

Appendix C
Calculation of Chemical Intake - Methodology

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C1.1 General Methodology

The following presents the general methodology adopted for the calculation of chemical intake via inhalation, ingestion and dermal exposure pathways. Most equations are derived from USEPA (1989).

C1.2 Intakes via Inhalation

The assessment of inhalation exposures assumes that exposures associated with the groundwater contamination and HCB car park are associated with volatile chemicals rather than particulates (more likely from combustion sources or dust emissions). On this basis, the following equation is used to calculate intake of volatile chemicals via all inhalation pathways:

$$\text{Daily Chemical Intake}_v = C_a \cdot \frac{\text{InhR} \cdot \text{ET} \cdot \text{FI} \cdot \text{EF} \cdot \text{ED}}{\text{BW} \cdot \text{AT}} \quad (\text{mg/kg/day})$$

where:

- Ca = Concentration of chemical in air (as relevant for each pathway assessed) (mg/m³)
- InhR= Inhalation rate (dependant on age and activity) (m³/hr)
- ET = Exposure time (dependant on activity) (hr/day)
- FI = Fraction inhaled from contaminated source assumed to be 1 or 100% unless noted otherwise (unitless)
- EF = Exposure frequency (days/year)
- ED = Exposure duration (years)
- BW = Body weight (dependant on age) (kg)
- AT = Averaging time for threshold and non-threshold exposures (days)

C1.3 Intakes via Ingestion

The assessment of ingestion exposures requires evaluation of a number of pathways that can loosely be grouped into the ingestion of water, ingestion of produce and the ingestion of soils and sediments.

C1.3.1 Ingestion of Water

This includes evaluation of the following pathways:

- Ingestion of groundwater extracted from a backyard bore; and
- Ingestion of surface water while playing, wading or swimming (it is proposed that unfiltered analytical data be used in this assessment to ensure ingestion of chemicals in water as well as suspended sediment are accounted for in the calculations).

The following equation is used to calculate intake of chemicals via the ingestion of water pathways:

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$$\text{Daily Chemical Intake}_{IW} = C_w \cdot \frac{IR_w \cdot B \cdot EF \cdot ED}{BW \cdot AT} \quad (\text{mg/kg/day})$$

where:

- C_w = Concentration of chemical in water (as relevant for each pathway assessed) (mg/L)
- IR_w = Ingestion rate of water (dependant on age and activity and may be derived using ingestion rate per hour and number of hours undertaking activity or simply an intake per day) (L/day)
- B = Bioavailability or absorption of chemical via ingestion assumed to be 1 or 100% unless noted otherwise (unitless)
- EF = Exposure frequency (days/year)
- ED = Exposure duration (years)
- BW = Body weight (dependant on age) (kg)
- AT = Averaging time for threshold and non-threshold exposures (days)

C1.3.2 Ingestion of Produce

This includes evaluation of the following pathways:

- Ingestion of home-grown fruit and vegetable crops
- Ingestion of recreationally caught fish and oysters

Home Grown Fruit and Vegetables

Assessment of intake via the ingestion of home-grown fruit and vegetable crops is evaluated using the following equation:

$$\text{Daily Chemical Intake}_{FV} = C_p \cdot \frac{IR_p \cdot FH \cdot B \cdot EF \cdot ED}{BW \cdot AT} \quad (\text{mg/kg/day})$$

where:

- C_p = Concentration of chemical in produce (as calculated) (mg/kg wet weight)
- IR_p = Ingestion rate of fruit and vegetable produce (dependant on age) (kg/day wet weight)
- FH = Fraction ingested which is home grown (unitless)
- B = Bioavailability or absorption of chemical via ingestion of product assumed to be 1 or 100% unless noted otherwise (unitless)
- EF = Exposure frequency (days/year)
- ED = Exposure duration (years)
- BW = Body weight (dependant on age) (kg)
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Recreationally Caught Fish and Oysters

The risk assessment will continue to provide an evaluation of exposure associated with this pathway despite a fish and shell fishing ban for the estuary (November 2004). It is assumed that people may still fish and collect oysters despite the ban.

