This report is the current version of the Work Package 1 report and represents the interim output of the first of three work packages that will be delivered as part of Defra R&D Project SP1010 – Development of Category 4 Screening Levels (C4SLs) for Assessment of Land Affected by Contamination, as follows:

WP1: Design of methodology
WP2: Develop methodology using at least two substances
WP3: Determine C4SLs for six substances

The aim of this research project is to provide technical guidance to support our recently revised Statutory Guidance (SG), in England and Wales, for Part 2A of the Environmental Protection Act 1990. For cases of potential harm to human health, the revised SG presents a new four category system for classifying land under Part 2A. These range from Category 4, describing land that is clearly not contaminated land (in the legal sense) to Category 1, describing land where there is a significant possibility of significant harm (SPOSH).

A key aspect of the project has been to re-consider and adapt the methodology used to derive soil guideline values (SGVs) and other generic assessment criteria, so that less conservative C4SLs can be derived. Six contaminants (arsenic, benzene, benzo(a)pyrene, cadmium, hexavalent chromium and lead) have been selected in order to test and refine the proposed approach and it is hoped that the final methodology will be published by Summer 2013.

The proposed C4SLs will represent a new set of generic screening levels that are more pragmatic (but still strongly precautionary) compared to the existing SGVs and other similarly derived numbers. They will consist of cautious estimates of contaminant concentrations in soil that are still considered to present an acceptable level of risk, within the context of Part 2A, by combining information on toxicology, exposure assessment and normal levels of exposure to these contaminants.

As the methodology is tested during Work Packages 2 & 3, **this report is likely to be substantially amended and therefore should not be considered a final version**. A final version of the report will be uploaded when the project concludes, at which point this version will be removed.

Therefore:

- **Do not cite or quote;**
- **Do not use as the basis for any decision-making on the contamination status of any land or site (under Part 2A or otherwise); and**
- **Should be read directly from the Defra website (if further circulation is necessary this document should not be downloaded but rather a link to the Defra web page circulated).**

The Project is being overseen by a Steering Group. The Steering Group members are:

- Department for Environment, Food & Rural Affairs
- Health Protection Agency
- Department for Communities & Local Government
- Homes & Communities Agency
- Food Standards Agency
- Environment Agency
- Environment Agency (Wales)
- Welsh Government

SP1010 – Development of Category 4 Screening Levels for Assessment of Land Affected by Contamination

Work Package 1 Report

FINAL

Contaminated Land: Applications in Real Environments (CL:AIRE)

7th December 2012

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ABBREVIATIONS

AC	Assessment Criteria
ADE	Average Daily Exposure
AGAC	Acute Generic Assessment Criterion
AQO	Air Quality Objectives
BMD	Benchmark Dose
BMDL	Lower Confidence Limit of BMD
BMR	Benchmark Response
BW	Body Weight
C4SL	Category 4 Screening Level
CLEA	Contaminated Land Exposure Assessment
COC	Committee on Carcinogenicity of Chemicals in Food, Consumer Products and the Environment
CR	Consumption Rate
CSAF	Chemical Specific Adjustment Factor
DCLG	Department for Communities and Local Government
DEFRA	Department for Environment, Food and Rural Affairs
DL	Dust Loading Factor
DQRA	Detailed Quantitative Risk Assessment
EA	Environment Agency
EAW	Environment Agency Wales
ELCR	Excess Lifetime Cancer Risk
EF	Exposure Frequency
FSA	Food Standards Agency
GAC	Generic Assessment Criterion
GQRA	Generic Quantitative Risk Assessment
HBGV	Health Based Guidance Value
HCA	Homes and Communities Agency
HCV	Health Criteria Value
HF	Homegrown Fraction
HPA	Health Protection Agency
ID	Index Dose
IGHRC	Interdepartmental Group on the Health Risks from Chemicals
IR	Intake Rate
LCD	Lifetime Cumulative Dose
LLTC	Low Level of Toxicological Concern
LOAEL	Lowest Observed Adverse Effect Level
MDI	Mean Daily Intake
MOE	Margin of Exposure
MRL	Minimum Risk Level
NBC	Normal Background Concentration
NOAEL	No Observed Adverse Effect Level
POD	Points of Departure
PRA	Preliminary Risk Assessment
PTWI	Provisional Tolerable Weekly Intake
RBA	Relative Bioavailability
RfC	Reference Concentrations
RfD	Reference Dose
SCL	Significant Contaminant Linkage
SG	Statutory Guidance
SGV	Soil Guideline Value
SoBRA	Society for Brownfield Risk Assessment

SPOSH	Significant Possibility of Significant Harm
SSAC	Site-Specific Assessment Criterion
TCA	Tolerable Concentration in Air
TDI	Tolerable Daily Intake
TF	Transport Factor
UF	Uncertainty Factor
USEPA	United States Environmental Protection Agency
WG	Welsh Government
WHO	World Health Organisation

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1. INTRODUCTION

This report presents a suggested methodology for the development of Category 4 Screening Levels (C4SLs). It has been produced in fulfilment of Work Package 1 (WP1) of Defra's C4SLs research project, SP1010, and it incorporates the results of consultations with both the project's Steering Group and the wider contaminated land community (via a Stakeholder Workshop held on 6 November 2012). The methodology will be finalised, demonstrated and further consulted upon, as part of Work Packages 2 and 3 (WP2 and WP3).

The project's Steering Group comprises individuals from the following organisations:

- Department for Environment, Food and Rural Affairs (Defra)
- Department for Communities and Local Government (DCLG)
- Welsh Government (WG)
- Environment Agency (EA)
- Environment Agency Wales (EAW)
- Health Protection Agency (HPA)
- Food Standards Agency (FSA)
- Homes and Communities Agency (HCA)

Attendees at the Stakeholder Workshop included representatives from trade and professional organisations involved in the management of land contamination, local authority "cluster groups", learned societies and university departments (as well as Steering Group members).

1.1 BACKGROUND AND OBJECTIVES

The overall aim of the C4SLs research project is to assist with the provision of technical guidance to support Defra's recently revised Statutory Guidance (SG) for Part 2A of the Environmental Protection Act 1990 (Part 2A) (Defra, 2012a). Specifically, the project aims to deliver:

- A methodology for deriving C4SLs (WP1); and
- C4SLs for six substances for four generic land-uses: residential, commercial, allotments and public open space (WP2 & 3).

Part 2A was originally introduced to ensure that significant risks from land contamination to human health, property and the environment are managed appropriately, with the revised SG being designed to address concerns regarding its real-world application. Details on some of these concerns and the importance of striking the right balance between the benefits and impacts of regulatory action under Part 2A were provided in the consultation document issued by Defra in connection with the planned revisions to the SG in 2010 (Defra, 2010a). The resulting revisions are believed to address them, as described in the Ministerial Foreword to the revised SG:

> *"It has been refined in order to give greater clarity to regulators as to how to decide when land is and is not actually contaminated land. It is shorter, simpler and more focused towards achieving optimum results in terms of dealing with sites most in need of remediation. Also included are various other improvements, reflecting the experience accumulated after eleven years of operating the regime and the progress in research and technology that we have seen in that time. They enable local authorities to take a more targeted approach which remains precautionary rather than a blanket approach which is over cautious."*

To help achieve a more targeted approach to identifying and managing contaminated land in relation to the risk (or possibility) of harm to human health, the revised SG

presents a new four category system for classifying land under Part 2A, ranging from Category 4, where there is no risk or the level of risk posed is acceptably low, to Category 1, where the level of risk is clearly unacceptable. More specific guidance on what type of land could be considered as Category 4 (Human Health) is provided in Paragraphs 4.21 and 4.22 of the revised SG:

"4.21 The local authority should consider that the following types of land should be placed into Category 4: Human Health:

(a) Land where no relevant contaminant linkage has been established.

(b) Land where there are only normal levels of contaminants in soil, as explained in Section 3 of this Guidance.

(c) Land that has been excluded from the need for further inspection and assessment because contaminant levels do not exceed relevant generic assessment criteria in accordance with Section 3 of this Guidance, or relevant technical tools or advice that may be developed in accordance with paragraph 3.30 of this Guidance.

(d) Land where estimated levels of exposure to contaminants in soil are likely to form only a small proportion of what a receptor might be exposed to anyway through other sources of environmental exposure (e.g. in relation to average estimated national levels of exposure to substances commonly found in the environment, to which receptors are likely to be exposed in the normal course of their lives).

4.22 The local authority may consider that land other than the types described in paragraph 4.21 should be placed into Category 4: Human Health if following a detailed quantitative risk assessment it is satisfied that the level of risk posed is sufficiently low."

