CHRYSENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC benzo(a)pyrene.

The TEF for chrysene is 0.1

BENZO(B)FLUORANTHENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC benzo(a)pyrene.

The TEF for benzo(b)fluoranthene is 0.1

BENZO(K)FLUORANTHENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC benzo(a)pyrene.

The TEF for benzo(k)fluoranthene is 0.1

INDENO(1,2,3-CD)PYRENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC benzo(a)pyrene.

The TEF for indeno(1,2,3-CD)pyrene is 0.1

DEBENZ(A,H)ANTHRACENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC *benzo(a)pyrene.*

The TEF for dibenz(a,h)anthracene is 1.0

BENZO(G,H,I)PERYLENE

There is currently no toxicological data available, hence Toxicity Equivalent Factors (TEF) have been used do derive an GAC based on the GAC benzo(a)pyrene.

The TEF for benzo(g,h,I)perylene is 0.1

HYDROCARBONS

AROMATIC EC5-EC7 (BENZENE)

The data collated from literature review of the toxicological properties of the aromatic EC5-EC7 (benzene) fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 11
European Commission Committees	No		
Other national organisations	No		
Authoritative organisations	N/A		

The oral index dose for benzene is 0.00029mg/kg bw/day and the inhalation index dose is 0.00091mg/kg bw/day.

The physical properties the aromatic EC5-EC7 fractions used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	125.89254	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	59	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.228	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$9.8x10^{-10}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$8.8x10^{-6}$	BP RISC V4.03 DATABASE
Saturated Vapor Pressure	95	BP RISC V4.03 DATABASE
Molecular Weight	78	BP RISC V4.03 DATABASE

AROMATIC EC7-EC8 (TOLUENE)

The data collated from literature review of the toxicological properties of the Aromatic EC7-EC8 (toluene) fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 14
European Commission Committees	No		
Other national organisations	No		
Authoritative organisations	N/A		

The oral tolerable daily intake for toluene is 200ug/kg bw/day and the inhalation tolerable daily intake is 74ug/kg bw/day.

The mean daily intake for toluene is 10ug/day for ingestion and 124ug/day for inhalation.

AROMATIC EC8-EC10

The data collated from literature review of the toxicological properties of the aromatic EC8-EC10 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aromatic EC8-EC10 fraction is 0.04mg/kg bw/day and the inhalation tolerable daily intake is 0.04mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties the aromatic EC8-EC10 fractions used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	1258.9254	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	1600	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.49	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	4.8	BP RISC V4.03 DATABASE
Molecular Weight	120	BP RISC V4.03 DATABASE

AROMATIC EC10-EC12

The data collated from literature review of the toxicological properties of the aromatic EC10-EC12 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aromatic EC10-EC12 fraction is 0.04mg/kg bw/day and the inhalation tolerable daily intake is 0.04mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties the aromatic EC10-EC12 fractions used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	3162.2777	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	2500	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.14	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1X10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1X10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	0.48	BP RISC V4.03 DATABASE
Molecular Weight	130	BP RISC V4.03 DATABASE

AROMATIC EC12-EC16

The data collated from literature review of the toxicological properties of the aromatic EC12-EC16 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aromatic EC12-EC16 fraction is 0.04mg/kg bw/day and the inhalation tolerable daily intake is 0.04mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties the aromatic EC12-EC16 fractions used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	7943.2823	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	5000	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.054	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	0.036	BP RISC V4.03 DATABASE
Molecular Weight	150	BP RISC V4.03 DATABASE

AROMATIC EC16-EC21

The data collated from literature review of the toxicological properties of the aromatic EC16-EC21 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aromatic EC16-EC21 fraction is 0.03mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties the aromatic EC16-EC21 fractions used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	50118.723	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	16000	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.013	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	$5.8x10^{-3}$	BP RISC V4.03 DATABASE
Molecular Weight	190	BP RISC V4.03 DATABASE

AROMATIC EC21-EC35

The data collated from literature review of the toxicological properties of the aromatic EC21-EC35 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aromatic EC21-EC35 fraction is 0.03mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties the aromatic EC21-EC35 fractions used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	1258925.4	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	130000	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	$6.8X10^{-4}$	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	$3.3X10^{-6}$	BP RISC V4.03 DATABASE
Molecular Weight	240	BP RISC V4.03 DATABASE

ALIPHATIC EC5-EC6

The data collated from literature review of the toxicological properties of the aliphatic EC5-EC6 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aliphatic EC5-EC6 fraction is 5mg/kg bw/day and the inhalation tolerable daily intake is 5.26mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties of the aliphatic EC5-EC6 fraction used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	1995.2623	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	790	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	34	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	270	BP RISC V4.03 DATABASE
Molecular Weight	81	BP RISC V4.03 DATABASE

ALIPHATIC EC6-EC8

The data collated from literature review of the toxicological properties of the aliphatic EC6-EC8 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aliphatic EC6-EC8 fraction is 5mg/kg bw/day and the inhalation tolerable daily intake is 5.26mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties of the aliphatic EC6-EC8 fraction used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	10000	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	4000	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	51	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	48	BP RISC V4.03 DATABASE
Molecular Weight	100	BP RISC V4.03 DATABASE

ALIPHATIC EC8-EC10

The data collated from literature review of the toxicological properties of the aliphatic EC8-EC10 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aliphatic EC8-EC10 fraction is 0.1mg/kg bw/day and the inhalation tolerable daily intake is 0.29mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties of the aliphatic EC8-EC10 fraction used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	63095.734	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	32000	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	82	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	4.8	BP RISC V4.03 DATABASE
Molecular Weight	130	BP RISC V4.03 DATABASE

ALIPHATIC EC10-EC12

The data collated from literature review of the toxicological properties of the aliphatic EC10-EC12 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aliphatic EC10-EC12 fraction is 0.1mg/kg bw/day and the inhalation tolerable daily intake is 0.29mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties of the aliphatic EC10-EC12 fraction used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	398107.17	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	$2.5X10^{5}$	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	130	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	0.49	BP RISC V4.03 DATABASE
Molecular Weight	160	BP RISC V4.03 DATABASE

ALIPHATIC EC12-EC16

The data collated from literature review of the toxicological properties of the aliphatic EC12-EC16 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aliphatic EC12-EC16 fraction is 0.1mg/kg bw/day and the inhalation tolerable daily intake is 0.29mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties of the aliphatic EC12-EC16 fraction used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	6309573.4	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	$5X10^{6}$	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	540	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	0.036	BP RISC V4.03 DATABASE
Molecular Weight	200	BP RISC V4.03 DATABASE

ALIPHATIC EC16-EC35

The data collated from literature review of the toxicological properties of the aliphatic EC16-EC35 fraction are summarized below;

	Data	Organisation	Reference
Authoritative UK Bodies	No		
European Commission Committees	No		
Other national organisations	Yes	TPHCWG	
Authoritative organisations	N/A		

The ingestion tolerable daily intake for the aliphatic EC16-EC35 fraction is 2.0mg/kg bw/day.

No data is available on the mean daily intake of this fraction, hence it will be assumed to be 80% of the tolerable daily intakes.

The physical properties of the aliphatic EC16-EC35 fraction used in the derivation of GAC's are presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	$10^{8.9}$	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	$1X10^{9}$	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	6400	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$1x10^{-9}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$1x10^{-5}$	BP RISC V4.03 DATABASE
Saturated Vapour Pressure	$5.8X10^{-3}$	BP RISC V4.03 DATABASE
Molecular Weight	270	BP RISC V4.03 DATABASE

XYLENES

The data collated from literature review of the toxicological properties of xylenes are summarised below;

	Data	Organisation	Reference
Authoritative UK Bodies	Yes	DEFRA	CLEA CLR TOX 20 – April 2002
European Commission Committees	N/A		
Other national organisations	N/A		
Authoritative organisations	N/A		

A summary of the toxicological properties for naphthalene is presented below;

The tolerable daily intake for ingestion and inhalation are 179ug/kg bw/day and 63ug/kg bw/day.

The mean daily intake for ingestion and inhalation are 20ug/day and 112ug/day.

The physical properties of xylenes used in the derivation of the GAC is presented below:

Property	Value	Source
Kow (octanol/water partition coefficient)	1995.2623	BP RISC V4.03 DATABASE
Koc (organic carbon-water partition coefficient)	240	BP RISC V4.03 DATABASE
Dimensionless Henry's constant	0.29	BP RISC V4.03 DATABASE
Diffusion coefficient in water	$8.5x10^{-10}$	BP RISC V4.03 DATABASE
Diffusion coefficient in soil air	$7.2x10^{-6}$	BP RISC V4.03 DATABASE
Molecular weight	106.2	BP RISC V4.03 DATABASE
Saturated vapour pressure	8.8	BP RISC V4.03 DATABASE

SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aliphatic EC5-EC6 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI). 5.00E+00 mg per kg body weight per day

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

[Y]

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

[0.485]

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)[a]

[ ] mg per kg body weight per day

[a] Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

[1] mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

[N]

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

[5.26E+00] mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

Y

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (Inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

1.052 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

Y

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{dirng} from this table, depending on your choice of land use

Land Use	SEI_{dirng} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{dirng} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

N

If Y insert the representative fraction here (default=1)

The amended SEI_{dirng} = SEI_{dirng} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{dirng} = RI_{ingest}/SEI_{dirng}

ASC_{dirng} = 1.00000E+00 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 101490.0249 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? *(Y or N)* **N**

Measured Concentration Factor for leafy vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) 1995.262315 l water per l octanol

a representative value of ϕ (soil density) 1.6 g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): 790 cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): 5.98802E-03 kg OC per kg soil

a representative value of θ (soil-water content by volume) 0.15 cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44}+(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= 0.818976571 [a] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= 0.023455113 [a] ug per g fresh weight plant per ug per g dry weight soil

[a] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	2.60996E-03
Cabbage	4.86885E-03	calc not required	2.49524E-03
Carrot	7.38094E-03	calc not required	7.06093E-05
Leafy salads	3.25677E-03	calc not required	4.66855E-04
Onion	3.69474E-03	calc not required	5.04372E-05
Potato	4.41616E-02	calc not required	3.88593E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	5.45443E-04
Allotments	5.45443E-04

SEI_{veg}= 5.45E-04 kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{organ}/SEI_{veg}$

ASC_{veg} = 1.00000E+00 mg per kg body weight per day / 5.45443E-04 kg soil per kg body weight per day = 1833.3712 mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$ = 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 1.00000E+00 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 887131.6833 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-5}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_s=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1 %		
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{air}=	0.31 unitless		
Water filled porosity	θ_{wat}=	0.15 unitless		
Total porosity	θ_{total}=	0.46 unitless		
Bulk soil density	ρ=	1.6 kg soil per l soil		

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	790 l water per kg OC
Dimensionless Henry's constant	H'=	34 l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09 m^2 per s
Diffusion coefficient in soil air	D_i=	1.00E-05 m^2 per s
Air in soil		9.52847E-02 unitless
Water in soil		8.47465E-03 unitless
Air term		9.52847E-07 m^2 per s
Water term		2.49254E-13 m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.52848E-07 m^2 per s
Molecular weight	MW=	81 g per mol
Saturated vapour pressure	SatVP	270 mmHg