Assessment of intake via the ingestion of recreationally caught fish (including shellfish, not oysters) is evaluated using the following equation:

$$\text{Daily Chemical Intake}_F = C_f \cdot \frac{IR_f \cdot FI \cdot B \cdot EF \cdot ED}{BW \cdot AT} \quad (\text{mg/kg/day})$$

where:

- C_f = Concentration of chemical in fish and shellfish (measured) (mg/kg wet weight)
- IR_f = Ingestion rate of recreationally caught fish (dependant on age) (kg/day wet weight)
- FI = Fraction of fish caught and ingested that is derived from Penrhyn Estuary (unitless)
- B = Bioavailability or absorption of chemical via ingestion assumed to be 1 or 100% unless noted otherwise (unitless)
- EF = Exposure frequency (days/year)
- ED = Exposure duration (years)
- BW = Body weight (dependant on age) (kg)
- AT = Averaging time for threshold and non-threshold exposures (days)

Assessment of intake via the ingestion of recreationally caught oysters in the estuary is evaluated using the following equation:

$$\text{Daily Chemical Intake}_O = C_o \cdot \frac{No \cdot Wo \cdot FI \cdot B \cdot EF \cdot ED}{BW \cdot AT} \quad (\text{mg/kg/day})$$

where:

- C_o = Concentration of chemical in oysters from site (Penrhyn Estuary, measured) (mg/kg wet weight)
- No = Number of oysters consumed per day (per day)
- Wo = Weight of oyster (kg wet weight)
- FI = Fraction of oysters caught and ingested that is derived from Penrhyn Estuary (unitless)
- B = Bioavailability or absorption of chemical via ingestion assumed to be 1 or 100% unless noted otherwise (unitless)
- EF = Exposure frequency (days/year)
- ED = Exposure duration (years)
- BW = Body weight (dependant on age) (kg)
- AT = Averaging time for threshold and non-threshold exposures (days)

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C1.3.3 Ingestion of Soils and Sediments

This includes evaluation of the following pathways:

- Ingestion of sediments
- Ingestion of soils (SRA area)

The following equation is used to calculate intake of chemicals via the ingestion of soils and sediment pathways:

$$\text{Daily Chemical Intake}_{IS} = C_s \cdot \frac{IRs \cdot FI \cdot B \cdot CF \cdot EF \cdot ED}{BW \cdot AT} \quad (\text{mg/kg/day})$$

where:

Cs = Concentration of chemical in soil or sediment (as relevant for each pathway assessed) (mg/kg)

IRs = Ingestion rate of soil or sediment (dependant on age and activity) (mg/day)

FI = Fraction of daily ingestion that is derived from contamination source assumed to be 1 or 100% unless noted otherwise (unitless)

B = Bioavailability or absorption of chemical via ingestion assumed to be 1 or 100% unless noted otherwise (unitless)

CF = Conversion factor of 1×10^{-6} to convert mg to kg

EF = Exposure frequency (days/year)

ED = Exposure duration (years)

BW = Body weight (dependant on age) (kg)

AT = Averaging time for threshold and non-threshold exposures (days)

C1.4 Intakes via Dermal Exposures

The assessment of dermal exposures involved quantification of intakes from sediments and water (extracted groundwater and surface water).

C1.4.1 Mechanisms of Dermal Absorption

Passive diffusion, as governed by Fick's First Law, is considered to be the main process whereby chemicals enter and permeate through the skin. The human skin is the largest organ of the body and it consists of a thin (approximately 100 μm) epidermal layer superimposed on a thick dermal layer (approximately 300-400 μm). The epidermis consists of four layers, the outermost layer being the stratum corneum (SC) (approximately 10-40 μm), which overlays the strata lucidum, granulosum, and germinativum (Figure 1). The SC layer is composed of flat highly keratinised squamous cells that are nonviable and are thought to maintain the barrier properties of the skin. If the SC layer is removed by tape stripping, for example, the permeability of the skin to chemicals increases dramatically.

Factors that have an effect on the dermal absorption of chemicals through the skin include:

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- Skin hydration with several studies indicating that skin hydration may increase skin permeability;
- Thickness of the SC and anatomic regions with higher absorption expected in areas unprotected by thick SC layers;
- Lipophilicity of chemical. The SC layer tends to be a lipid-rich milieu and hence provides a barrier to hydrophilic compounds but permits the entry of lipophilic compounds;
- Degree of sediment binding;
- The presence of surface slicks typically comprised of fatty substances (e.g., lipids from decomposed organisms and oil from petroleum contamination) which typically cover the surface of all natural bodies of water.
- Environmental factors that include water temperature, pH, turbidity, flow rate (current), and degree of solar illumination.
- Physiologic factors include genetic-related sensitivity (e.g., tendency to sunburn) and individual differences (e.g., age, the presence of skin disease, skin abrasions).