The C4SLs are intended as "relevant technical tools" (in relation to Paragraph 4.21c of the revised SG) to help local authorities and others when deciding to stop assessing a site, on the grounds that it could not pose the level of risk to human health required for determination under Part 2A (i.e. a "significant possibility of significant harm" [SPOSH]).

The Impact Assessment (IA) which was produced to secure sign off of the revised SG (Defra, 2012b) provides further information on the nature and potential role of the C4SLs. Paragraph 47(h) of the IA states that:

> *"The new statutory guidance will bring about a situation where the current SGVs/GACs are replaced with more pragmatic (but still strongly precautionary) Category 4 screening levels (C4SLs) which will provide a higher simple test for deciding that land is suitable for use and definitely not contaminated land."*

A key distinction between the Soil Guideline Values (SGVs), derived in accordance with the EA SR2 and SR3 documents, and the C4SLs, is the level of risk that they describe. As described by the Environment Agency (2009a):

> *"SGVs are guidelines on the level of long-term human exposure to individual chemicals in soil that, unless stated otherwise, are tolerable or pose a minimal risk to human health."*

The implication of Paragraph 47(h) of the IA (see above) is that minimal risk is well within Category 4 and that the C4SLs should describe a higher level of risk which, whilst not minimal, can still be considered low enough to allow a judgement to be made that land containing substances at, or below, the C4SLs is a "Category 4: Human Health" case (see Paragraph 4.20 of the revised SG).

Thus, the C4SLs will consist of cautious estimates of contaminant concentrations in soil that are not considered to represent an unacceptable level of risk within the context of the policy objectives of Part 2A. It is important to note that such C4SLs should not be

viewed as “SPOSH levels” or “Part 2A levels” and they should not, on their own, be used as a legal trigger for the determination of land under Part 2A.

1.2 UK APPROACH TO CONTAMINATED LAND RISK ASSESSMENT

As outlined in the revised SG and the Environment Agency CLR11 document (EA, 2004), a “staged” or “tiered” approach is recommended for assessing risks from land contamination in the UK. After each stage, or tier, of assessment, the decision is made as to whether further action is required, and whether this should entail further assessment (such as gathering more data or proceeding to the next stage or tier) or risk mitigation (such as remediation or the implementation of risk control measures).

The revised SG and CLR11 describe three stages or tiers of assessment:

- **Preliminary Risk Assessment (PRA).** A primary objective of a PRA is to gather as much information as possible about a site so that a *conceptual model* can be developed that represents site characteristics and shows the possible relationships between contaminants, pathways and receptors. On the basis of the conceptual model, any need for further assessment (e.g. intrusive investigation) is then identified or a remedial strategy is developed.

- **Generic Quantitative Risk Assessment (GQRA).** In the event that the PRA indicates the existence of *plausibly significant contaminant linkages* (and remediation is not planned), GQRA is then carried out by comparison of measured concentrations (in, for example, soil, water or soil vapour) with generic screening values appropriate for the pollutant linkage(s) being assessed. In simple terms, provided the measured concentrations are below the generic screening criteria, the risk from the pollutant linkages(s) being assessed are unlikely to be significant. Note that GQRA often involves an element of statistics to estimate the representative exposure concentration for comparison with the generic screening values.

- **Detailed Quantitative Risk Assessment (DQRA).** If contaminant levels exceed the generic screening values, or where generic screening values are not appropriate for a particular site, then DQRA may be carried out and site-specific assessment criteria (SSAC) developed. The outcome of the DQRA is a final decision regarding which, if any, of the plausible contaminant linkages identified in the PRA and GQRA are significant. If any are thought to be significant, then the process proceeds to options appraisal. In the event that no significant contaminant linkages (SCLs) are identified, then no further action is required.

The SGVs (and Generic Assessment Criteria - GACs) are risk-based generic screening values used within a GQRA to assess the risks to human health from chronic exposure to contaminants in soil. These are typically derived using the CLEA methodology as described in the Environment Agency SR2, SR3 and SR7 reports (EA, 2009b & c; EA, 2008). The CLEA methodology follows the paradigm for chemical risk assessment proposed by the National Academy of Sciences (NAS, 1983; IPCS, 1999; EA, 2009b) which can be summarised as three key stages:

- *Toxciological Assessment.* This consists of two steps:

    - *Hazard identification* involves identifying the potential toxic effects of a chemical e.g. whether the chemical is mutagenic, carcinogenic or toxic to organs and physiological systems etc.; and

    - *Hazard characterisation* involves understanding the identified hazards in terms of dose, exposure route, duration and timing of exposure i.e. it explores how the dose or length of exposure affects the probability, magnitude and severity of effects. It should,

where possible, include a dose-response assessment in the study design. There are a number of steps involved in hazard characterisation, resulting, in the case of CLEA, in the derivation of Health Criteria Values (HCVs).

- *Exposure Assessment.* This involves the evaluation and quantification of exposure from a defined scenario. Human exposure to chemicals may occur via ingestion, inhalation and dermal entry, and also involves an appreciation of the 'bioavailability' of the chemical. The CLEA model uses a series of equations to estimate exposure via a number of potential pathways.

- *Risk Characterisation.* This involves comparison of estimated exposure with the health criteria. In simple terms, the SGV is the concentration of contaminant in soil that may result in human exposure that is equivalent to the HCV.

It is anticipated that C4SLs will also be adopted as generic screening levels that can be used within a GQRA, albeit that they describe a higher level of risk than the SGVs.

1.2.1 SUMMARY OF PROPOSED APPROACH TO DERIVE C4SL

Our suggested approach to the development of C4SLs consists of the retention and use of the CLEA framework, as explained principally in SR2 and SR3 (EA, 2009b & c) and associated documents (which outline the basic principles of land contamination risk assessment), modified according to considerations of the underlying science within the context of Defra's policy objectives relating to the revised SG.

Ultimately, the development of C4SLs may be achieved in one of three ways, namely:

- by carrying out modifications to the exposure parameters (and maintaining current toxicological "minimal risk" interpretations);
- by carrying out modifications to the toxicological parameters and going above minimum risk (and maintaining current exposure parameters); and
- by modifying both exposure and toxicology parameters.

The remainder of this report outlines the work that has been undertaken to develop our suggested methodology for the development of C4SLs. We outline the current methodology used in the CLEA framework for both exposure modelling and toxicological assessment and propose suggestions where this may be modified in order to achieve the project's objectives. These suggestions are summarised in the orange boxes that appear throughout the text. Note that the initial draft report has been amended in the light of comments from the Steering Group and Stakeholders and the orange boxes indicate whether the proposed modifications have been retained, revised or rejected, based on these comments.

2. EXPOSURE MODELLING

Exposure modelling is an integral part of the assessment of risks to human health from soil contamination. It is the mathematical representation of the conceptual model of exposure (IPCS, 2008) and involves the use of equations and associated input parameter values to estimate the intake (and/or uptake) dose of contaminant to a human receptor for a given exposure scenario. There are two general approaches to exposure modelling: a 'forward' modelling approach can be used to predict the actual exposure at a site from measured or estimated soil concentrations. The exposure can then be combined or compared with toxicological dose-response data to characterise risk. Alternatively, a 'reverse' modelling approach can be used to estimate the theoretical soil concentration at which the estimated exposure equals some predefined toxicological benchmark. Both approaches can be used with the CLEA model, but it is the latter approach that is used to derive soil assessment criteria, which in simplified terms, estimates the theoretical soil concentration at which the Average Daily Exposure (ADE) from soil contamination would equal the HCV. This soil concentration can be adopted as a GAC or SGV which, depending on the input parameters used, is land-use specific. As described in Section 1.2, SGVs and/or GACs are used as part of GQRAs for comparison with measured soil concentrations at a site to help characterise risk.

As discussed in Section 1.1, the CLEA model and associated land-use and contaminant specific parameter values have been chosen by the Environment Agency to derive GACs that represent minimal or tolerable risk. This chapter assesses whether the CLEA model and associated parameter values are a suitable basis for estimating exposure for derivation of the C4SLs. Proposals for modifications to the CLEA methodology and parameter values are presented. As will be explained these broadly relate to (a) an update in existing parameters in line with more recent evidence; and (b) a move towards central tendency estimates for parameter values. It will also be explained that the overall level of precaution in a C4SL is governed by the combined effect of uncertainties, including the assumptions made in the exposure modelling. As discussed in Section 6 probabilistic exposure modelling is proposed to ensure that the approach used for the exposure modelling for deriving C4SL is suitably precautionary.