Pathway parameters

Dilution ratio	DR=	20000 unitless		
Temperature	Temp=	12 °C + 273 =	285	K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3 m per s		

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 3.05254E-05 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAloutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residential without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air
using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

2.22048E-03 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air
using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 1.05200E+00 mg per kg body weight per day / 2.22048E-03 kg soil per kg body weight per day = 473.7714317 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 0.139133498 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 2.979375121 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 4.14697E-02 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 1.05200E+00 mg per kg body weight per day / 4.14697E-02 kg soil per kg body weight per day = 25.3678985 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^6)/(760mmHg \times R \times Temp)$

C_{sat}= 1.23044E+09 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 7.55805E+01 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 6.14258E-08 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/ 101490.0249	=	9.85319E-06	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/ 1833.3712	=	5.45443E-04	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/ 887131.6833	=	1.12723E-06	kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$=	1/ 473.7714317	=	2.11072E-03	kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$=	1/ 25.3678985	=	3.94199E-02	kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39	For the residential with plant uptake land use the $SSAC_{rwp}$ =		mg per kg soil
40	For the allotments land use the $SSAC_{all}$ =		mg per kg soil
41	For the residential without plant uptake land use the $SSAC_{other}$ =	24.07290734	mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for liphatic EC5-EC in the Residential without plant uptake scenario is 24.07291 mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	=		kg soil per mg

The integrated Site Specific Assessment Criterion

43	For the residential with plant uptake land use the $SSAC_{rwp}$ =		mg per kg soil
	For the allotments land use the $SSAC_{all}$ =		mg per kg soil
	For the residential without plant uptake land use the $SSAC_{other}$ =		mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

The Level 1 Site Specific Assessment Criterion for Aliphatic EC5-EC in the scenario is mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aliphatic EC6-EC8 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion 5.00E+00 mg per kg body weight per day
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

[Y]

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

[0.485]

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

[1] mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

[N]

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

[5.26E+00] mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

[Y]

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

[0.362]

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

1.052 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-5}? (Yor N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

Y

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{dirg} from this table, depending on your choice of land use

Land Use	SEI_{dirg} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{dirg} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

N

If Y insert the representative fraction here (default=1)

The amended SEI_{dirg} = SEI_{dirg} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{dirg} = RI_{ingest}/SEI_{dirg}

ASC_{dirg} = 1.00000E+00 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 101490.0249 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **10000** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **4333** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(\log K_{ow}-1.78)^2/2.44}+(10^{0.95\log K_{ow}-2.05}+0.82)*(\phi/(\theta+\phi K_{oc} f_{oc}))$

CF_{leafy}= **0.228221055** [b] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77\log K_{ow}-1.52}+0.82)*(\phi/(\theta+\phi K_{oc} f_{oc}))*0.01$

CF_{root}= **0.014258068** [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc} f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	7.27306E-04
Cabbage	4.86885E-03	calc not required	6.95340E-04
Carrot	7.38094E-03	calc not required	4.29225E-05
Leafy salads	3.25677E-03	calc not required	1.30097E-04
Onion	3.69474E-03	calc not required	3.06602E-05
Potato	4.41616E-02	calc not required	2.36221E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	1.67044E-04
Allotments	1.67044E-04

SEI_{veg}= **1.67E-04** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = **1.00000E+00** mg per kg body weight per day / **1.67044E-04** kg soil per kg body weight per day = **5986.428908** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 1.00000E+00 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 887131.6833 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-5}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15	metres
Depth to subsurface contamination	d_z=	1	metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{air}=	0.31	unitless	
Water filled porosity	θ_{wat}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ_b=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	4333	l water per kg OC
Dimensionless Henry's constant	H'=	48	l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s
Diffusion coefficient in soil air	D_i=	1.00E-05	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		9.52847E-07	m^2 per s
Water term		1.76555E-13	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.52847E-07	m^2 per s
Molecular weight	MW=	100	g per mol
Saturated vapour pressure	SatVP	48	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height — TAH= 0.93 m
Height of mixing zone — h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 1.39159E-05 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residential without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent intake

Calculate the soil equivalent intake for inhalation of outdoor air
using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

1.01227E-03 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air
using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 1.05200E+00 mg per kg body weight per day / 1.01227E-03 kg soil per kg body weight per day = 1039.244296 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 0.540543912 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 1.356239761 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 1.89053E-02 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 1.05200E+00 mg per kg body weight per day / 1.89053E-02 kg soil per kg body weight per day = 55.64590863 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^{3})/(760mmHg \times R \times Temp)$

C_{sat}= 2.70054E+08 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 7.55805E+01 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 2.79871E-07 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/ 101490.0249	=	9.85319E-06	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/ 5986.428908	=	1.67044E-04	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/ 887131.6833	=	1.12723E-06	kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$ =	1/ 1039.244296	=	9.62238E-04	kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$ =	1/ 55.64590863	=	1.79708E-02	kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39	For the residential with plant uptake land use the $SSAC_{rep}$ =		mg per kg soil
40	For the allotments land use the $SSAC_{all}$ =		mg per kg soil
41	For the residential without plant uptake land use the $SSAC_{other}$ =	52.79032785	mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for **liphatic EC6-EC** in the **Residential without plant uptake** scenario is 52.79033 mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/	=		kg soil per mg

The integrated Site Specific Assessment Criterion

43	For the residential with plant uptake land use the $SSAC_{rep}$ =	mg per kg soil
	For the allotments land use the $SSAC_{all}$ =	mg per kg soil
	For the residential without plant uptake land use the $SSAC_{other}$ =	mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=	mg per kg soil

The Level 1 Site Specific Assessment Criterion for **Aliphatic EC6-EC** in the scenario is mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aliphatic EC8-EC10 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion 1.00E-01 mg per kg body weight per day
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

Y

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

0.02 mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

N

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

2.90E-01 mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

Y

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0.058 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

Y

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{dirng} from this table, depending on your choice of land use

Land Use	SEI_{dirng} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{dirng} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

[ ]

If Y insert the representative fraction here (default=1)

[ ]

The amended SEI_{dirng} = SEI_{dirng} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{dirng} = RI_{ingest}/SEI_{dirng}

ASC_{dirng} = 2.00000E-02 (mg per kg body weight per day) / 9.85319E-06 (kg soil per kg body weight per day) = 2029.800499 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] *Note - See 18 below*

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient)	63095.73445	l water per l octanol
a representative value of ϕ (soil density)	1.6	g dry weight per cm^3
a representative value of K_{oc} (organic carbon-water partition coefficient):	3.20E+04	cm^3 per g dry weight
a representative value of f_{oc} (fraction of organic carbon in soil):	5.98802E-03	kg OC per kg soil
a representative value of θ (soil-water content by volume)	0.15	cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44}+(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= 0.031061606 [b] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= 0.007865426 [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	1.00901E-04
Cabbage	4.86885E-03	calc not required	9.64863E-05
Carrot	7.38094E-03	calc not required	2.36781E-05
Leafy salads	3.25677E-03	calc not required	1.80487E-05
Onion	3.69474E-03	calc not required	1.69136E-05
Potato	4.41616E-02	calc not required	1.30311E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	3.46474E-05
Allotments	3.46474E-05

SEI_{veg}= 3.46E-05 kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = 2.00000E-02 mg per kg body weight per day / 3.46474E-05 kg soil per kg body weight per day = 577.2441854 mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 2.00000E-02 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 17742.63367 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-5}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_z=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{air}=	0.31	unitless	
Water filed porosity	θ_{wet}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	32000	l water per kg OC
Dimensionless Henry's constant	H'=	82	l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s
Diffusion coefficient in soil air	D_s=	1.00E-05	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		9.52847E-07	m^2 per s
Water term		1.03349E-13	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.52847E-07	m^2 per s
Molecular weight	MW=	130	g per mol
Saturated vapour pressure	SatVP	4.8	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 4.04694E-06 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residential without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air
using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

2.94383E-04 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air
using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 5.80000E-02 mg per kg body weight per day / 2.94383E-04 kg soil per kg body weight per day = 197.0224539 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{sv} \times f_{ow}/H'$

SF= 2.336789835 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.39499414 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 5.49790E-03 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 5.80000E-02 mg per kg body weight per day / 5.49790E-03 kg soil per kg body weight per day = 10.54948549 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^6)/(760mmHg \times R \times Temp)$

C_{sat}= 3.51071E+07 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 4.16696E+00 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 1.18694E-07 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/ 2029.800499	=	4.92659E-04	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/ 577.2441854	=	1.73237E-03	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/ 17742.63367	=	5.63614E-05	kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$=	1/ 197.0224539	=	5.07556E-03	kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$=	1/ 10.54948549	=	9.47914E-02	kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39	For the residential with plant uptake land use the $SSAC_{rwp}$ =		mg per kg soil
40	For the allotments land use the $SSAC_{alt}$ =		mg per kg soil
41	For the residential without plant uptake land use the $SSAC_{other}$ =	9.964171275	mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for **liphatic EC8-EC** in the **Residential without plant uptake** scenario is **9.964171** mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	=		kg soil per mg

The integrated Site Specific Assessment Criterion

43	For the residential with plant uptake land use the $SSAC_{rwp}$ =		mg per kg soil
	For the allotments land use the $SSAC_{alt}$ =		mg per kg soil
	For the residential without plant uptake land use the $SSAC_{other}$ =		mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

The Level 1 Site Specific Assessment Criterion for **liphatic EC8-EC1** in the scenario is mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aliphatic EC10-EC12 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion 1.00E-01 mg per kg body weight per day
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

Y

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

0.02 mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

N

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

2.90E-01 mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

[Y]

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

[0.362]

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0.058 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

Y

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{ding} from this table, depending on your choice of land use

Land Use	SEI_{ding} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{ding} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

If Y insert the representative fraction here (default=1)

The amended SEI_{ding} = SEI_{ding} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{ding} = RI_{ingest}/SEI_{ding}

ASC_{ding} = 2.00000E-02 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 2029.800499 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses; residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables ug per g (dry or fresh)* weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables ug per g (dry or fresh)* weight plant per ug per g dry weight soil

* Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **398107.1706** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **2.50E+05** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44})(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= **0.002475843** ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= **0.004143085** * ug per g fresh weight plant per ug per g dry weight soil

* Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}

The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	7.89014E-06
Cabbage	4.86885E-03	calc not required	7.54335E-06
Carrot	7.38094E-03	calc not required	1.24723E-05
Leafy salads	3.25677E-03	calc not required	1.41135E-06
Onion	3.69474E-03	calc not required	8.90916E-06
Potato	4.41616E-02	calc not required	6.86407E-05

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	9.58449E-06
Allotments	9.58449E-06

SEI_{veg}= **9.58E-06** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{irgest}/SEI_{veg}$