Models that are used to estimate dermal absorption of chemicals present in water and soils/sediment are simplifications of the more complex dermal absorption processes.

C1.4.2 Dermal Contact with Water

The following equation (as detailed in USEPA 1989 and 1992b) is used to calculate intake of chemicals via dermal exposure to chemicals in water:

$$\text{Daily Chemical Intake}_{DW} = C_w \cdot \frac{SA_w \cdot ET \cdot K_p \cdot CF \cdot EF \cdot ED}{BW \cdot AT} \quad (\text{mg/kg/day})$$

where:

C_w = Concentration in water (mg/L)

SA_w = Surface area of body in contact with water (cm²)

ET = Exposure time in contact with water (hr/day)

K_p = Dermal permeability/absorption via skin for each chemical in water (cm/hr)

CF = Conversion factor of 1×10^{-3} to convert cm³ to L

EF = Exposure frequency (days/year)

ED = Exposure duration (years)

BW = Body weight (dependant on age) (kg)

AT = Averaging time for threshold and non-threshold exposures (days)

K_p is a chemical-specific factor that has been derived for a wide range of chemicals. Values for chemicals evaluated have been obtained from the Risk Assessment Information System (RAIS) database available on the website (<http://risk.lsd.ornl.gov/index.shtml>) which is maintained by the Oak Ridge Operations of the US Department of Energy, current to February 2005.

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C1.4.3 Dermal Contact with Sediment

Dermal absorption of chemicals from soil depends on the area of contact, duration of contact, bond between chemical and the soil and the ability of the chemical to penetrate the skin. The assessment of dermal absorption of chemicals in sediments has followed the approach adopted for the evaluation of dermal absorption of chemicals in soils.

USEPA Approach

The USEPA (1989 and 2004) define a simple approach to the evaluation of dermal absorption associated with soil contact. This is presented in the following equation:

$$\text{Daily Chemical Intake} = C_s \cdot \frac{SAs \cdot AF \cdot ABSd \cdot CF \cdot EF \cdot ED}{BW \cdot AT} \quad (\text{mg/kg/day})$$

where:

Cs = Concentration in soil (mg/kg)

SAs = Surface area of body exposed to soil (cm²)

AF = Adherence factor, amount of soil that adheres to the skin per unit area which depends on soil properties and area of body (mg/cm² per event)

ABSd = Dermal absorption fraction (unitless – refer to discussion below)

CF = Conversion factor of 1x10⁻⁶ to convert mg to kg

EF = Exposure frequency (days/year)

ED = Exposure duration (years)

BW = Body weight (dependant on age) (kg)

AT = Averaging time for threshold and non-threshold exposures (days)

Dermal Absorption Fraction (ABSd)

The approach undertaken by the USEPA utilises a dermal absorption fraction typically derived from experimental studies on different chemicals. On the basis of the studies undertaken and a number of simplifications, ABSd values have been recommended for a range of 10 chemicals and default values for other semi-volatile chemicals. No default is defined (in USEPA 2004) for volatile organic chemicals or inorganic chemicals. It is considered that, with regards to soil exposures, volatile organic chemicals would volatilise from soil on skin and should be accounted for in the assessment of inhalation exposures. For inorganics, the speciation is very important to dermal absorption and hence no generic default values have been determined.

More commonly used values for the assessment of dermal exposure to organics and inorganics utilise defaults for ABSd for organics of 0.01 and inorganics of 0.001 as presented on RAIS (Risk Assessment Information System derived from USEPA 1992), along with the few chemical-specific values available.

The value of ABSd has no consideration of exposure time. Experimental studies used to define ABSd values are associated with dermal application over 24 hours (i.e. the event is considered to be a 24 hour day by default). Due to the lack of information about the rate and relationship of absorption of chemicals

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through the skin over shorter exposure periods, the USEPA methodology does not recommend adjusting the ABSd to account for exposures over times less than 24 hours, rather it recommended adjusting exposure frequency and exposure duration to reflect site conditions. This approach is utilised to evaluate dermal intake per exposure event (commonly adopted as a day) and is considered to be conservative in the assessment of exposure events that are less than 24 hours in duration or multiple short-term exposure events where absorption would be “double-counted”.