2.1 BRIEF OVERVIEW OF CLEA

Common to all models for quantifying exposure from soil contamination, CLEA uses a series of equations to predict exposure to a 'critical' receptor from a given soil concentration via a number of exposure pathways. The critical receptor is dependent on land-use. SGVs have been derived for three generic land-uses: residential, allotments and commercial. The critical receptor is generally assumed to be a 0 to 6 year old child for residential and allotments land-uses[1] and a 16 to 65 year old adult for commercial land-use.

CLEA considers up to ten exposure pathways (soil and dust ingestion are combined), although not all may be active depending on the generic land-use modelled (Table 2.1). Other pathways not considered within the CLEA software may also be active at a specific site, such as consumption of eggs or diffusion of contaminants through water supply pipes. As described in Environment Agency guidance on using SGVs (EA, 2009a), the assessor should assess the applicability of assessment criteria derived using CLEA in the context of the conceptual model of risk developed for the site.

[1] Cadmium is an exception. The cadmium SGVs for residential and allotments land-uses are based on exposure over a lifetime (i.e. a 0 to 75 year old) – see Section 2.5.1.2.

Table 2.1: Exposure pathways modelled in CLEA

Exposure Pathway	Generic Land-use		
	Residential	Allotments	Commercial
Direct ingestion of soil (outdoors) and dust derived from soil (indoors)	✓	✓	✓
Ingestion of soil attached to fruit/vegetables	✓	✓	
Ingestion of fruit/vegetables	✓	✓	
Dermal contact with dust derived from soil (indoors)	✓		✓
Dermal contact with soil (outdoors)	✓	✓	✓
Inhalation of dust derived from soil (indoors)	✓		✓
Inhalation of dust derived from soil (outdoors)	✓	✓	✓
Inhalation of vapours (indoors)	✓		✓
Inhalation of vapours (outdoors)	✓	✓	✓

CLEA is used for deriving assessment criteria relating to human health from chronic exposure, and as such estimates daily exposure averaged over a number of years for comparison with the HCV. This is termed the ADE and it has units of mg kg^{-1} d^{-1} for direct comparison with the HCV. The generalised equation for estimating ADE for each exposure pathway is given below:

$$ADE_i = \frac{IR_i.EF_i.ED}{BW.AT}$$

Where,

ADE_i = Average daily exposure from pathway i (mg kg^{-1} d^{-1})
IR_i = chemical intake/uptake rate for pathway i (mg d^{-1})
EF_i = exposure frequency for pathway i (d yr^{-1})
ED = exposure duration (yr)
BW = body weight (kg)
AT = averaging time (d)

CLEA averages ADE over a series of age classes that represent the critical receptor. Where the critical receptor is a 0 to 6 year old child, 6 age classes of 1 year duration each are used (age classes 1 to 6). Where the critical receptor is a 16 to 65 year old adult (age class 17), 1 age class of 49 years duration is used. Finally, for lifetime averaging, 18 age classes are used: age classes 1 to 16 for the 0 to 16 year old, age class 17 for the 16 to 65 year old and age class 18 for the 65 to 75 year old.

Each exposure pathway has a unique equation (or series of equations) and associated input parameters for estimating the intake rate (IR). Exposure frequency may also vary between pathways. CLEA adds up ADE for groups of pathways and compares with the HCVs for oral and/or inhalation exposure. For compounds exhibiting a threshold health effect[2], an allowance for background exposure from non soil sources is also included in the ADE calculation. CLEA derives two assessment criteria (AC), as follows:

[2] i.e. an effect where there is a threshold dose below which adverse effects are not discernible (see Section 3)

- AC_{oral}. This is the soil concentration at which the sum of the ADE equals the oral HCV[3].
- AC_{inhal}. This is the soil concentration at which the sum of the ADE equals the inhalation HCV.

The use of these assessment criteria to derive the GAC or SGV is dependent on whether the toxicological effects are systemic or localised. Where both oral and inhalation HCVs are based on systemic toxicological effects, the assessment criteria are "integrated" to derive the GAC[4]. Where one or more HCV are based on localised effects, the lowest of the two assessment criteria are used as the GAC.

In total there are approximately 100 parameters used in the equations for predicting exposure in CLEA, however many of these apply to only one or two pathways. The parameters can be sub-divided into three broad types:

- **Contaminant specific**. Parameters related to the physico-chemical properties of the contaminant such as solubility, air-water partition coefficient and dermal absorption factor;
- **Receptor specific**. Parameters related to the critical receptor such as body weight, respiration rate and consumption rate of fruit and vegetables. CLEA allows different values to be attributed to each age class for the majority of these parameters; and
- **Site specific**. Parameters relating to the site itself such as soil properties (e.g. soil porosity, permeability and organic carbon content) and building properties (e.g. dimensions of buildings, pressure differential and rate of air exchange).

CLEA allows almost all the parameter values to be adjusted by the user but has an in-built set of "default" values for calculating SGV and GAC for the generic land-uses.

2.2 UNCERTAINTY IN ESTIMATING EXPOSURE

CLEA is a deterministic model and as such provides one estimate of exposure from one set of parameter input values for one type of critical receptor. The extent to which this estimate of exposure is accurate for an individual within the critical receptor group will be dependent on a number of factors:

- Uncertainty in the conceptual model. As shown in Table 2.1, CLEA assumes that exposure occurs via up to ten exposure pathways (although soil and dust ingestion are combined). As described in the EA SR3 report (EA, 2009c), these pathways are assumed to represent typical exposure scenarios for each of the generic land-uses. When applying the SGV or GAC it is important to consider the applicability of these pathways to the site in question. For example, as described in Section 2.1, there may be residential properties where chickens are kept and where the ingestion of eggs is a potentially significant route of exposure. Equally, there may be residential properties where there is no garden or exposed soils and thus virtually no plausibly significant exposure pathways (other than perhaps intrusion of vapours through the building foundations). Likewise, for allotments it may be reasonable to assume that a negligible proportion of allotment soils is tracked back to the residential property, but there may be some allotment holders who live adjacent to their allotment where tracking back of soils may be more significant. The CLEA framework regards such

[3] Due to the general sparsity in dermal toxicity data for chronic exposure, health criteria for oral intake are typically used for assessing dermal as well as oral exposures.

[4] See for example method given in Chen, 2010, which can be simplified to GAC = 1 / ($1/AC_{oral}$ + $1/AC_{inhal}$)

uncertainties as being most effectively assessed and managed when applying soil screening criteria on a particular site.

For the purposes of this project, the exposure pathways modelled for the SGV are also considered appropriate for derivation of the C4SLs. However, as with the SGV, assessors should check the applicability of the C4SLs for GQRA in the context of the conceptual model for the site.

- Uncertainty in the ability of the CLEA equations to accurately predict exposure. For some exposure pathways (such as incidental ingestion of soil and dust) the equations are relatively simple and robust, with the accuracy of prediction largely dependent on the input parameters rather than the equation itself. For other pathways, such as vapour inhalation, the equations are relatively complex and the accuracy of prediction is not only dependent on the input parameters but also on the validity of the assumptions underpinning those equations. Deviation from these underlying assumptions can lead to a significant under- or over- estimation of exposure

- Uncertainty in the input parameter values. This can be sub-divided into:

    - Aleatoric uncertainty (aka variability). This type of uncertainty can be measured but not reduced. Body weight, for example, is variable within each age class - not all 2 to 3 year old children weigh the same. With sufficient measurement we can estimate average body weight within each age class to a reasonable degree of accuracy. We can also estimate the probability of a random individual within an age class having a body weight in excess of a given value.
    - Epistemic uncertainty (aka systematic uncertainty). This is uncertainty that exists due to lack of data or difficulties in measurement/estimation of parameter values. It may be small for some parameters but more significant for others. For example, relatively few studies have been conducted to estimate the amount of soil that children ingest on a day to day basis (see Section 2.5.2.2). These studies were conducted outside the UK and in summer months only. We can use these studies to estimate average daily soil ingestion rate for UK children but there will be relatively large epistemic uncertainty in this estimate.

It should also be recognised that uncertainty associated with the use of GAC is typically greater than that associated with the use of site specific assessment criteria (SSAC) within a DQRA. The incorporation of site specific information, such as details of the exposure scenario, receptor behaviour, soil type and foundation construction in the derivation of SSAC allows a more realistic (and hence accurate) estimate of risk to be made than with the use of GAC which are derived to be broadly applicable to a wide range of sites. The more encompassing a GAC, the less applicable it will be to any individual site and the greater the uncertainty becomes. Furthermore, it is highly unlikely that the overall generic scenario could ever be verified in the real world as most verification work applies to individual pathways in a specific set of circumstances.