ASC_{veg} = **2.00000E-02** mg per kg body weight per day / **9.58449E-06** kg soil per kg body weight per day = **2086.705472** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 2.00000E-02 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 17742.63367 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area					
	Source zone width parallel to wind direction	W=	15	metres	
	Depth to subsurface contamination	d_z=	1	metres	
Soil Matrix					
	Soil organic matter content	SOM=	1	%	
	Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
	Air filled porosity	θ_{vap}=	0.31	unitless	
	Water filled porosity	θ_{wat}=	0.15	unitless	
	Total porosity	θ_{total}=	0.46	unitless	
	Bulk soil density	ρ=	1.6	kg soil per l soil	
Contaminant					
	Organic carbon/water partition coefficient	K_{oc}=	250000	l water per kg OC	
	Dimensionless Henry's constant	H'=	130	l water per l air	
	Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s	
	Diffusion coefficient in soil air	D_i=	1.00E-05	m^2 per s	
	Air in soil		9.52847E-02	unitless	
	Water in soil		6.47465E-03	unitless	
	Air term		9.52847E-07	m^2 per s	
	Water term		6.51896E-14	m^2 per s per (l water per l air)	
	Effective diffusion coefficient	D_{eff}=	9.52847E-07	m^2 per s	
	Molecular weight	MW=	160	g per mol	
	Saturated vapour pressure	SatVP	0.49	mmHg	
Pathway parameters					
	Dilution ratio	DR=	20000	unitless	
	Temperature	Temp=	12	°C + 273 =	285 K
	Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 8.74949E-07 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAloutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residental without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

6.36456E-05 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the *nominal assessment sub-criteria* for intake via outdoor air using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 5.80000E-02 mg per kg body weight per day / 6.36456E-05 kg soil per kg body weight per day = 911.2963863 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 11.51543068 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.085397812 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 1.18865E-03 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 5.80000E-02 mg per kg body weight per day / 1.18865E-03 kg soil per kg body weight per day = 48.7949847 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^3)/(760mmHg \times R \times Temp)$

C_{sat}= 4.41089E+06 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 4.16698E+00 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 9.44704E-07 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/ 2029.800499	=	4.92659E-04	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/ 2086.705472	=	4.79224E-04	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/ 17742.63367	=	5.63614E-05	kg soil per mg
inhalation of outdoor air	$1/ASC_{out}$=	1/ 911.2963863	=	1.09734E-03	kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$=	1/ 48.7949847	=	2.04939E-02	kg soil per mg

The Integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

40 For the allotments land use the $SSAC_{all}$ = mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = 45.28184344 mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for **phatic EC10-EC** in the **Residential without plant uptake** scenario is 45.28184 mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	=		kg soil per mg

The Integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

For the allotments land use the $SSAC_{all}$ = mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

The Level 1 Site Specific Assessment Criterion for **liphatic EC10-EC1** in the scenario is mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aliphatic EC12-EC16 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion. For a non threshold substance the relevant health criterion is the Index Dose (ID). For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI). 1.00E-01 mg per kg body weight per day

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses. Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

Y

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

0.02 mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

N

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

2.90E-01 mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

Y

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

mg per kg body weight per day

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0.058 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

Y

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{dirng} from this table, depending on your choice of land use

Land Use	SEI_{dirng} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{dirng} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

If Y insert the representative fraction here (default=1)

The amended SEI_{dirng} = SEI_{dirng} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{dirng} = RI_{ingest}/SEI_{dirng}

ASC_{dirng} = 2.00000E-02 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 2029.800499 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables _____ ug per g (dry or fresh)* weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables _____ ug per g (dry or fresh)* weight plant per ug per g dry weight soil

* Note - See 18 below

17 *Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.*

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **6309573.445** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **5.00E+06** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(\log Kow-1.78)^2/2.44}+(10^{0.95\log Kow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= **2.21671E-05** ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77\log Kow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= **0.001737055** * *ug per g fresh weight plant per ug per g dry weight soil*

* Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	7.06432E-08
Cabbage	4.86885E-03	calc not required	6.75383E-08
Carrot	7.38094E-03	calc not required	5.22923E-06
Leafy salads	3.25677E-03	calc not required	1.26363E-08
Onion	3.69474E-03	calc not required	3.73532E-06
Potato	4.41816E-02	calc not required	2.87787E-05

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	3.39857E-06
Allotments	3.39857E-06

SEI_{veg}= **3.40E-06** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{irgest}/SEI_{veg}$

ASC_{veg} = **2.00000E-02** mg per kg body weight per day / **3.39857E-06** kg soil per kg body weight per day = **5884.825504** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 2.00000E-02 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 17742.63367 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_z=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{vap}=	0.31	unitless	
Water filed porosity	θ_{wat}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	5000000	l water per kg OC
Dimensionless Henry's constant	H'=	540	l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s
Diffusion coefficient in soil air	D_i=	1.00E-05	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		9.52847E-07	m^2 per s
Water term		1.56938E-14	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.52847E-07	m^2 per s
Molecular weight	MW=	200	g per mol
Saturated vapour pressure	SatVP	3.60E-02	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 1.84145E-07 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residental without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

1.33951E-05 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 5.80000E-02 mg per kg body weight per day / 1.33951E-05 kg soil per kg body weight per day = 4329.946503 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 55.44466622 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.017973137 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 2.50167E-04 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 5.80000E-02 mg per kg body weight per day / 2.50167E-04 kg soil per kg body weight per day = 231.8451665 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^3)/(760mmHg \times R \times Temp)$

C_{sat}= 4.05082E+05 mm Hg g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 4.16698E+00 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 1.02868E-05 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/ 2029.800499	=	4.92659E-04	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/ 5884.825504	=	1.69929E-04	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/ 17742.63367	=	5.63614E-05	kg soil per mg
inhalation of outdoor air	$1/ASC_{outdv}$=	1/ 4329.946503	=	2.30950E-04	kg soil per mg
inhalation of indoor air	$1/ASC_{indv}$=	1/ 231.8451665	=	4.31322E-03	kg soil per mg

The Integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

40 For the allotments land use the $SSAC_{ah}$ = mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = 198.5374776 mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for phatic EC12-EC in the Residential without plant uptake scenario is 198.5375 mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	=		kg soil per mg

The Integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

For the allotments land use the $SSAC_{ah}$ = mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

The Level 1 Site Specific Assessment Criterion for liphatic EC12-EC in the scenario is mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aliphatic EC16-EC35 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Y or N) N

5a Insert the relevant health criterion for ingestion 2.00E+00 mg per kg body weight per day
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

[Y]

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

[0.485]

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{Ingest}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{Ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)[a]

[ ] mg per kg body weight per day

[a] Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{Ingest}=0.2TDI

[0.4] mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

[N]

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

[0.00E+00] mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

Y

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

		mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.		
		mg per kg body weight per day

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

	0	mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

N	Inhalation pathway should not be selected if H' < 1E-3

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{dring} from this table, depending on your choice of land use

Land Use	SEI_{dring} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{dring} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

	N

If Y insert the representative fraction here (default=1)

The amended SEI_{dring} = SEI_{dring} * bioaccessibility fraction

9.85319E-06	kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{dring} = RI_{ingest}/SEI_{dring}

ASC_{dring} =		/		=		
	4.00000E-01		9.85319E-06		40596.00998	mg per kg soil
	mg per kg body weight per day		kg soil per kg body weight per day			

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **794328234.7** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **1.00E+09** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44}+(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= **3.19947E-10** [b] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= **0.000359516** [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	1.01962E-12
Cabbage	4.86885E-03	calc not required	9.74808E-13
Carrot	7.38094E-03	calc not required	1.08229E-06
Leafy salads	3.25677E-03	calc not required	1.82385E-13
Onion	3.69474E-03	calc not required	7.73093E-07
Potato	4.41616E-02	calc not required	5.95629E-06

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	7.00598E-07
Allotments	7.00598E-07

SEI_{veg}= **7.01E-07** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = **4.00000E-01** mg per kg body weight per day / **7.00598E-07** kg soil per kg body weight per day = **570940.5202** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect}$ = $RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 4.00000E-01 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 354852.6733 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_s=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{air}=	0.31	unitless	
Water filed porosity	θ_{wat}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	1000000000	l water per kg OC
Dimensionless Henry's constant	H'=	6.40E+03	l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s
Diffusion coefficient in soil air	D_i=	1.00E-05	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		6.47465E-03	unitless
Air term		9.52847E-07	m^2 per s
Water term		1.32416E-15	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.52847E-07	m^2 per s
Molecular weight	MW=	270	g per mol
Saturated vapour pressure	SatVP	5.80E-03	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 1.09482E-08 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residental without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air
using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

7.96394E-07 *kg soil per (kg body weight per day)*

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air
using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 0.00000E+00 mg per kg body weight per day / 7.96394E-07 kg soil per kg body weight per day = 0 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 935.6287425 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.001068579 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 1.48735E-05 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{lv}/SEI_{inv}$

ASC_{inv} = 0.00000E+00 mg per kg body weight per day / 1.48735E-05 kg soil per kg body weight per day = 0 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
C_{sat} = (SatVP x MW x 10^3)/(760mmHg x R x Temp)

C_{sat}= 8.81053E+04 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 0.00000E+00 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 0 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/		=	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/		=	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/		=	kg soil per mg
inhalation of outdoor air	$1/ASC_{outdv}$=	1/		=	kg soil per mg
inhalation of indoor air	$1/ASC_{indv}$=	1/		=	kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

40 For the allotments land use the $SSAC_{all}$ = mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for phatic EC16-EC in the scenario is mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	40596.00998	=	2.4633E-05 kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	570940.5202	=	1.7515E-06 kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	354852.6733	=	2.81807E-06 kg soil per mg

The integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

For the allotments land use the $SSAC_{all}$ = mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = 40596.00998 mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

The Level 1 Site Specific Assessment Criterion for liphatic EC16-EC3 in the Residential without plant uptake scenario is 40596.01 mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aromatic EC5-EC7 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) **Y**

5a Insert the relevant health criterion for ingestion
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI). **2.90E-04** mg per kg body weight per day

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

0.00E+00 mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

0.00029 mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

Y

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

9.10E-04 mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero) 0.00E+00 mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

0.00091 mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

mg per kg body weight per day

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

Y

Intake via Soil and Dust Ingestion

12 *Select a value for SEI_{ding} from this table, depending on your choice of land use*

Land Use	SEI_{ding} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{ding} = 9.85E-06

13 *Is site specific* data on the bioaccessibility of the contaminant in soil available? (Y or N)

N

If Y insert the representative fraction here (default=1)

The amended SEI_{ding} = SEI_{ding} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{ding} = RI_{ingest}/SEI_{ding}

ASC_{ding} = 2.90000E-04 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 29.43210723 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables ____ ug per g (dry or fresh)* weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables ____ ug per g (dry or fresh)* weight plant per ug per g dry weight soil

* Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **125.8925412** *l water per l octanol*

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **59** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44})*(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc} f_{oc}))$

CF_{leafy}= **1.278848457** ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc} f_{oc}))*0.01$

CF_{root}= **0.02070259** * ug per g fresh weight plant per ug per g dry weight soil

* Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc} f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}

The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	4.07550E-03
Cabbage	4.86885E-03	calc not required	3.89637E-03
Carrot	7.38094E-03	calc not required	6.23231E-05
Leafy salads	3.25677E-03	calc not required	7.29004E-04
Onion	3.69474E-03	calc not required	4.45183E-05
Potato	4.41616E-02	calc not required	3.42991E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	8.20691E-04
Allotments	8.20691E-04