Further Review of Dermal Absorption

In reviewing the approach to the assessment of dermal exposure presented in source documents “The Health Risk Assessment and Management of Contaminated Sites” (CSMS, 1991, 1993, 1996, 1998 and enHealth 2002) that are referenced in enHealth (2002) it is noted that the approach suggested by Hawley (1985) has been adopted. The approach is similar to the USEPA approach presented above, with some differences with respect to the evaluation of absorption.

Hawley (1985) provides a review of dermal uptake from soils for organic chemicals based on studies of a number of compounds by humans, rats, rabbits and pigs. The absorption rates obtained for application of a pure compound (or in acetone solvent) were determined to be 11% for an adult over 24 hours. For a 12 hour contact time, the dermal absorption rate was taken to half or 6% (as rounded up from half of 11%) of the applied dose. For children a higher rate was assumed to account for more permeable skin of a young child. For children the absorption rate was taken to be twice that of the adult, or 12% of the compound on the skin over 12 hours.

Absorption of contaminants in soils or dust (and sediments) was discussed by Hawley to limited by the physical-chemical binding to the matrix. On this basis Hawley also applied use of a factor to account for the matrix effect of absorption from soils (or relevant matrix) by comparison to the absorption study data that used the pure compound or solvent solution. The value used by Hawley (for TCDD and other organic compounds where no data is available) was 15%.

This approach is also adopted in the assessment of dermal intake of organic chemicals presented in the Dutch sediment exposure model SEDISOIL (1996) and the soil exposure model CSOIL (2001). These models express the dermal absorption of organics presented by Hawley as an absorption rate per hour. Hence for children the absorption rate is 0.01 or 1% per hour and for adults the absorption rate is 0.005 or 0.5% per hour.

This approach was generally utilised by Fitzgerald D.J (CSMS 1991) in the setting of a response level for benzo(a)pyrene where intake via skin absorption for a 2 ½ and 6 year old child utilises the dermal absorption value over 24 hours. For an adult the intake via skin absorption considers exposure to soils over 12 hours and adjusts the intake using a linear relationship for absorption. While many other response levels (in various papers in CSMS) have been established following this approach, they are typically set for a 2 ½ year old child where dermal absorption associated with soils over 24 hours is considered to be relevant. Other references where dermal absorption over shorter exposure periods than 24 hours (using the linear approach) are presented in the following:

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- Di Marco P.N. and Buckett K.J in CSMS 1996 in “Derivation of Health Investigation Levels for Beryllium and Beryllium Compounds”
- Di Marco P.N. in CSMS 1993 in “The Assessment and Management of Organochlorine Termiticides” where exposures over 24 hours (children), 8 and 10 hours (adults).
- Di Marco P.N. and Buckett K.J in CSMS 1993 in “Derivation of A Health Investigation Level for PCBs”

It is proposed that the methodology presented by Hawley (1985), SEDISOIL (1996) and CSOIL (2001) be adopted for the assessment of dermal exposures to chemicals identified in sediments. On this basis, dermal intake from exposure to sediment will be determined using the following equation:

$$\text{Daily Chemical Intake}_{Ds} = C_s \cdot \frac{SAs \cdot AF \cdot Abs \cdot ET \cdot ME \cdot CF \cdot EF \cdot ED}{BW \cdot AT} \quad (\text{mg/kg/day})$$

where:

- Cs = Concentration in sediment (mg/kg)
- SAs = Surface area of body exposed to sediment (cm²)
- AF = Adherence factor, amount of sediment that adheres to the skin per unit area which depends on soil/sediment properties and area of body (mg/cm² per event)
- Abs = Dermal absorption rate (per hour) – based on chemicals specific information or use of default values of 0.01 per hour for children and 0.005 per hour for adults (as above)
- ET = Exposure time to sediments (hours/day)
- ME = Matrix effect (unitless) – dependant on the nature of dermal data available, by default 0.15 or 15% assumed (discussed above)
- CF = Conversion factor of 1x10⁻⁶ to convert mg to kg
- EF = Exposure frequency (days/year)
- ED = Exposure duration (years)
- BW = Body weight (dependant on age) (kg)
- AT = Averaging time for threshold and non-threshold exposures (days)

For the chemicals expected to be evaluated in Penrhyn Estuary, there are no chemical-specific dermal absorption parameters available and hence default values as noted above will be used in the assessment.

C1.5 References

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