There are a variety of approaches that can be used to assess and manage uncertainty in exposure modelling. Probabilistic modelling, such as Monte Carlo analysis, can help to quantify uncertainty in the exposure estimates caused by variability and (to a certain extent) epistemic uncertainty in the model parameter inputs. In an earlier version of CLEA (CLEAUK) variability in a limited number of input parameters was modelled using Monte Carlo analysis to produce a frequency plot of ADE (Figure 2.1). In that model, the upper bound 95th percentile estimated ADE was used to calculate the SGV. Note that the resultant frequency distribution of ADE would likely have had a greater spread of values if uncertainty in all model input parameters had been taken into account.

Although uncertainty cannot be quantified using deterministic modelling, it can be managed. Adopting conservative values for all input parameter values decreases the probability of the model under-predicting exposure for an individual within the critical receptor group. The current configuration of CLEA uses a mixture of "central tendency" and "reasonable worst case" values and as a result likely over-predicts exposure for the majority of individuals within each critical receptor group. However, the degree of conservatism in the estimates of ADE and the probability that it under-predicts exposure for a randomly selected individual from the critical receptor group is not known (see Figure 2.2). A better understanding of these aspects is required to help assess the suitability of the current CLEA model configuration for the derivation of C4SLs. This has been achieved by conducting the following work:

- Pathway analyses to identify the key pathways involved in deriving GAC for the generic land-uses
- Sensitivity analyses to identify the key pathways and parameters that lead to significant uncertainty in the estimates of exposure;
- Critical review of the ability of the CLEA equations to accurately predict exposure for the key pathways; and
- Critical review of the key parameter values and in particular an appraisal of their level of conservatism for predicting exposure to the critical receptor groups.

This work is described in the following sections. As described in Section 6.1 probabilistic modelling is also proposed to ensure that the set of deterministic exposure parameter values chosen results in a C4SL with a suitable level of precaution.

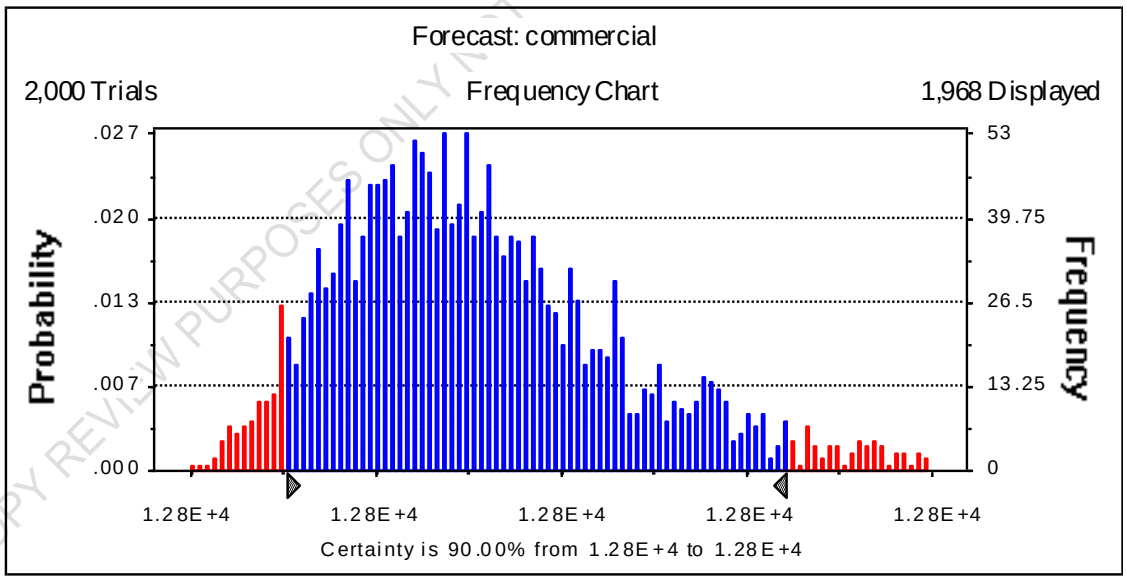


Figure 2.1: Frequency distribution of ADE from CLEAUK

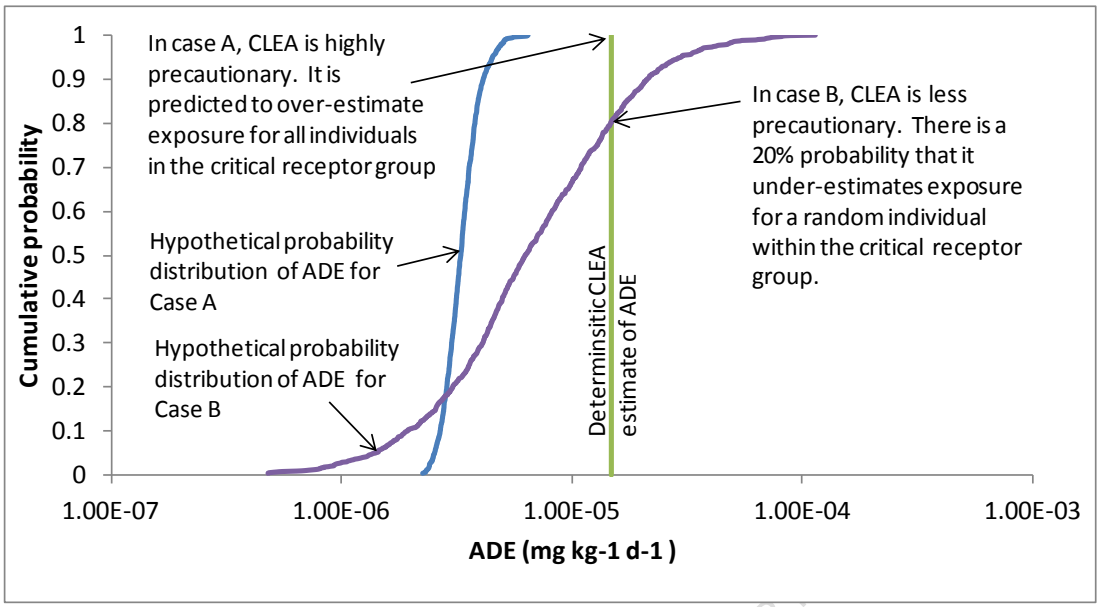


Figure 2.2: Schematic graph illustrating probability that CLEA under predicts exposure for a randomly selected individual from the critical receptor group

2.3 PATHWAY ASSESSMENT

As discussed in Section 2.1, CLEA models exposure via a number of pathways. The relative importance of each pathway to overall risk is dependent on the particular configuration of input parameters and will vary depending on contaminant and land-use. Figures 2.3 to 2.5 show the relative importance of each pathway to the derivation of GACs for the six contaminants suggested by Defra as the focus of this work (arsenic, benzene, benzo(a)pyrene, cadmium, chromium (VI) and lead) for residential, allotments and commercial land-uses (the standard land-uses in CLEA). As can be seen, the following pathways are important for one or more contaminants for one or more land-uses:

- direct soil and dust ingestion
- consumption of homegrown produce
- dermal contact outdoors
- inhalation of dust indoors
- inhalation of vapours indoors

These can be considered the key pathways and are considered further in this review.

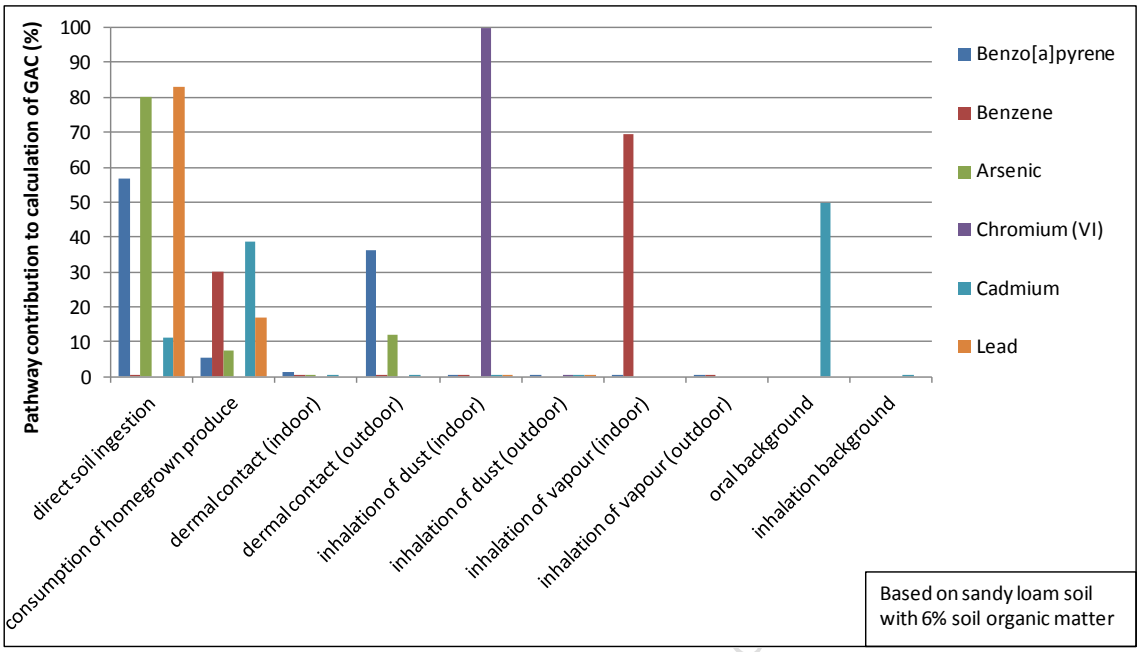


Figure 2.3: Relative importance of exposure pathways to GAC for Residential land-use with consumption of homegrown produce