SEI_{veg}= **8.21E-04** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = **2.90000E-04** mg per kg body weight per day / **8.20691E-04** kg soil per kg body weight per day = **0.353360747** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 2.90000E-04 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 257.2681881 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_z=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{esp}=	0.31	unitless	
Water filed porosity	θ_{wet}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	59	l water per kg OC
Dimensionless Henry's constant	H'=	0.228	l water per l air
Diffusion coefficient in water	D_{wat}=	9.80E-10	m^2 per s
Diffusion coefficient in soil air	D_i=	8.80E-06	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		8.38506E-07	m^2 per s
Water term		3.64261E-11	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	8.38542E-07	m^2 per s
Molecular weight	MW=	78	g per mol
Saturated vapour pressure	SatVP	95	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 4.18503E-06 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residential without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ *here* 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent intake

Calculate the soil equivalent intake for inhalation of outdoor air using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

3.04427E-04 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air using the formula: $ASC_{outv} = RI_{out}/SEI_{outv}$

ASC_{outv} = 9.10000E-04 mg per kg body weight per day / 3.04427E-04 kg soil per kg body weight per day = 2.989217672 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 1.549532514 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.464151982 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 6.46050E-03 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 9.10000E-04 mg per kg body weight per day / 6.46050E-03 kg soil per kg body weight per day = 0.140855926 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^{3})/(760mmHg \times R \times Temp)$

C_{sat}= 4.16896E+08 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 6.53786E-02 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 1.56822E-10 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/ 29.43210723	=	3.39765E-02	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/ 0.353360747	=	2.82997E+00	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/ 257.2681881	=	3.88699E-03	kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$=	1/ 2.989217672	=	3.34536E-01	kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$=	1/ 0.140855926	=	7.09945E+00	kg soil per mg

The Integrated Site Specific Assessment Criterion (SSAC)

39	For the residential with plant uptake land use the $SSAC_{rwp}$ =		mg per kg soil
40	For the allotments land use the $SSAC_{alt}$ =		mg per kg soil
41	For the residential without plant uptake land use the $SSAC_{other}$ =	0.133905287	mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for romatic EC5-EC in the Residential without plant uptake scenario is 0.133905 mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	=		kg soil per mg

The Integrated Site Specific Assessment Criterion

43	For the residential with plant uptake land use the $SSAC_{rwp}$ =		mg per kg soil
	For the allotments land use the $SSAC_{alt}$ =		mg per kg soil
	For the residential without plant uptake land use the $SSAC_{other}$ =		mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

The Level 1 Site Specific Assessment Criterion for Aromatic EC5-EC in the scenario is mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site. Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aromatic EC8-EC10 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion 4.00E-02 mg per kg body weight per day
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

	mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

Y

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15	kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: $RI_{ingest}=ID$

	mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: $RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)^{a}$

	mg per kg body weight per day

[a] Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: $RI_{ingest}=0.2TDI$

0.008	mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

N

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

6.00E-02	mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/Industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

Y

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0.012 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Yor N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

Y

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{ding} from this table, depending on your choice of land use

Land Use	SEI_{ding} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{ding} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

[ ]

If Y insert the representative fraction here (default=1)

[ ]

The amended SEI_{ding} = SEI_{ding} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{ding} = RI_{ingest}/SEI_{ding}

ASC_{ding} = 8.00000E-03 (mg per kg body weight per day) / 9.85319E-06 (kg soil per kg body weight per day) = 811.9201995 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **1258.925412** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **1600** *cm^3 per g dry weight*

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44}+(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= **0.344272232** [b] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= **0.008457281** [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	1.09714E-03
Cabbage	4.86885E-03	calc not required	1.04892E-03
Carrot	7.38094E-03	calc not required	2.54598E-05
Leafy salads	3.25677E-03	calc not required	1.96251E-04
Onion	3.69474E-03	calc not required	1.81863E-05
Potato	4.41616E-02	calc not required	1.40116E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	2.26554E-04
Allotments	2.26554E-04

SEI_{veg}= **2.27E-04** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = **8.00000E-03** mg per kg body weight per day / **2.26554E-04** kg soil per kg body weight per day = **35.31163297** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect}$ = $RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 8.00000E-03 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 7097.053466 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15	metres
Depth to subsurface contamination	d_z=	1	metres

Soil Matrix

Soil organic matter content	SOM=	1	%		
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03	kg OC per kg soil
Air filled porosity	θ_{vap}=	0.31	unitless		
Water filed porosity	θ_{wat}=	0.15	unitless		
Total porosity	θ_{total}=	0.46	unitless		
Bulk soil density	ρ=	1.6	kg soil per l soil		

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	1600	l water per kg OC
Dimensionless Henry's constant	H'=	0.49	l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s
Diffusion coefficient in soil air	D_i=	1.00E-05	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		9.52847E-07	m^2 per s
Water term		1.72952E-11	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.52865E-07	m^2 per s
Molecular weight	MW=	120	g per mol
Saturated vapour pressure	SatVP	4.8	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless		
Temperature	Temp=	12	°C + 273 =	285	K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s		

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 5.13886E-07 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAloutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residental without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air

using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

3.73811E-05 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air

using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 1.20000E-02 mg per kg body weight per day / 3.73811E-05 kg soil per kg body weight per day = 321.0178624 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 19.55273127 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.050155965 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 6.98118E-04 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 1.20000E-02 mg per kg body weight per day / 6.98118E-04 kg soil per kg body weight per day = 17.18907829 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^{3})/(760mmHg \times R \times Temp)$

C_{sat}= 3.24065E+07 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 8.62135E-01 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 2.66037E-08 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/ 811.9201995	=	1.23165E-03	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/ 35.31163297	=	2.83193E-02	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/ 7097.053466	=	1.40904E-04	kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$=	1/ 321.0178624	=	3.11509E-03	kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$=	1/ 17.18907829	=	5.81765E-02	kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39	For the residential with plant uptake land use the $SSAC_{rep}$ =		mg per kg soil
40	For the allotments land use the $SSAC_{NR}$ =		mg per kg soil
41	For the residential without plant uptake land use the $SSAC_{other}$ =	15.99405902	mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for **omaric EC8-EC** in the **Residential without plant uptake** scenario is 15.99406 mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	=		kg soil per mg

The integrated Site Specific Assessment Criterion

43	For the residential with plant uptake land use the $SSAC_{rep}$ =		mg per kg soil
	For the allotments land use the $SSAC_{NR}$ =		mg per kg soil
	For the residential without plant uptake land use the $SSAC_{other}$ =		mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

The Level 1 Site Specific Assessment Criterion for **romaric EC8-EC1** in the scenario is mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aromatic EC8-EC10 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI). 4.00E-02 mg per kg body weight per day

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

	mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

Y

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15	kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

	mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

	mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

0.008	mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

N

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID). For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

6.00E-02	mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

[Y]

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF)
which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

[0.362]

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	48.4

[11.15] kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0.012 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

Y

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{dring} from this table, depending on your choice of land use

Land Use	SEI_{dring} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{dring} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

[ ]

If Y insert the representative fraction here (default=1)

[ ]

The amended SEI_{dring} = SEI_{dring} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{dring} = RI_{ingest}/SEI_{dring}

ASC_{dring} = 8.00000E-03 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 811.9201995 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25 .
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient)	3162.27766	l water per l octanol
a representative value of ϕ (soil density)	1.6	g dry weight per cm^3
a representative value of K_{oc} (organic carbon-water partition coefficient):	2500	cm^3 per g dry weight
a representative value of f_{oc} (fraction of organic carbon in soil):	5.98802E-03	kg OC per kg soil
a representative value of θ (soil-water content by volume)	0.15	cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44})*(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= 0.304585014 ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= 0.010477002 [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	9.70603E-04
Cabbage	4.86885E-03	calc not required	9.27943E-04
Carrot	7.38094E-03	calc not required	3.15400E-05
Leafy salads	3.25677E-03	calc not required	1.73616E-04
Onion	3.69474E-03	calc not required	2.25295E-05
Potato	4.41616E-02	calc not required	1.73578E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	2.06261E-04
Allotments	2.06261E-04

SEI_{veg}= 2.06E-04 kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = 8.00000E-03 mg per kg body weight per day / 2.06261E-04 kg soil per kg body weight per day = 38.78581788 mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$ = 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 8.00000E-03 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 7097.053466 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_z=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{air}=	0.31	unitless	
Water filled porosity	θ_{wat}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	2500	l water per kg OC
Dimensionless Henry's constant	H'=	0.14	l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s
Diffusion coefficient in soil air	D_s=	1.00E-05	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		9.52847E-07	m^2 per s
Water term		6.05332E-11	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.52908E-07	m^2 per s
Molecular weight	MW=	130	g per mol
Saturated vapour pressure	SatVP	0.48	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height — TAH= 0.93 m

Height of mixing zone — h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 9.50551E-06 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residental without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air — 6.91450E-06 kg soil per (kg body weight per day)

using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air

using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 1.20000E-02 mg per kg body weight per day / 6.91450E-06 kg soil per kg body weight per day = 1735.482331 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{ov}/H'$

SF= 106.9289991 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.009277093 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 1.29127E-04 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 1.20000E-02 mg per kg body weight per day / 1.29127E-04 kg soil per kg body weight per day = 92.93157419 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^6)/(760mmHg \times R \times Temp)$

C_{sat}= 3.51071E+06 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 8.62135E-01 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 2.45573E-07 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	811.9201995	=	1.23165E-03 kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	38.78581768	=	2.57826E-02 kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	7097.053466	=	1.40904E-04 kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$=	1/	1735.482331	=	5.76209E-04 kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$=	1/	92.93157419	=	1.07606E-02 kg soil per mg

The Integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

40 For the allotments land use the $SSAC_{alt}$ = mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = 79.56422841 mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for omatic EC8-EC in the Residential without plant uptake scenario is 79.56423 mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/		=	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/		=	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/		=	kg soil per mg

The Integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

For the allotments land use the $SSAC_{alt}$ = mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

The Level 1 Site Specific Assessment Criterion for romatic EC8-EC1 in the scenario is mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aromatic EC12-EC16 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI). 4.00E-02 mg per kg body weight per day

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

Y

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

0.008 mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

N

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

6.00E-02 mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/Industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

Y

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0.012 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-5}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

[Y]

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{dring} from this table, depending on your choice of land use

Land Use	SEI_{dring} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{dring} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

[ ]

If Y insert the representative fraction here (default=1)

[ ]

The amended SEI_{dring} = SEI_{dring} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{dring} = RI_{ingest}/SEI_{dring}

