

SNIFFER Method - Organics

Project Ref: **A385-00**

Run No: **Tier 1**

1 This worksheet may be used for organic contaminants

2 This worksheet has been completed by **Chris Hepworth** on **25/04/2006**
 and has been checked by **Sarah MacInnes** on **18/05/2006**

3 It relates to **Nitroglycerine** found at **Bishopton**

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 **9.00E-04** 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	Y	2190	Y
Residential without plant uptake	0-6		2190	
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 unknown? (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: $RI_{ingest}=(TDI-((MDI/70 \times 46.4) \times CF)/TABW)^a$

9.00000E-04 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: $RI_{ingest}=0.2TDI$

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

9.00E-04 mg per kg body weight per day

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).

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	Y	2190	Y
Residential without plant uptake	0-6		2190	
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)

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: $RI_{ingest} = (TDI - ((MDI/70 \times 46.4) \times CF) / TABW)^*$

* 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.

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

$SEI_{ding} =$

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 $SEI_{ding} = SEI_{ding} \times$ bioaccessibility fraction

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: $ASC_{ding} = RI_{ingest} / SEI_{ding}$

$ASC_{ding} =$ mg per kg body weight per day

/

kg soil per kg body weight per day

=

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)

50 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):

589 cm^3 per g dry weight

a representative value of f_{oc} (fraction of organic carbon in soil):

0.006 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 $CF_{leafy} = (0.784 \cdot 10^{-0.434 \cdot (\log K_{ow} - 1.78)})^{2/2.44} \cdot (10^{0.99 \log K_{ow} - 2.05} + 0.82)^{\psi / (\theta + \psi K_{oc} f_{oc})}$
 $CF_{leafy} =$ 0.255718639 ug per g fresh weight plant per ug per g dry weight soil

For root vegetables $CF_{root} = (10^{0.77 \log K_{ow} - 1.52} + 0.82)^{\psi / (\theta + \psi K_{oc} f_{oc})} \cdot 0.01$
 $CF_{root} =$ 0.003953014 ug per g fresh weight plant per ug per g dry weight soil

^b Note - If the soil correction factor ($\psi / (\theta + \psi K_{oc} f_{oc})$) 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	8.14937E-04
Cabbage	4.86885E-03	calc not required	7.79119E-04
Carrot	7.38094E-03	calc not required	1.19002E-05
Leafy salads	3.25677E-03	calc not required	1.45772E-04
Onion	3.69474E-03	calc not required	8.50045E-06
Potato	4.41616E-02	calc not required	6.54917E-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	1.63742E-04
Allotments	1.63742E-04

$SEI_{veg} =$ 1.64E-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: $ASC_{veg} = R_{Ingest} / SEI_{veg}$

$ASC_{veg} =$ 9.00000E-04 / 1.63742E-04 = 5.496463102 mg per kg soil
 mg per kg body weight per day / kg soil per kg body weight per day

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 $SEI_{indirect} = SEI_{indirect} \times$ 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: $ASC_{indirect} = RI_{ingest}/SEI_{indirect}$

$$ASC_{indirect} = \frac{9.00000E-04 \text{ mg per kg body weight per day}}{1.12723E-06 \text{ kg soil per kg body weight per day}} = 798.4173594 \text{ mg per kg soil}$$

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
Depth to subsurface contamination

$W =$ metres
 $d_s =$ metres

Soil Matrix

Soil organic matter content
Mass fraction of organic carbon in soil
Air filled porosity
Water filled porosity
Total porosity
Bulk soil density

$SOM =$ %
 $f_{oc} =$ /167 $0.00000E+00$ kg OC per kg soil
 $\theta_{vap} =$ unitless
 $\theta_{wat} =$ unitless
 $\theta_{total} = 0$ unitless
 $\rho =$ kg soil per l soil

Contaminant

Organic carbon/water partition coefficient
Dimensionless Henry's constant
Diffusion coefficient in water
Diffusion coefficient in soil air
Air in soil
Water in soil
Air term
Water term
Effective diffusion coefficient
Molecular weight
Saturated vapour pressure

$K_{oc} =$ l water per kg OC
 $H' =$ l water per l air
 $D_{wat} =$ m² per s
 $D_s =$ m² per s
#DIV/0! unitless
#DIV/0! unitless
#DIV/0! m² per s
#DIV/0! m² per s per (l water per l air)
 $D_{eff} =$ m² per s
MW = g per mol
SatVP = mmHg

Pathway parameters

Dilution ratio
Temperature
Ambient air velocity in the mixing zone (default from CLEA is 3 m per s)

DR = unitless
Temp = °C + 273 = 273 K
 $V_{air} =$ m per s

Receptor characteristics

Time-averaged body height
Height of mixing zone

TAH= m
h= /2 = m

26 Contaminant Volatilisation Factor (CVF)

CVF= kg soil per l air

27 Time-Averaged Air Intake Outdoors

Landuse	TAAI _{outv} 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 m³ 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} x CVF x 1000

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} = / = mg per kg soil
mg per kg body weight per day kg soil per kg body weight per day

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 m³ 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 = l air per kg soil

33 Soil vapour partition coefficient

The soil vapour partition coefficient (SVPC) is

SVPC = 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} = kg soil/(kg body weight per day)

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

$ASC_{inv} =$

 mg per kg body weight per day
 /

 kg soil per kg body weight per day
 =

 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} = 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} = 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} = (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 10³

soil ingestion pathway	1/ASC _{ding} =	1/		=		kg soil per mg
homegrown vegetable consumption pathway	1/ASC _{vveg} =	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 _{ouV} =	1/		=		kg soil per mg
inhalation of indoor air	1/ASC _{iv} =	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_{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 **Nitroglycerine** in the scenario is mg per kg soil

Integrated site specific assessment criteria for substances with dimensionless Henry's constant less than 10³

soil ingestion pathway	1/ASC _{ding} =	1/	<input type="text" value="91.34097688"/>	=	<input type="text" value="0.010947989"/>	kg soil per mg
homegrown vegetable consumption pathway	1/ASC _{vveg} =	1/	<input type="text" value="5.496463102"/>	=	<input type="text" value="0.181935179"/>	kg soil per mg
ingestion of soil attached to vegetables	1/ASC _{indirect} =	1/	<input type="text" value="798.4173594"/>	=	<input type="text" value="0.001252478"/>	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 **Nitroglycerine** in the **Residential with plant uptake** 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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