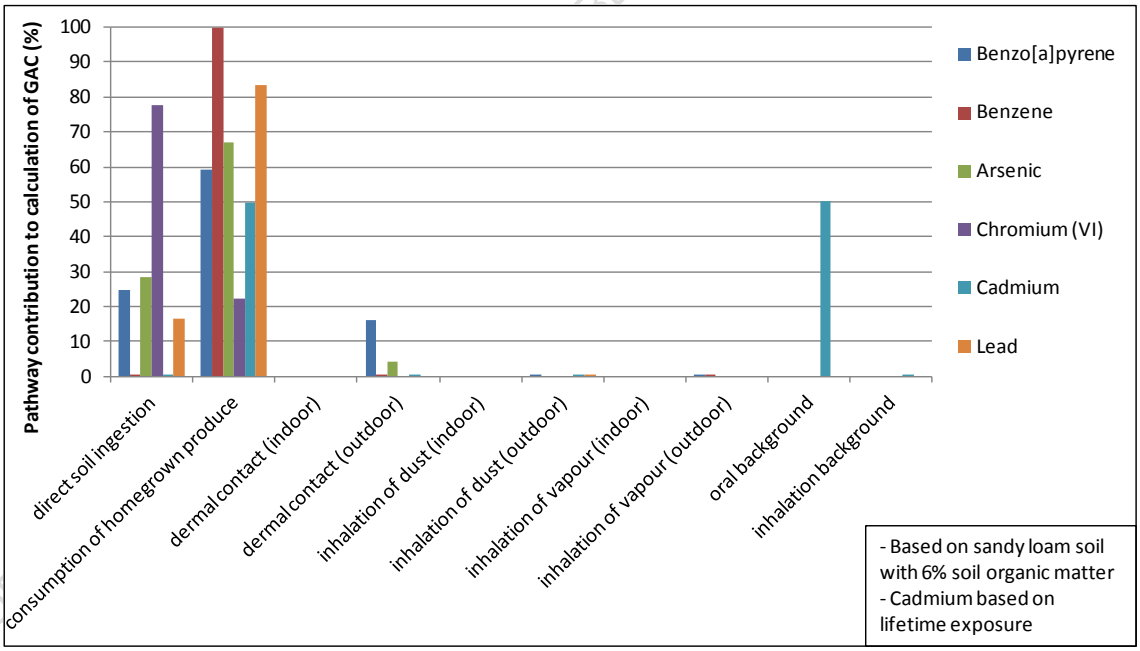


Figure 2.4: Relative importance of exposure pathways to GAC for Allotments land-use

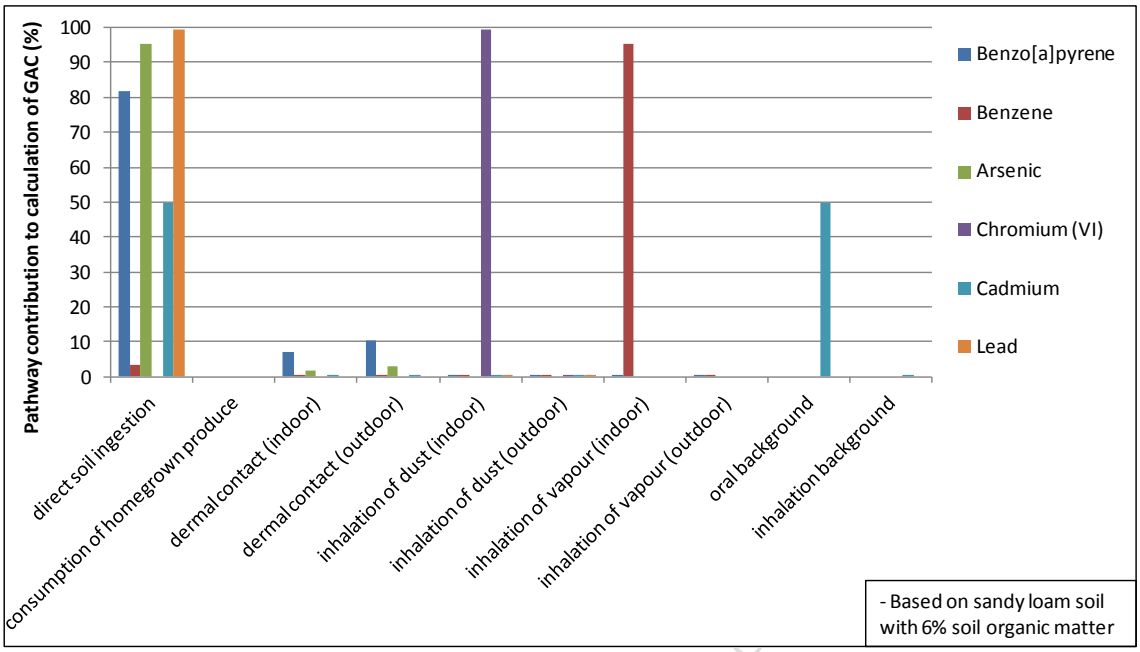


Figure 2.5: Relative importance of exposure pathways to GAC for Commercial land-use.

2.4 SENSITIVITY ANALYSIS

Sensitivity analysis provides a method for identifying key sources of uncertainty in the estimates of ADE. Sensitivity analysis has been conducted using CLEA for the residential, allotments and commercial land-uses. The sensitivity analysis has been conducted by varying one input parameter at a time between a reasonable minimum and maximum value and assessing what effect this has on the GAC for each of the six focus contaminants. Only parameters that are used in the calculation of ADE from soil for the six focus contaminants have been tested. For example, empirical soil to plant concentrations factors have been used for the inorganic contaminants and this negates the need for parameters only used by the PRISM plant uptake model such as the soil-water partition coefficient (Kd) and root to shoot correction factors. A total of 58 parameters have been tested in the sensitivity analyses. The range of values tested and justification for each range are provided in Appendix 1.

Figures A2.1 to A2.3 show the results of the sensitivity analyses. These show the ratio of modified GAC to original GAC for each parameter. Note that many parameter values used in CLEA already represent the reasonable maximum value (such as an exposure frequency of 365 days per year) and in these cases only one sensitivity run (using the minimum value) has been conducted.

The results of the sensitivity analyses show that there are a number of key parameters/assumptions that cause uncertainty in the derivation of GAC. These are listed below (with key associated pathways in brackets)

- Body weight (all pathways)
- Averaging time (all pathways)
- Soil and dust ingestion rate (soil & dust ingestion)
- Exposure frequency outdoors (dermal contact outdoors)
- Skin adherence outdoors (dermal contact outdoors)
- Maximum exposed skin fraction outdoors (dermal contact outdoors)
- Dermal absorption fraction (dermal contact outdoors)
- Inhalation rate (vapour and dust inhalation indoors)
- Dust loading factor (dust inhalation indoors)
- Soil to dust transport factor (dust inhalation indoors)

- Soil to indoor air correction factor (vapour inhalation indoors)
- Building footprint (vapour inhalation indoors)
- Living space height (vapour inhalation indoors)
- Soil to plant concentration factors (consumption of homegrown produce)
- Homegrown fraction (consumption of homegrown produce)
- Soil type (vapour inhalation indoors)[5]
- Produce consumption rate (consumption of homegrown produce)
- Soil organic matter (vapour inhalation indoors & consumption of homegrown produce).

As expected, these parameters are all related to the five key pathways identified in Section 2.3. The exposure models and associated parameter values used for these 5 key pathways are considered further in Section 2.5.