ASC_{dring} = 9.80000E-03 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 811.9201995 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient)	7943.282347	l water per l octanol
a representative value of ϕ (soil density)	1.6	g dry weight per cm^3
a representative value of K_{oc} (organic carbon-water partition coefficient):	5000	cm^3 per g dry weight
a representative value of f_{oc} (fraction of organic carbon in soil):	5.98802E-03	kg OC per kg soil
a representative value of θ (soil-water content by volume)	0.15	cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44}+(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= 0.190590674 ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= 0.010397878 [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	6.07384E-04
Cabbage	4.86885E-03	calc not required	5.80688E-04
Carrot	7.38094E-03	calc not required	3.13018E-05
Leafy salads	3.25677E-03	calc not required	1.08646E-04
Onion	3.69474E-03	calc not required	2.23593E-05
Potato	4.41816E-02	calc not required	1.72287E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	1.36560E-04
Allotments	1.36560E-04

SEI_{veg}= 1.37E-04 kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = 8.00000E-03 mg per kg body weight per day / 1.36560E-04 kg soil per kg body weight per day = 58.5822401 mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 8.00000E-03 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 7097.053466 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15	metres
Depth to subsurface contamination	d_z=	1	metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{air}=	0.31	unitless	
Water filed porosity	θ_{wat}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	5000	l water per kg OC
Dimensionless Henry's constant	H'=	0.054	l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s
Diffusion coefficient in soil air	D_i=	1.00E-05	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		9.52847E-07	m^2 per s
Water term		1.56938E-10	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.53004E-07	m^2 per s
Molecular weight	MW=	150	g per mol
Saturated vapour pressure	SatVP	0.036	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 1.84178E-06 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residential without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

1.33975E-06 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air using the formula: $ASC_{outv} = RI_{out}/SEI_{outv}$

ASC_{outv} = 1.20000E-02 mg per kg body weight per day / 1.33975E-06 kg soil per kg body weight per day = 8956.883984 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 554.4486622 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.001797344 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 2.50171E-05 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 1.20000E-02 mg per kg body weight per day / 2.50171E-05 kg soil per kg body weight per day = 479.6715723 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^{6})/(760mmHg \times R \times Temp)$

C_{sat}= 3.03811E+05 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 8.62135E-01 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 2.83773E-06 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	811.9201995	=	1.23165E-03 kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	58.5822401	=	1.70700E-02 kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	7097.053466	=	1.40904E-04 kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$=	1/	8956.883984	=	1.11646E-04 kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$=	1/	479.6715723	=	2.08476E-03 kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39	For the residential with plant uptake land use the $SSAC_{rwp}$ =		mg per kg soil
40	For the allotments land use the $SSAC_{all}$ =		mg per kg soil
41	For the residential without plant uptake land use the $SSAC_{other}$ =	291.7107007	mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for omatic EC12-EC in the Residential without plant uptake scenario is 291.7107 mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/		=	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/		=	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/		=	kg soil per mg

The integrated Site Specific Assessment Criterion

43	For the residential with plant uptake land use the $SSAC_{rwp}$ =	mg per kg soil
	For the allotments land use the $SSAC_{all}$ =	mg per kg soil
	For the residential without plant uptake land use the $SSAC_{other}$ =	mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=	mg per kg soil

The Level 1 Site Specific Assessment Criterion for omatic EC12-EC in the scenario is mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aromatic EC16-EC21 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI). 3.00E-02 mg per kg body weight per day

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

[Y]

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

[0.485]

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

[0.006] mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

[N]

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

[0.00E+00] mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/Industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

Y

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

N

Inhalation pathway should not be selected if H' < 1E-3

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{ding} from this table, depending on your choice of land use

Land Use	SEI_{ding} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{ding} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

N

If Y insert the representative fraction here (default=1)

The amended SEI_{ding} = SEI_{ding} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{ding} = RI_{ingest}/SEI_{ding}

ASC_{ding} = 6.00000E-03 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 608.9401496 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables _____ ug per g (dry or fresh)* weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables _____ ug per g (dry or fresh)* weight plant per ug per g dry weight soil

* Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **50118.72336** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **16000** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44}+(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= **0.06490442** * ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= **0.013182501** * ug per g fresh weight plant per ug per g dry weight soil

* Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.64750E-03	calc not required	2.06541E-04
Cabbage	4.86885E-03	calc not required	1.97750E-04
Carrot	7.38094E-03	calc not required	3.96846E-05
Leafy salads	3.25677E-03	calc not required	3.69986E-05
Onion	3.69474E-03	calc not required	2.83473E-05
Potato	4.41616E-02	calc not required	2.18401E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	6.52935E-05
Allotments	6.52935E-05

SEI_{veg}= **6.53E-05** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = **8.00000E-03** mg per kg body weight per day / **6.52935E-05** kg soil per kg body weight per day = **91.89281415** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$ = 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) — N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction — 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 6.00000E-03 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 5322.7901 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_z=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{vap}=	0.31	unitless	
Water filed porosity	θ_{wat}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	16000	l water per kg OC
Dimensionless Henry's constant	H'=	0.013	l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s
Diffusion coefficient in soil air	D_i=	1.00E-05	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		9.52847E-07	m^2 per s
Water term		6.61696E-10	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.53499E-07	m^2 per s
Molecular weight	MW=	190	g per mol
Saturated vapour pressure	SatVP	5.80E-03	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 1.38975E-07 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residential without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air

using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

1.01093E-07 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air

using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 0.00000E+00 mg per kg body weight per day / 1.01093E-07 kg soil per kg body weight per day = 0 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF = K_{oc} \times f_{oc} / H'$

SF= 7369.875633 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.000135551 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 1.88673E-06 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 0.00000E+00 mg per kg body weight per day / 1.88673E-06 kg soil per kg body weight per day = 0 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^6)/(760mmHg \times R \times Temp)$

C_{sat}= 6.20000E+04 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 0.00000E+00 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 0 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	=	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	=	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	=	kg soil per mg
inhalation of outdoor air	$1/ASC_{outA}$=	1/	=	kg soil per mg
inhalation of indoor air	$1/ASC_{inA}$=	1/	=	kg soil per mg

The Integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

40 For the allotments land use the $SSAC_{all}$ = mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for omatic EC16-EC in the scenario is mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/ 608.9401496	=	0.001642198 kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/ 91.89281415	=	0.010882244 kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/ 5322.7901	=	0.000187871 kg soil per mg

The Integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

For the allotments land use the $SSAC_{all}$ = mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = 608.9401496 mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

The Level 1 Site Specific Assessment Criterion for omatic EC16-EC in the Residential without plant uptake scenario is 608.94015 mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Aromatic EC21-EC35 found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Y or N) N

5a Insert the relevant health criterion for ingestion
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI). 3.00E-02 mg per kg body weight per day

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

[Y]

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

[0.485]

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)[a]

[ ] mg per kg body weight per day

[a] Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

[0.005] mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

[N]

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

[0.00E+00] mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

[Y]

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

[0.362]

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

N

Inhalation pathway should not be selected if H' < 1E-3

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{ding} from this table, depending on your choice of land use

Land Use	SEI_{ding} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{ding} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

N

If Y insert the representative fraction here (default=1)

The amended SEI_{ding} = SEI_{ding} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{ding} = RI_{ingest}/SEI_{ding}

ASC_{ding} = 6.00000E-03 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 608.9401466 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Y or N) **N**

Measured Concentration Factor for leafy vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **1258925.412** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **1.30E+05** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(\log Kow-1.78)^2/2.44}+(10^{0.95\log Kow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= **0.002683127** ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77\log Kow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= **0.0193178** [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}

The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	8.55072E-06
Cabbage	4.86885E-03	calc not required	8.17490E-06
Carrot	7.38094E-03	calc not required	5.81543E-05
Leafy salads	3.25677E-03	calc not required	1.52951E-06
Onion	3.69474E-03	calc not required	4.15405E-05
Potato	4.41616E-02	calc not required	3.20048E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	3.92823E-05
Allotments	3.92823E-05

SEI_{veg}= **3.93E-05** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = **6.00000E-03** mg per kg body weight per day / **3.92823E-05** kg soil per kg body weight per day = **152.7403895** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$ = 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 6.00000E-03 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 5322.7901 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_s=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{air}=	0.31	unitless	
Water filed porosity	θ_{wat}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	130000	l water per kg OC
Dimensionless Henry's constant	H'=	6.80E-04	l water per l air
Diffusion coefficient in water	D_{wat}=	1.00E-09	m^2 per s
Diffusion coefficient in soil air	D_i=	1.00E-05	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		9.52847E-07	m^2 per s
Water term		1.24627E-08	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	9.65310E-07	m^2 per s
Molecular weight	MW=	240	g per mol
Saturated vapour pressure	SatVP	3.30E-06	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height — TAH= 0.93 m

Height of mixing zone — h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 9.06586E-12 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residental without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

6.59469E-10 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air using the formula: $ASC_{outv} = RL_{out}/SEI_{outv}$

ASC_{outv} = 0.00000E+00 mg per kg body weight per day / 6.59469E-10 kg soil per kg body weight per day = 0 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 1144769.285 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 8.73433E-07 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 1.21573E-08 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 0.00000E+00 mg per kg body weight per day / 1.21573E-08 kg soil per kg body weight per day = 0 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^6)/(760mmHg \times R \times Temp)$

C_{sat}= 4.45590E+01 mm Hg g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 0.00000E+00 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 0 (mg per l air) per (mm Hg g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/		=	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/		=	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/		=	kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$ =	1/		=	kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$ =	1/		=	kg soil per mg

The Integrated Site Specific Assessment Criterion (SSAC)

39	For the residential with plant uptake land use the $SSAC_{rwp}$ =		mg per kg soil
40	For the allotments land use the $SSAC_{all}$ =		mg per kg soil
41	For the residential without plant uptake land use the $SSAC_{other}$ =		mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for omatic EC21-EC in the scenario is mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/	608.9401496	=	0.001642198 kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/	152.7403895	=	0.006547057 kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/	5322.7901	=	0.000187871 kg soil per mg

The Integrated Site Specific Assessment Criterion

43	For the residential with plant uptake land use the $SSAC_{rwp}$ =		mg per kg soil
	For the allotments land use the $SSAC_{all}$ =		mg per kg soil
	For the residential without plant uptake land use the $SSAC_{other}$ =	608.9401496	mg per kg soil
	For the commercial/industrial land use the $SSAC_{other}$=		mg per kg soil

The Level 1 Site Specific Assessment Criterion for omatic EC21-EC in the Residential without plant uptake scenario is 608.94015 mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 01/09/2006

and has been checked by Christopher Bolan on 01/09/2006

3 It relates to Naphthalene found at Residential without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) **N**

5a Insert the relevant health criterion for ingestion
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI). **2.00E-02** mg per kg body weight per day

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

7.00E-03 mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

N

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

1.97982E-02 mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

N

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

8.60E-04 mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

2.80E-03 mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

N

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

7.99742E-04 mg per kg body weight per day

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

[ ] mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

Y

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{ding} from this table, depending on your choice of land use

Land Use	SEI_{ding} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{ding} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

N

If Y insert the representative fraction here (default=1)

The amended SEI_{ding} = SEI_{ding} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{ding} = RI_{ingest}/SEI_{ding}

ASC_{ding} = 1.97982E-02 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 2009.316808 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] *Note - See 18 below*

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **2511** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **2000** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(\log Kow-1.78)^2/2.44}+(10^{0.95\log Kow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc} f_{oc}))$

CF_{leafy}= **0.353737193** [b] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77\log Kow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc} f_{oc}))*0.01$

CF_{root}= **0.011059014** [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc} f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.94750E-03	calc not required	1.12731E-03
Cabbage	4.86885E-03	calc not required	1.07776E-03
Carrot	7.38094E-03	calc not required	3.32921E-05
Leafy salads	3.25677E-03	calc not required	2.01647E-04
Onion	3.69474E-03	calc not required	2.37810E-05
Potato	4.41616E-02	calc not required	1.83221E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	2.37400E-04
Allotments	2.37400E-04

SEI_{veg}[a] **2.37E-04** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = **1.97962E-02** mg per kg body weight per day / **2.37400E-04** kg soil per kg body weight per day = **83.39591004** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect}$ = RI_{ingest}/$SEI_{indirect}$

$ASC_{indirect}$ = 1.97982E-02 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 17563.58424 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_z=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1 %	
Mass fraction of organic carbon in soil	f_{oc}=	1 /167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{air}=	0.31 unitless	
Water filed porosity	θ_{wat}=	0.15 unitless	
Total porosity	θ_{total}=	0.46 unitless	
Bulk soil density	ρ=	1.6 kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	2000 l water per kg OC
Dimensionless Henry's constant	H'=	0.0198 l water per l air
Diffusion coefficient in water	D_{wat}=	7.50E-10 m^2 per s
Diffusion coefficient in soil air	D_i=	5.90E-06 m^2 per s
Air in soil		9.52847E-02 unitless
Water in soil		8.47465E-03 unitless
Air term		5.62180E-07 m^2 per s
Water term		3.21010E-10 m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	5.62501E-07 m^2 per s
Molecular weight	MW=	128.2 g per mol
Saturated vapour pressure	SatVP	0.085 mmHg

Pathway parameters

Dilution ratio	DR=	20000 unitless	
Temperature	Temp=	12 °C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3 m per s	

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 9.91893E-09 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residental without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

7.21524E-07 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 7.99742E-04 mg per kg body weight per day / 7.21524E-07 kg soil per kg body weight per day = 1108.407959 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 604.8509043 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.001639037 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 2.28262E-05 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 7.99742E-04 mg per kg body weight per day / 2.28262E-05 kg soil per kg body weight per day = 35.03619167 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^6)/(760mmHg \times R \times Temp)$

C_{sat}= 6.13080E+05 mm Hg.g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 5.74571E-02 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 9.37189E-08 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/ 2009.316808	=	4.97682E-04	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/ 83.39591004	=	1.19910E-02	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/ 17563.58424	=	5.69360E-05	kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$ =	1/ 1108.407959	=	9.02195E-04	kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$ =	1/ 35.03619167	=	2.85419E-02	kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{nvp}$ = [ ] mg per kg soil

40 For the allotments land use the $SSAC_{all}$ = [ ] mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = [33.39813533] mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= [ ] mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for **Naphthalene** in the **Residential without plant uptake** scenario is **33.39814** mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/	=		kg soil per mg

The integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{nvp}$ = [ ] mg per kg soil

For the allotments land use the $SSAC_{all}$ = [ ] mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = [ ] mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= [ ] mg per kg soil

The Level 1 Site Specific Assessment Criterion for **Naphthalene** in the [ ] scenario is [ ] mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Anthracene found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI). 3.00E-01 mg per kg body weight per day

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

		mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

Y		

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485		

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15		kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

		mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

		mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

0.06		mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

N		

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

0.00E+00		mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

[Y]

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

[0.362]

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathway is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

mg per kg body weight per day

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathway is calculated using the formula: RI_{inhal}=0.2TDI

0 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

N

Inhalation pathway should not be selected if H' < 1E-3

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{ding} from this table, depending on your choice of land use

Land Use	SEI_{ding} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{ding} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

N

If Y insert the representative fraction here (default=1)

The amended SEI_{ding} = SEI_{ding} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{ding} = RI_{ingest}/SEI_{ding}

ASC_{ding} = 6.00000E-02 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 6089.401466 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16** or **17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables ____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **39810** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **30000** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44}+(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= **0.03522914** [b] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= **0.005898408** [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	1.12270E-04
Cabbage	4.86885E-03	calc not required	1.07335E-04
Carrot	7.38094E-03	calc not required	1.77566E-05
Leafy salads	3.25677E-03	calc not required	2.00823E-05
Onion	3.69474E-03	calc not required	1.26838E-05
Potato	4.41616E-02	calc not required	9.77220E-05

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	3.29910E-05
Allotments	3.29910E-05

SEI_{veg}= **3.30E-05** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = **6.00000E-02** mg per kg body weight per day / **3.29910E-05** kg soil per kg body weight per day = **1818.675551** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$ = 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 6.00000E-02 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 53227.901 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_s=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1 %		
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{vap}=	0.31 unitless		
Water filed porosity	θ_{wat}=	0.15 unitless		
Total porosity	θ_{total}=	0.46 unitless		
Bulk soil density	ρ_b=	1.6 kg soil per l soil		

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	30000 l water per kg OC
Dimensionless Henry's constant	H'=	0.00267 l water per l air
Diffusion coefficient in water	D_{wat}=	7.70E-10 m^2 per s
Diffusion coefficient in soil air	D_i=	3.20E-06 m^2 per s
Air in soil		9.52847E-02 unitless
Water in soil		8.47465E-03 unitless
Air term		3.04911E-07 m^2 per s
Water term		2.44400E-09 m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	3.07355E-07 m^2 per s
Molecular weight	MW=	178.2 g per mol
Saturated vapour pressure	SatVP	0.0000027 mmHg

Pathway parameters

Dilution ratio	DR=	20000 unitless		
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3 m per s		

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 4.90947E-11 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAloutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residential without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	*8.45534E-03*

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent intake

Calculate the soil equivalent intake for inhalation of outdoor air using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

3.57125E-09 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 0.00000E+00 mg per kg body weight per day / 3.57125E-09 kg soil per kg body weight per day = 0 mg per kg soil

Intake via Inhalation of Indoor Air

30 Indoor inhalation of vapour

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 Time-averaged air intake indoors

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 Soil Factor

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 67281.168 l air per kg soil

33 Soil vapour partition coefficient

The soil vapour partition coefficient (SVPC) is

SVPC= 1.48552E-05 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 2.06769E-07 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculatec using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 0.00000E+00 mg per kg body weight per day / 2.06769E-07 kg soil per kg body weight per day = 0 mg per kg soil

36 Saturated vapour concentration

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^6)/(760mmHg \times R \times Temp)$

C_{sat}= 2.70696E+01 mm Hg.g per mol

37 Equilibrium contaminant concentration in soil vapour

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 0.00000E+00 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 0 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/		≈	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/		≈	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/		≈	kg soil per mg
inhalation of outdoor air	$1/ASC_{outdv}$=	1/		≈	kg soil per mg
inhalation of indoor air	$1/ASC_{indv}$=	1/		≈	kg soil per mg

The Integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

40 For the allotments land use the $SSAC_{allt}$ = mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for **Anthracene** in the scenario is mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/	6089.401496	≈	0.00016422 kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/	1818.675551	≈	0.000549851 kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/	53227.901	≈	1.87871E-05 kg soil per mg

The Integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

For the allotments land use the $SSAC_{allt}$ = mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = 6089.401496 mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

The Level 1 Site Specific Assessment Criterion for **Anthracene** in the **Residential without plant uptake** scenario is 6089.4015 mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Fluoranthene found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion 3.00E-01 mg per kg body weight per day
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

Y

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

0.06 mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Yor N)

N

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

0.00E+00 mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

Y

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

N

Inhalation pathway should not be selected if H' < 1E-3

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{ding} from this table, depending on your choice of land use

Land Use	SEI_{ding} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{ding} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

N

If Y insert the representative fraction here (default=1)

The amended SEI_{ding} = SEI_{ding} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{ding} = RI_{ingest}/SEI_{ding}

ASC_{ding} = 6.00000E-02 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 6089.401496 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient)	125892	l water per l octanol
a representative value of ϕ (soil density)	1.6	g dry weight per cm^3
a representative value of K_{oc} (organic carbon-water partition coefficient):	110000	cm^3 per g dry weight
a representative value of f_{oc} (fraction of organic carbon in soil):	5.98802E-03	kg OC per kg soil
a representative value of θ (soil-water content by volume)	0.15	cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784 * 10^{-0.434*(\log Kow-1.78)^2/2.44} + (10^{0.95\log Kow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc} f_{oc}))$

CF_{leafy}= 0.008139681 [b] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root} = (10^{0.77\log Kow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc} f_{oc}))*0.01$

CF_{root}= 0.003887348 [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc} f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.84756E-03	calc not required	2.59399E-05
Cabbage	4.86885E-03	calc not required	2.47998E-05
Carrot	7.38094E-03	calc not required	1.17025E-05
Leafy salads	3.25677E-03	calc not required	4.64000E-06
Onion	3.69474E-03	calc not required	8.35925E-06
Potato	4.41616E-02	calc not required	6.44037E-05

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	1.25422E-05
Allotments	1.25422E-05

SEI_{veg}= 1.25E-05 kg soil per kg body weight per day

20 *The nominal assessment sub criterion for intake via consumption of* homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = 6.00000E-02 mg per kg body weight per day / 1.25422E-05 kg soil per kg body weight per day = 4783.860035 mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$= 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect}$ = $RI_{oral}/SEI_{indirect}$

$ASC_{indirect}$ = 6.00000E-02 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 53227.901 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15	metres		
Depth to subsurface contamination	d_z=	1	metres		

Soil Matrix

Soil organic matter content	SOM=	1	%		
Mass fraction of organic carbon in soil	f_{oc}=	1		/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{vap}=	0.31	unitless		
Water filed porosity	θ_{wat}=	0.15	unitless		
Total porosity	θ_{total}=	0.46	unitless		
Bulk soil density	ρ=	1.6	kg soil per l soil		

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	110000	l water per kg OC
Dimensionless Henry's constant	H'=	0.00267	l water per l air
Diffusion coefficient in water	D_{wat}=	6.40E-10	m^2 per s
Diffusion coefficient in soil air	D_i=	3.00E-06	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		2.85854E-07	m^2 per s
Water term		2.03138E-09	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	2.87886E-07	m^2 per s
Molecular weight	MW=	202.3	g per mol
Saturated vapour pressure	SatVP	1.20E-08	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless		
Temperature	Temp=	12		°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s		

Receptor characteristics

Time-averaged body height — TAH= 0.93 m

Height of mixing zone — h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 1.25461E-11 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residential without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air
using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

9.12629E-10 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air
using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 0.00000E+00 mg per kg body weight per day / 9.12629E-10 kg soil per kg body weight per day = 0 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF=K_{oc} \times f_{oc}/H'$

SF= 246697.616 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 4.05297E-06 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$

SEI_{inv}= 5.64130E-08 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$

ASC_{inv} = 0.00000E+00 mg per kg body weight per day / 5.64130E-08 kg soil per kg body weight per day = 0 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^6)/(760mmHg \times R \times Temp)$