2.5 REVIEW OF EXPOSURE MODELS AND ASSUMPTIONS FOR KEY PATHWAYS

2.5.1 ESTIMATING AVERAGE DAILY EXPOSURE

As discussed in Section 2.1, ADE is estimated using the following generalised equation:

$$ADE_i = \frac{IR_i.EF_i.ED}{BW.AT}$$

This can be regarded as the internationally recognised standard equation for estimating ADE for chronic exposure durations and there is little doubt in its validity. Exposure frequency and the pathway specific equations used for estimating exposure rate (IR) are discussed in Sections 2.5.2 to 2.5.6. The remaining parameter values used within the generalised ADE equation are discussed below.

2.5.1.1 Exposure Duration

CLEA uses the above equation to estimate ADE for up to 18 age classes which range in exposure duration from 1 year for the 0 to 16 year old age classes, 10 years for the 65 to 75 year old age class and 49 years for the 16 to 65 year old age class. The subdivision of ADE calculations into so many age classes is unique to CLEA. The exposure durations used in CLEA are effectively equal to the duration of age class and are thus irrefutable.

2.5.1.2 Averaging Time

The averaging time can have a large influence on the ADE estimates derived. USEPA guidance allows averaging time to be greater than exposure duration when estimating the excess lifetime cancer risk from land contamination. For example, exposure duration of 30 years (6 years for a child and 24 years for an adult) versus an averaging time of 70 years (assumed lifetime) is a common assumption when assessing carcinogens in the USA. This effectively assumes that there is no exposure from land contamination for 40 years of the receptor's lifetime, and is judged to be a reasonable worst case assumption regarding household mobility in the USA.

Even where averaging time is equal to exposure duration, the period over which exposure is averaged can have a large influence on the ADE. This arises because ADE is generally higher for children (due to higher exposure rate to body weight

[5] The sensitivity analysis was conducted for soil type by assessing the change in GAC using the CLEA default parameter values for a clay and sandy soil respectively.

ratios) than adults as exemplified in Figure 2.6. Indeed CLEA predicts the average ADE over the first 6 years of a child's life to be 2.3 to 5.1 times higher (for the six focus contaminants under the residential scenario) than lifetime averaged ADE (assuming the receptor remains in the same residential property and that soil concentrations remain unchanged for their lifetime).

Lifetime averaging has been assumed by the Environment Agency for the derivation of the cadmium SGV for residential and allotments land-uses. This is justified on the basis that the critical toxicological effect is based on body burden of cadmium built up over a lifetime. There may also be an argument for the use of lifetime averaged ADE for some non threshold compounds, depending on the substance specific toxicological review. This is discussed further in Section 3.2.5.

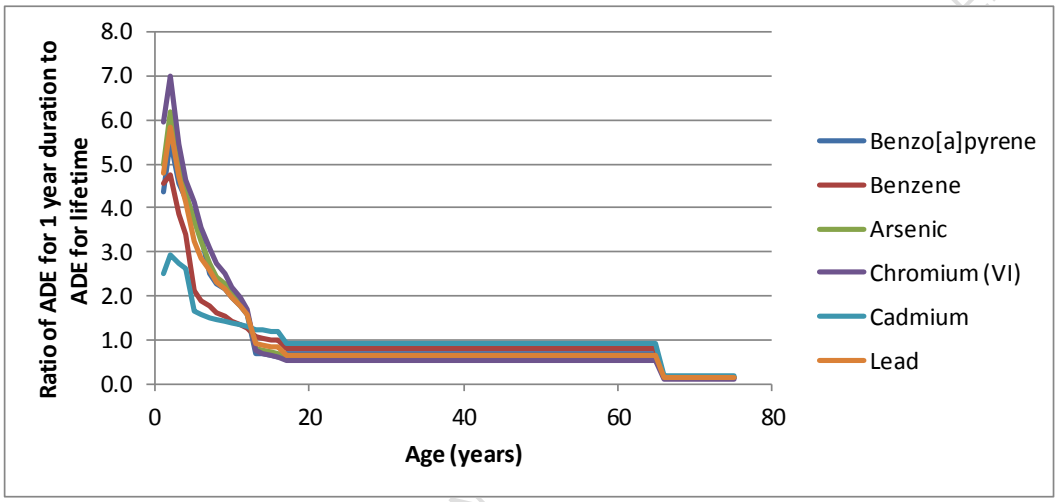


Figure 2.6: Total soil derived ADE with age predicted by CLEA for residential land-use

2.5.1.3 Body Weight

Body weight varies between individuals and this will be one factor that leads to uncertainty in estimates of ADE. The current configuration of CLEA uses the arithmetic mean female body weight for each age class taken from the Health Survey for England 2003 (EA, 2009c). Whilst this represents central tendency for females it will tend towards an over-estimation of ADE for males whose arithmetic mean body weights are approximately 7 to 20% higher depending on age class. The use of central tendency values will tend to result in an over-estimation of ADE for some (lighter than average) individuals and an under-estimation for others (heavier than average). The sensitivity analyses showed that use of the 5th and 95th percentile bodyweights generally changed the ADE estimates by less than ± 30% and thus variability in body weight is unlikely to cause significant uncertainty in exposure estimates.

2.5.2 SOIL AND DUST INGESTION

Soil and soil derived dust ingestion is a key exposure pathway for four of the six compounds considered. In CLEA, the exposure rate for this pathway is estimated using the following equation:

$$IR_{direct\_s\&d\_ing} = C_{soil} . RBA_{soil} . S_{ING}$$

Where

$IR_{direct\_s\&d\_ing}$ = exposure rate for soil and dust ingestion (mg d^{-1})
C_{soil} = concentration in soil (mg g^{-1})
RBA_{soil} = relative bioavailability of the contaminant in soil (fraction)
S_{ING} = direct soil and soil derived dust ingestion rate (g d^{-1})

This equation is based on simple mass balance and there is no reason to doubt its ability to predict exposure accurately. Rather, it is uncertainty in the associated input parameters that affect uncertainty in the estimates of ADE as discussed below.

Note that CLEA uses a combined soil and soil derived dust ingestion rate. This is justified on the basis that it is difficult to differentiate between these two types of exposure. However, as discussed below, there may be merit in considering both exposures separately to allow a more realistic assessment of exposure.

2.5.2.1 Soil Concentration

CLEA uses iteration to calculate the soil concentration at which the sum of ADE equals the relevant HCV. Thus, soil concentration is an output rather than an input when CLEA is used in reverse mode. In GQRA, uncertainty in the soil concentration at a particular site is considered when estimating the "representative exposure concentration" from measured concentrations for comparison with the GAC. As discussed in Section 7.1 work is underway to review the methods used for estimating the representative exposure concentration and associated uncertainty and this will be reported in WP2.

It is important to note that the soil concentration used in the soil and dust ingestion exposure equation is the concentration of contaminant in soil (and soil derived dust) that is actually ingested, which may not necessarily be the same as the concentration in bulk soil samples. Incidental ingestion of soil and dust is likely to be limited to finer particles, which may have relatively higher or lower concentrations than the average concentration in bulk samples (SoBRA, 2011 & 2012). This uncertainty should be considered when developing the sample plan for the site and when conducting the GQRA.

2.5.2.2 Soil and Dust Ingestion Rate

The soil and dust ingestion rate is a key uncertainty highlighted by the sensitivity analysis. CLEA assumes an average daily soil and dust ingestion rate of 100 mg d^{-1} for 0 to 11 year old children and 50 mg d^{-1} for 12 to 75 year olds. These values are consistent with central tendency values recommended by the USEPA and Netherlands (USEPA 2008, 2011; Lijzen *et al.*, 2001).

Relatively few studies on soil and dust ingestion rate have been conducted. Most of these are based on mass balance using tracer compounds naturally present in soil. Typically, the mass of tracer compounds (such as aluminium, silicon and titanium) are measured in the faeces, urine and non soil dietary intake of children over a 1 day to 2 week basis. Any excess excreted relative to intake is assumed to be due to ingestion of soil and dust. This excess mass is divided by the measured fraction in soil and dust to estimate the mass of soil and dust ingested per day.

Of the studies on children reviewed by the USEPA (2011), there appear to be five key studies on which their recommendations for a soil ingestion rate are based. These studies show considerable variability in ingestion rate on a day to day basis for each child and in the time averaged values between children. Considerable variability was also observed between tracers used.

Figure 2.7 presents the variability in the estimates of mean soil and dust ingestion rate derived from these key studies. The tracer compound used accounts for much of the variability. For example Calabrese *et al.* (1989) used 8 different tracers and this gave 8 different estimates of soil ingestion rate varying from -496 mg d^{-1} (using manganese as the tracer) to 483 mg d^{-1} (using silicon as the tracer). The large variability between tracers and the occurrence of negative estimates highlights the large measurement error and uncertainty in these studies.