C_{sat}= 1.36580E-01 mm Hg g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 0.00000E+00 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 0 (mg per l air) per (mm Hg.g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/		=	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/		=	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/		=	kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$=	1/		=	kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$=	1/		=	kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

40 For the allotments land use the $SSAC_{all}$ = mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for **Fluoranthene** in the scenario is mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$=	1/ 6089.401496	=	0.00016422	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$=	1/ 4783.860035	=	0.000209036	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$=	1/ 53227.901	=	1.87871E-05	kg soil per mg

The integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

For the allotments land use the $SSAC_{all}$ = mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = 6089.401496 mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$= mg per kg soil

The Level 1 Site Specific Assessment Criterion for **Fluoranthene** in the **Residential without plant uptake** scenario is 6089.4015 mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Fluorene found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) N

5a Insert the relevant health criterion for ingestion 4.00E-02 mg per kg body weight per day
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

[ ] mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

[Y]

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

[0.485]

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

[11.15] kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

[ ] mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

[ ] mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

[0.008] mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Y or N)

[N]

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

[0.00E+00] mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

Y

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

mg per kg body weight per day

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

0 mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

N

Inhalation pathway should not be selected if H' < 1E-3

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{dring} from this table, depending on your choice of land use

Land Use	SEI_{dring} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{dring} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

If Y insert the representative fraction here (default=1)

The amended SEI_{dring} = SEI_{dring} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{dring} = RI_{ingest}/SEI_{dring}

ASC_{dring} = 8.00000E-03 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 811.9201995 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient)	15848	l water per l octanol
a representative value of ϕ (soil density)	1.6	g dry weight per cm^3
a representative value of K_{oc} (organic carbon-water partition coefficient):	14000	cm^3 per g dry weight
a representative value of f_{oc} (fraction of organic carbon in soil):	5.98802E-03	kg OC per kg soil
a representative value of θ (soil-water content by volume)	0.15	cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44}+(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= 0.074613187 [b] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= 0.006264839 [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}
The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.64750E-03	calc not required	2.37781E-04
Cabbage	4.86885E-03	calc not required	2.27330E-04
Carrot	7.38094E-03	calc not required	1.88597E-05
Leafy salads	3.25677E-03	calc not required	4.25331E-05
Onion	3.69474E-03	calc not required	1.34717E-05
Potato	4.41616E-02	calc not required	1.03793E-04

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	5.77371E-05
Allotments	5.77371E-05

SEI_{veg}= 5.77E-05 kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{England}/SEI_{veg}$

ASC_{veg} = 8.00000E-03 mg per kg body weight per day / 5.77371E-05 kg soil per kg body weight per day = 138.5591475 mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$ = 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 8.0000E-03 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 7097.053466 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area

Source zone width parallel to wind direction	W=	15 metres
Depth to subsurface contamination	d_z=	1 metres

Soil Matrix

Soil organic matter content	SOM=	1	%	
Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
Air filled porosity	θ_{air}=	0.31	unitless	
Water filed porosity	θ_{wat}=	0.15	unitless	
Total porosity	θ_{total}=	0.46	unitless	
Bulk soil density	ρ=	1.6	kg soil per l soil	

Contaminant

Organic carbon/water partition coefficient	K_{oc}=	14000	l water per kg OC
Dimensionless Henry's constant	H'=	0.0261	l water per l air
Diffusion coefficient in water	D_{wat}=	7.90E-10	m^2 per s
Diffusion coefficient in soil air	D_i=	3.60E-06	m^2 per s
Air in soil		9.52847E-02	unitless
Water in soil		8.47465E-03	unitless
Air term		3.43025E-07	m^2 per s
Water term		2.56512E-10	m^2 per s per (l water per l air)
Effective diffusion coefficient	D_{eff}=	3.43282E-07	m^2 per s
Molecular weight	MW=	166.2	g per mol
Saturated vapour pressure	SatVP	0.0084	mmHg

Pathway parameters

Dilution ratio	DR=	20000	unitless	
Temperature	Temp=	12	°C + 273 =	285 K
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height TAH= 0.93 m

Height of mixing zone h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 1.14785E-09 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAIoutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residential without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

8.34966E-08 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 0.00000E+00 mg per kg body weight per day / 8.34966E-08 kg soil per kg body weight per day = 0 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{iov}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{iov}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF = K_{oc} \times f_{oc}/H'$

SF= 3211.966871 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 0.000310969 kg soil per l air

34 The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{iov} = (TAAI_{iov} \times 1000 \times SVPC)/DR$

SEI_{iov}= 4.32836E-06 kg soil/(kg body weight per day)

35 The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{iov} = RI_{iov}/SEI_{iov}$

ASC_{iov} = 0.00000E+00 mg per kg body weight per day / 4.32836E-06 kg soil per kg body weight per day = 0 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^6)/(760mmHg \times R \times Temp)$

C_{sat}= 7.85453E+04 mm Hg g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{iov} \times SVPC$

C_{sv}= 0.00000E+00 mg per l air

38 Saturated vapour concentration compared to the equilibrium contaminant concentration in soil vapour: C_{sv} / C_{sat}

C_{sv}/C_{sat}= 0 (mg per l air) per (mm Hg g per mol)

If the ratio is greater than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/	=		kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$ =	1/	=		kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$ =	1/	=		kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

40 For the allotments land use the $SSAC_{all}$ = mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$ = mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for **Fluorene** in the scenario is mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/ 811.9201995	=	0.001231648	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/ 138.5591475	=	0.007217134	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/ 7097.053466	=	0.000140904	kg soil per mg

The integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{rwp}$ = mg per kg soil

For the allotments land use the $SSAC_{all}$ = mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = 811.9201995 mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$ = mg per kg soil

The Level 1 Site Specific Assessment Criterion for **Fluorene** in the **Residential without plant uptake** scenario is 811.9202 mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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SNIFFER Method - Organics

Project Ref: GAC **Run No:** 1

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by Paul Brew on 08/07/2006

and has been checked by Christopher Bolan on 08/07/2006

3 It relates to Benzo(a)pyrene found at Residential Without Plant Uptake Site

INGESTION PATHWAYS

Toxicology for Ingestion Pathways

4a Is the substance a non threshold substance? (Yor N) Y

5a Insert the relevant health criterion for ingestion 2.00E-05 mg per kg body weight per day
For a non threshold substance the relevant health criterion is the Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

Land Use

6a The Table below lists the default exposure durations and averaging times, used in the method for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/industrial	16-59		15695	

Background Exposure for Ingestion

7a Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

0.00E+00 mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unkown? (Y or N)

8a Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (ingestion)
0-6	0.485
16-59	1

0.485

Receptor Body Weight

9a Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Ingestion

10a For non threshold substances the Reference Intake (RI) for the ingestion pathway is calculated using the formula: RI_{ingest}=ID

0.00002 mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

mg per kg body weight per day

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI, or the MDI is unknown, the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=0.2TDI

mg per kg body weight per day

INHALATION PATHWAYS

Toxicology for Inhalation Pathways

4b Is the substance a non threshold substance. (Y or N)

Y

5b Insert the relevant health criterion for inhalation
For a non threshold substance the relevant health criterion is the (indicative) Index Dose (ID).
For threshold substances the relevant health criterion is the Tolerable Daily Intake (TDI).

7.00E-06 mg per kg body weight per day

Land Use

6b The Table below lists the default exposure durations and averaging times, used in the level 1 methodology for standard land uses.
Please insert Y to indicate your choice of land use and acceptance of the default assumptions.

Land Use	Exposure duration (years)		Averaging time (days)	
Residential with plant uptake	0-6		2190	
Residential without plant uptake	0-6	Y	2190	Y
Allotments	0-6		2190	
Commercial/Industrial	16-59		15695	

Background Exposure for inhalation

7b Insert Mean Daily Intake (MDI) from non-soil sources
(If the contaminant is a non threshold substance insert zero)

0.00E+00 mg per day

Is the MDI equal to or greater than 80% of the TDI or is the MDI unknown? (Y or N)

8b Because the MDI for children is lower than that for adults, the MDI will need to be corrected by a Childhood Factor (CF) which depends on exposure duration. Insert the appropriate factor here:

Exposure duration (years)	Childhood Factor (inhalation)
0-6	0.362
16-59	1

0.362

Receptor Body Weight

9b Insert the Time-Averaged (female) Body Weight (TABW) depending on the chosen exposure duration

Exposure duration (years)	TABW
0-6	11.15
16-59	46.4

11.15 kg body weight

Reference Intake for Inhalation

10b For non threshold substances the Reference Intake (RI) for the inhalation pathway is calculated using the formula: RI_{inhal}=ID

0.000007 mg per kg body weight per day

For threshold substances the Reference Intake (RI) for ingestion pathways is calculated using the formula: RI_{ingest}=(TDI-((MDI/70x46.4)xCF)/TABW)*

* Note - The background component is in line with the approach in CLR 9, namely that the MDI is corrected by the relevant adult body weight.

mg per kg body weight per day

For threshold substances where the background exposure (MDI) is greater than or equal to 80% of the TDI the Reference Intake (RI) for inhalation pathways is calculated using the formula: RI_{inhal}=0.2TDI

mg per kg body weight per day

Pathway Check

11 The relevant pathways for calculating Site Specific Assessment Criteria depend on the land-use scenarios and the relative tendency of a substance to exist as vapour molecules as opposed to being dissolved in water, as expressed in Henry's Law constant.

Is the dimensionless Henry's constant H' greater than or equal to 10^{-3}? (Y or N)
If the answer is Y, include vapour inhalation pathways. If it is N, do not.

N

Inhalation pathway should not be selected if H' < 1E-3

Intake via Soil and Dust Ingestion

12 Select a value for SEI_{ding} from this table, depending on your choice of land use

Land Use	SEI_{ding} (kg soil/kg body weight/day)
Residential with plant uptake	9.85319E-06
Residential without plant uptake	9.85319E-06
Allotments	9.85319E-06
Commercial/Industrial	5.43222E-07

SEI_{ding} = 9.85E-06

13 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N)

N

If Y insert the representative fraction here (default=1)

The amended SEI_{ding} = SEI_{ding} * bioaccessibility fraction

9.85319E-06 kg soil per kg body weight per day

14 The nominal assessment sub criterion for intake via soil and dust ingestion is calculated using the formula: ASC_{ding} = RI_{ingest}/SEI_{ding}

ASC_{ding} = 2.00000E-05 mg per kg body weight per day / 9.85319E-06 kg soil per kg body weight per day = 2.029800499 mg per kg soil

Intake via Consumption of Homegrown Vegetables

15 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to question 25.
Select the basis for the Concentration Factor from **16 or 17** below. Select **one** option only

16 Are measured site specific Concentration Factors for leafy and root plant uptake of organics available? (Yor N) **N**

Measured Concentration Factor for leafy vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

Measured Concentration Factor for root vegetables _____ ug per g (dry or fresh)[a] weight plant per ug per g dry weight soil

[a] Note - See 18 below

17 Where measured site specific Concentration Factors are not available the following formulae can be used to calculate Concentration Factors for leafy and root vegetable uptake of organics using the Briggs and Ryan approach.