Van Wijnen *et al.* (1990) is the only key study outside of the US. They conducted mass balance studies for three groups of children in the Netherlands: children in

day care, children on campsites and children in hospital. They used titanium, aluminium and acid insoluble residue as the tracer compounds. Their methods differed slightly to those used in the US making direct comparison between studies difficult. Firstly, they do not report soil ingestion rate estimated from each tracer but instead report the lowest soil ingestion rate from all tracers. Secondly, they did not attempt to estimate mass of tracer ingested via food per individual but instead used the mean concentration of each tracer in the faeces of children in hospital to estimate dietary intake from non soil sources. Despite these differences the arithmetic mean soil ingestion rates derived by Van Wijnen *et al.* (1990) are similar to those from other studies.

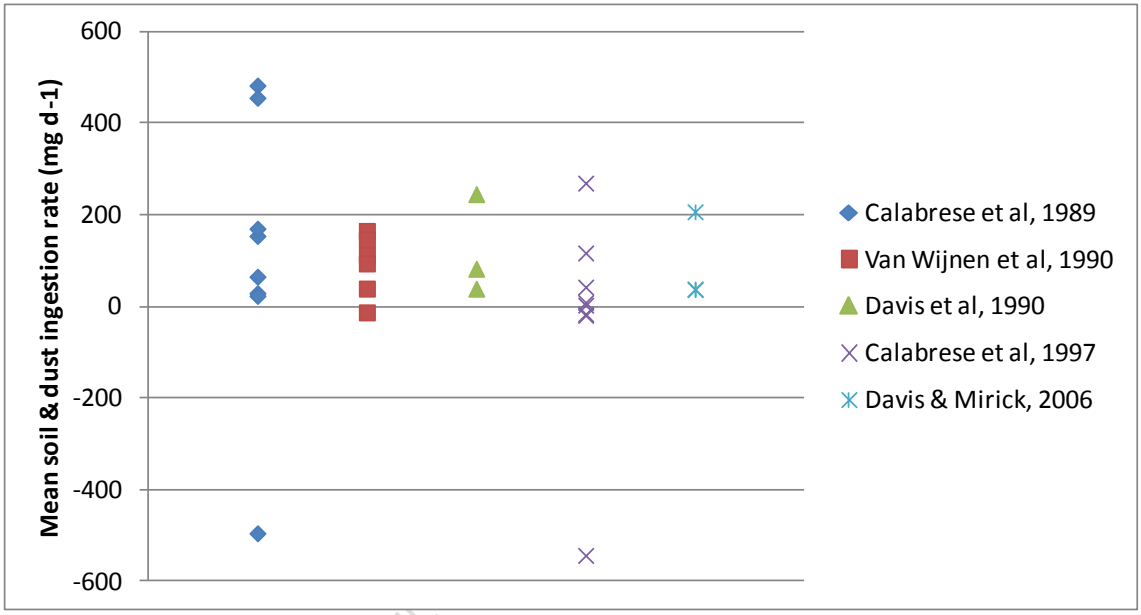


Figure 2.7: Estimates of soil ingestion rate in children from mass balance studies

An interesting finding from the Van Wijnen *et al.,* (1990) study was the difference between soil ingestion rates in children in day care and those in campsites. Samples of faeces were taken from children in day care on two occasions, one in early summer and one in late summer. The results were markedly different. The early summer estimates were similar to those of the campsite cohort, whilst the estimates from late summer were similar to those for the children in hospital. Van Wijnen *et al*.(1990) noted that the weather was poorer during the second sampling round, with a higher number of rainy days. They attributed the lower soil ingestion rate to less time spent outdoors.

This is an important consideration as all of the key studies reviewed by the US were conducted during summer months when contact with soil is likely to be greater (either directly outdoors or with soil that has been tracked into the house). Thus, whilst a value of 100 mg d^{-1} may be a reasonable central tendency estimate of soil ingestion rate during summer months, it may be an over-estimate during winter months when children spend less time outdoors.

Another consideration when evaluating the soil ingestion studies is the source of the soil ingested. Van Wijnen *et al.,* (1990) found little difference in soil ingestion rate between children who resided in houses with and without gardens and assumed that the majority of soil ingestion occurred whilst outdoors at day care. Thus, it is reasonable to assume that a proportion of soil ingested by a 0 to 6 year old child will come from locations other than the home, such as the play park, streets, shops, day care and schools.

In summary, whilst there is much uncertainty over soil ingestion rate it is likely that the current assumptions of 100 mg d^{-1} for 365 days per year for residential land-use and 50 mg d^{-1} for 230 days per year for commercial land–use will tend towards an over-estimation of exposure for the majority of cases. It may be more realistic to use a weighted estimate of soil and dust ingestion rate based on assumed exposure frequencies indoors and outdoors. This could be calculated as follows:

$$S_{ING} = \frac{S_{ING\_indoors}.EF_{indoors} + S_{ING\_outdoors}.EF_{outdoors}}{EF_{soil\&dust.ing}}$$

Where,

S_{ING} = direct soil and soil derived dust ingestion rate (g d^{-1})
$S_{ING\_indoors}$ = direct soil derived dust ingestion rate indoors (g d^{-1})
$S_{ING\_outdoors}$ = direct soil ingestion rate outdoors (g d^{-1})
$EF_{indoors}$ = exposure frequency indoors (d yr^{-1})
$EF_{outdoors}$ = exposure frequency outdoors (d yr^{-1})
$EF_{soil\&dust.ing}$ = exposure frequency assumed for soil and dust ingestion pathway (d yr^{-1})

The USEPA (2011) recommend central tendency values of soil and indoor dust ingestion rates of 50 and 60 mg d^{-1} for children and 20 and 30 mg d^{-1} for adults, respectively. Whilst an exposure frequency of 365 d yr^{-1} may not be unreasonable for indoor exposure for residential land-use (see Section 2.5.2.4), this is likely to be highly precautionary for outdoor exposure. Data on which to base exposure frequency for a child outdoors are lacking but it is not unreasonable to assume that this would be no greater than 170 days (approximately 50% of the year). For commercial land-use, based on the existing parameter values used within CLEA, it is not unreasonable to assign exposure frequencies of 230 and 170 d yr^{-1} for indoor and outdoor exposure, respectively. Use of these parameter values with the equation above results in weighted soil and dust ingestion rates for residential and commercial land-uses of approximately 80 and 40 mg d^{-1} for these land-uses, respectively. These soil and dust ingestion rates are still likely to be conservative estimates of central tendency as they do not account for the proportion of soil and dust ingested that comes from off-site sources.

For allotments land-use, CLEA assumes that exposure via direct ingestion of soil and soil derived dust only occurs whilst at the allotment, i.e. the tracking back of soils to the residential property is negligible. CLEA assumes that children ingest 100 mg d^{-1} soil from the allotment. Whilst this is higher than the central tendency value recommended by the USEPA (50 mg d^{-1}), it seems reasonable to assume that children might have greater regular contact with soils at an allotment than in a garden, and thus the CLEA value of 100 mg d^{-1} is considered reasonable for this scenario.

Suggested C4SL CLEA Modification 1: Reduce average soil and dust ingestion rates from 100 to 80 mg d^{-1} for residential land-use and 50 to 40 mg d^{-1} for commercial land-use to account for lower exposure in winter months.

Whilst there was general support for this proposed modification from the steering group, there was mixed support from stakeholders. Some felt that tracking back of soil could be higher in winter months and thus the logic that soil and dust ingestion in winter being less may not apply. Given the relatively high degree of uncertainty involved with this parameter it has been considered prudent to ***reject*** *this proposed modification and retain the existing soil ingestion rates used within CLEA which are accepted as being precautionary.*

2.5.2.3 Relative Bioavailability

Bioavailability is a consideration of how much enters the systemic blood circulation and organs after absorption of the chemical through the gut, lungs or skin. The Relative BioAvailability (RBA) is the ratio of the bioavailability of the contaminant in soil to the bioavailability of the contaminant in the critical study used to derive the HCV. In the case of the soil and dust ingestion pathway, it is the relative bioavailability of the contaminant to oral exposure that is relevant. The published SGVs are all based on the assumption of an RBA of 100%, i.e. that the bioavailability of the contaminant in soil is equal to that in the critical toxicological study. Toxicology studies for oral exposure are based on oral intakes of the contaminant dissolved in different media (e.g. water, oil, diet), where bioavailability can often be greater than contaminants in soil. Thus, the assumption of an RBA of 100% is most likely conservative.