To use the formulae for plant uptake of organics the following data are required:

a representative value for K_{ow} (octanol/water partition coefficient) **1258925** l water per l octanol

a representative value of ϕ (soil density) **1.6** g dry weight per cm^3

a representative value of K_{oc} (organic carbon-water partition coefficient): **1000000** cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil): **5.98802E-03** kg OC per kg soil

a representative value of θ (soil-water content by volume) **0.15** cm^3 per cm^3

For leafy vegetables $CF_{leafy} = (0.784*10^{-0.434*(logKow-1.78)^2/2.44}+(10^{0.95logKow-2.05}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))$

CF_{leafy}= **0.000348843** [b] ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root}=(10^{0.77logKow-1.52}+0.82)*(\phi/(\theta+\phi K_{oc}f_{oc}))*0.01$

CF_{root}= **0.002511577** [b] ug per g fresh weight plant per ug per g dry weight soil

[b] Note - If the soil correction factor ($\phi/(\theta+\phi K_{oc}f_{oc})$) is greater than 1 a default value of 1 is used.

18 For calculation of the SEI_{veg} the units for CF_{leafy} and CF_{root} must be ug per g fresh weight plant over ug per g dry weight soil.
It may be necessary to use a dry weight conversion factor when using **measured** CF values.
Is a dry weight conversion required? (Y or N) **N**

Calculation of SEI_{veg}

The Time Averaged Vegetable Consumption Rate for homegrown vegetables is given in the Table below.

Vegetable Type	TAVCR (kg FW/day)	TAVCR*HF*CF*DW	TAVCR*HF*CF
Brussel sprouts	5.04750E-03	calc not required	1.11171E-06
Cabbage	4.86885E-03	calc not required	1.06285E-06
Carrot	7.38094E-03	calc not required	7.56085E-06
Leafy salads	3.25877E-03	calc not required	1.98857E-07
Onion	3.69474E-03	calc not required	5.40083E-06
Potato	4.41616E-02	calc not required	4.16106E-05

19 Select a value for SEI_{veg} from this table for the contaminant of concern, depending on your choice of land use and toxicological endpoint

Landuse	SEI_{veg} (kg soil per kg body weight per day)
Residential with plant uptake	5.10724E-06
Allotments	5.10724E-06

SEI_{veg}= **5.11E-06** kg soil per kg body weight per day

20 The nominal assessment sub criterion for intake via consumption of homegrown vegetables is calculated using the formula: $ASC_{veg} = RI_{ingest}/SEI_{veg}$

ASC_{veg} = **2.00000E-05** mg per kg body weight per day / **5.10724E-06** kg soil per kg body weight per day = **3.916010858** mg per kg soil

Intake via Ingestion of Soil Attached to Vegetables

21 This pathway only applies to two land uses: residential with plant uptake and allotments. For other land uses go directly to paragraph 25.

22 Select a value for $SEI_{indirect}$ from this table, depending on your choice of land use

Land Use	$SEI_{indirect}$ (kg soil per kg body weight per day)
Residential with plant uptake	1.12723E-06
allotments	1.12723E-06

$SEI_{indirect}$ = 1.1272E-06 kg soil per kg body weight per day

23 Is site specific data on the bioaccessibility of the contaminant in soil available? (Y or N) N

Insert the representative fraction here (default=1)

The amended $SEI_{indirect}$ = $SEI_{indirect}$ * bioaccessibility fraction 1.12723E-06 kg soil per kg body weight per day

24 The nominal assessment sub criterion for intake via indirect soil ingestion using the formula: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$ASC_{indirect}$ = 2.00000E-05 mg per kg body weight per day / 1.12723E-06 kg soil per kg body weight per day = 17.74263367 mg per kg soil

Intake via Inhalation of Outdoor Air

25 This pathway only applies to substances with H' greater than or equal to 10^{-3}.
To use the formulae for inhalation of outdoor air, the following site parameters are required:

Source Area					
	Source zone width parallel to wind direction	W=	15	metres	
	Depth to subsurface contamination	d_z=	1	metres	
Soil Matrix					
	Soil organic matter content	SOM=	1	%	
	Mass fraction of organic carbon in soil	f_{oc}=	1	/167	5.98802E-03 kg OC per kg soil
	Air filled porosity	θ_{air}=	0.31	unitless	
	Water filed porosity	θ_{wat}=	0.15	unitless	
	Total porosity	θ_{total}=	0.46	unitless	
	Bulk soil density	ρ=	1.6	kg soil per l soil	
Contaminant					
	Organic carbon/water partition coefficient	K_{oc}=	1000000	l water per kg OC	
	Dimensionless Henry's constant	H'=	0.0000463	l water per l air	
	Diffusion coefficient in water	D_{wat}=	9.00E-10	m^2 per s	
	Diffusion coefficient in soil air	D_a=	4.30E-06	m^2 per s	
	Air in soil		9.52847E-02	unitless	
	Water in soil		8.47465E-03	unitless	
	Air term		4.09724E-07	m^2 per s	
	Water term		1.64734E-07	m^2 per s per (l water per l air)	
	Effective diffusion coefficient	D_{eff}=	5.74458E-07	m^2 per s	
	Molecular weight	MW=	252.3	g per mol	
	Saturated vapour pressure	SatVP	5.50E-09	mmHg	
Pathway parameters					
	Dilution ratio	DR=	20000	unitless	
	Temperature	Temp=	12	°C + 273 =	285 K
	Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)	V_{air}=	3	m per s	

Receptor characteristics

Time-averaged body height — TAH= 0.93 m

Height of mixing zone — h= 0.93 /2 = 0.465 m

26 Contaminant Volatilisation Factor (CVF)

CVF= 4.77599E-14 kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAloutv m^3 air per (kg body weight per day)
Residential with plant uptake	7.27421E-02
Residental without plant uptake	7.27421E-02
Allotments	1.55763E-02
Commercial/Industrial	6.45534E-03

Insert the appropriate $TAAI_{outv}$ here 7.27E-02 m^3 air per (kg body weight per day)

28 Soil equivalent Intake

Calculate the soil equivalent intake for inhalation of outdoor air using the formula: $SEI_{outv} = TAAI_{outv} \times CVF \times 1000$

3.47416E-12 kg soil per (kg body weight per day)

29 Nominal Assessment Sub Criterion

Calculate the nominal assessment sub-criteria for intake via outdoor air using the formula: $ASC_{outv} = RI_{outv}/SEI_{outv}$

ASC_{outv} = 7.00000E-06 mg per kg body weight per day / 3.47416E-12 kg soil per kg body weight per day = 2014878.081 mg per kg soil

Intake via Inhalation of Indoor Air

30 **Indoor inhalation of vapour**

This pathway **only** applies to substances with dimensionless Henry's constant **equal to or greater than 10^{-3}** and to the following land-use scenarios:
Residential with plant uptake, Residential without plant uptake, Commercial/industrial

31 **Time-averaged air intake indoors**

Landuse	$TAAI_{inv}$ m3 air per (kg body weight per day)
Residential with plant uptake	2.78379E-01
Residential without plant uptake	2.78379E-01
Commercial/industrial	4.34795E-02

Insert the appropriate $TAAI_{inv}$ here: 2.78E-01 m^3 air per (kg body weight per day)

32 **Soil Factor**

Soil Factor is calculated using the formula $SF = K_{oc} \times f_{oc} / H'$

SF= 129330970.9 l air per kg soil

33 **Soil vapour partition coefficient**

The soil vapour partition coefficient (SVPC) is

SVPC= 7.73198E-09 kg soil per l air

34 **The soil equivalent intakes for inhalation of indoor air is calculated using the formula: $SEI_{inv} = (TAAI_{inv} \times 1000 \times SVPC)/DR$**

SEI_{inv}= 1.07621E-10 kg soil/(kg body weight per day)

35 **The nominal assessment sub criterion for intake via indoor air is calculated using the formula: $ASC_{inv} = RI_{inv}/SEI_{inv}$**

ASC_{inv} = 7.00000E-06 mg per kg body weight per day / 1.07621E-10 kg soil per kg body weight per day = 65043.11264 mg per kg soil

36 **Saturated vapour concentration**

Saturated vapour concentration is calculated using the formula
$C_{sat} = (SatVP \times MW \times 10^3)/(760mmHg \times R \times Temp)$

C_{sat}= 7.80710E-02 mm Hg g per mol

37 **Equilibrium contaminant concentration in soil vapour**

Equilibrium contaminant concentration in soil vapour is calculated using the formula $C_{sv} = ASC_{inv} \times SVPC$

C_{sv}= 5.02912E-04 mg per l air

38 ***Saturated vapour concentration compared to the equilibrium*** **contaminant concentration in soil vapour: C_{sv} / C_{sat}**

C_{sv}/C_{sat}= 0.006441722 (mg per l air) per (mm Hg g per mol)

If the ratio is greated than 1, Level 1 risk assessment is not appropriate. It should be noted for further site-specific risk assessment that a C_{sv}/C_{sat} ratio greater than 1 may indicate the presence of a free product.

Integrated site specific assessment criteria (SSAC) for substances with dimensionless Henry's constant greater than or equal to 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/	=		kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/	=		kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/	=		kg soil per mg
inhalation of outdoor air	$1/ASC_{outv}$ =	1/	=		kg soil per mg
inhalation of indoor air	$1/ASC_{inv}$ =	1/	=		kg soil per mg

The integrated Site Specific Assessment Criterion (SSAC)

39 For the residential with plant uptake land use the $SSAC_{rep}$ = mg per kg soil

40 For the allotments land use the $SSAC_{alt}$ = mg per kg soil

41 For the residential without plant uptake land use the $SSAC_{other}$ = mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$ = mg per kg soil

42 The Level 1 Site Specific Assessment Criterion for Benzo(a)pyrene in the scenario is mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10^{-3}

soil ingestion pathway	$1/ASC_{ding}$ =	1/ 2.029800499	=	0.492659254	kg soil per mg
homegrown vegetable consumption pathway	$1/ASC_{veg}$ =	1/ 3.916010858	=	0.255361907	kg soil per mg
ingestion of soil attached to vegetables	$1/ASC_{indirect}$ =	1/ 17.74283367	=	0.056361418	kg soil per mg

The integrated Site Specific Assessment Criterion

43 For the residential with plant uptake land use the $SSAC_{rep}$ = mg per kg soil

For the allotments land use the $SSAC_{alt}$ = mg per kg soil

For the residential without plant uptake land use the $SSAC_{other}$ = 2.029800499 mg per kg soil

For the commercial/industrial land use the $SSAC_{other}$ = mg per kg soil

The Level 1 Site Specific Assessment Criterion for Benzo(a)pyrene in the Residential without plant uptake scenario is 2.0298005 mg per kg soil

Risk Evaluation

44 Justify your use of the defaults on the worksheet and characterise the risk associated with the site.
Include the following:

	Justification provided (Y or N)
i. Choice of Relevant Health Criteria value	Y
ii. Site use (current and intended), comment on compatibility with land use selected	Y
iii. Critical Receptor	Y
iv. Pathways included/omitted (including bioaccessibility if used)	Y
v. Soil Parameters, e.g. pH	Y

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