For some substances (notably metals), *in-vitro* bioaccessibility data can be generated (Wragg *et al.,* 2009) and this is an evaluation of the proportion of chemical that stays in the soil matrix vs the amount that is free to be absorbed into the body. The amount free to absorb and become 'bioavailable' is said to be the 'bioaccessible' fraction. As such, bioaccessibility testing can provide an indication of the bioavailability of the contaminant in soil and can be used to refine the value of RBA used in CLEA. Bioaccessibility can be highly variable, depending on soil properties and the speciation of the contaminant and thus it may be more appropriate for use as part of a site specific DQRA than for derivation of a generic screening value.

However, consideration could be given to use of conservative generic estimates of RBA to derive C4SLs, where there is strong evidence (e.g. from *in-vivo* studies) that the bioavailability of the contaminant in soil is significantly lower than that associated with the critical toxicological studies.

> Suggested C4SL CLEA Modification 2: Utilise conservative generic chemical-specific RBA estimates, where feasible and supportable, rather than the current default of 100%.
>
> *There was mixed support for this modification from the steering group and stakeholders. Most agreed that the use of in-vitro bioaccessibility data was unlikely to form an appropriate basis for reducing the RBA for derivation of the C4SL. However, this modification is* ***retained*** *as there may be contaminants where there is sufficient in-vivo data to demonstrate that the bioavailability of the contaminant in soil is less than that associated with the critical toxicological study.*

2.5.2.4 Exposure Frequency

The SGVs and GACs for residential land-use are based on the assumption that children aged 1 to 6 years are exposed to soil and soil derived dust at their home 365 days per year. Whilst this is a worst case assumption, sensitivity analysis has shown that reducing this value to 350 days per year (which is likely to be closer to central tendency for the UK population) has a negligible effect on the GAC derived.

As discussed above, there is some evidence that the average soil and dust ingestion rate is correlated to amount of time spent outdoors, with the implication that the daily ingestion rate of soil derived dust indoors is significantly lower than that outdoors. Whilst an exposure frequency of 365 days per year may not be unreasonable for exposure to indoor dust, it is likely to be highly conservative for exposure outdoors. As discussed in Section 2.5.2.2 typical values for exposure frequency outdoors are likely to be less than 170 days per year. There may therefore be merit in calculating a weighted soil and dust ingestion rate based on different indoor and outdoor ingestion rates, as described above.

For commercial land-use, an exposure frequency of 230 d per year is assumed. This is based on an adult working 5 days per week for 46 weeks of the year and is likely to be a reasonable estimate of central tendency for indoor exposure to soil derived dust. As discussed above, there may be merit in weighting the soil and dust ingestion rate to account for differences in indoor and outdoor exposure frequencies. Note that CLEA currently assumes an outdoor exposure frequency of 170 days per year for dermal contact outdoors for commercial land-use.

For allotments land-use, the exposure frequency varies according to age class. An exposure frequency of 258 days per year has been assumed as a reasonable worst case for adults, based on an activity survey from 1993 (EA, 2009c). Exposure frequencies for children are based on some proportion of this time, and range from 25 to 130 days per year. The highest frequency of 130 days per year is assumed for the 1 to <4 year old child, based on 50% of the adult exposure frequency. Whilst there may be some children who accompany their parents/guardians to the allotment 130 days per year, this is likely to be rare. Whilst the percentage of allotment holders with young families is rising, the activity data from 1993 is likely to be strongly biased towards retired adults. Central tendency exposure frequency for adults with young children visiting allotments is likely to be significantly lower than 258 days. Halving the current set of exposure frequencies for allotments land-use would still likely be a conservative estimate of central tendency exposure frequencies for the 0 to 6 year old child.

> Suggested C4SL CLEA Modification 3: Halve exposure frequencies for children on allotments to better reflect likely central tendency behaviour.
>
> *There was mixed support for this modification from the steering group and stakeholders. Some raised concerns that the increasing trend in use of allotments by young families would mean that the proposed modification would not be sufficiently precautionary. There was also concern that there was large uncertainty in this parameter due to lack of relevant recent activity data. Given these concerns this proposed modification has been* ***rejected*** *and the original CLEA value retained as a suitably precautionary value.*

2.5.3 DERMAL CONTACT OUTDOORS

Dermal contact outdoors is a key exposure pathway for benzo(a)pyrene for residential land-use. In CLEA, the exposure rate for this pathway is estimated using the following equation:

$$IR_{dermal\_out} = C_s.n.AF.ABS_d.A_{skin}$$

Where

IR_{dermal_out} = chemical uptake rate from outdoor dermal contact with soil (mg d^{-1})
C_s = concentration in soil (mg g^{-1})
n = number of daily soil contact events (d^{-1})
AF = soil to skin adherence factor (mg cm^{-2})
ABS_d = dermal absorption fraction (dimensionless)
A_{skin} = exposed skin area (m^2)

This equation is based on the assumption that a proportion of mass of contaminant in soil on skin (ABS_d) will enter the bloodstream in a single event. It is a simplification of the skin diffusion process and does not explicitly describe the influence that partitioning and diffusion kinetics have on uptake. For example, the duration of adherence event is theoretically a key factor in the amount of

contaminant that can enter the bloodstream but this is not a variable used in this equation. Rather, it is implicitly considered in the selection of the dermal absorption factor.

It is interesting to note that the original published CLEA methodology used an equation for dermal contact that did account for partitioning and diffusion kinetics (EA, 2002a). This was based on USEPA protocol but the USEPA (2004) later abandoned this method for soils in favour of the simplified version now used by CLEA, presumably because the increased model uncertainty associated with the simplified version was more than off-set by the decreased uncertainty in parameter value uncertainty. Nevertheless, the validity of the assumption that a fixed proportion of the mass of contaminant in soil adhered to the skin entering the bloodstream should be considered and is discussed further below in the context of the dermal absorption factor.

2.5.3.1 Soil Concentration

As discussed for soil and dust ingestion, soil concentration is an output and not an input in the CLEA model when used to derive GAC. Similar to soil and dust ingestion, it is likely to be the finer particles of soil that remain attached to skin and thus it is the concentration of contaminant in these finer particles that is important when predicting exposure via dermal contact.

2.5.3.2 Number of Daily Soil Contact Events

CLEA assumes that one exposure event occurs per day that exposure occurs, i.e. that soil adherence occurs and remains on the skin for a period of time before being washed off and that this happens once per day. This is consistent with the experimental methodology used to derive the dermal absorption factor (Section 2.5.3.6) and USEPA protocol (USEPA, 2004) and is therefore considered reasonable.

2.5.3.3 Soil to Skin Adherence Factor

The value of the soil to skin adherence factor (AF) is a key uncertainty highlighted by the sensitivity analysis. This factor refers to the amount of soil that adheres to the skin per unit of surface area. The soil to skin adherence factor varies with soil properties, different parts of the body and the activity undertaken (USEPA, 2004).

The CLEA model assumes an adherence factor of 1 mg cm^{-2} for children aged 0 to 12 years for residential and allotments land-uses. This is the approximate mid-point between the USEPA (1992) estimated upper 95^{th} percentile estimates for children playing on wet and dry soils. The most recent version of the USEPA Exposure Factors Handbook (USEPA, 2011) gives recommended central tendency values of soil adherence for common activities, including children in day care playing inside and outside and children playing soccer. The central tendency adherence estimates for children in daycare varied from 0.02 to 0.099 mg cm^{-2} depending on body part (Holmes *et al.* 1999). Central tendency estimates for children playing soccer varied from 0.011 to 0.031 mg cm^{-2} depending on body part (Kissel *et al*. 1996). The highest adherence occurred for hands. Based on this information a value of 0.1 mg cm^{-2} may be reasonable for a central tendency estimate of soil adherence for children in residential gardens. A higher value may be expected for children at allotments where more direct contact with soil is expected and thus it may be appropriate to retain the assumption of 1 mg cm^{-2} for allotments.

It should be noted that the estimates are based on very limited datasets. Holmes *et al*.(1999) tested 21 children in daycare. The children were washed beforehand and then re-washed (collecting the water from each body part) at the end of the day. The dry residue in the wash water was used to estimate the average soil adherence factor for each body part. The same method was used by Kissel *et al.* (1996) for 8 children playing soccer. The USEPA considered there to be

insufficient data to describe probability functions of soil adherence for these activities and therefore only provide recommended central tendency estimates.

> Suggested C4SL CLEA Modification 4: Reduce soil adherence factors in children for residential land-use from 1 to 0.1 mg cm^{-2} to better reflect "central tendency".
>
> *Whilst there was general support for this proposed modification from the steering group, there was mixed support from stakeholders. The majority of concern related to whether the move towards central tendency would be sufficiently precautionary. Whilst a move towards central tendency is less precautionary it should be recognised that use of upper bound estimates for all parameters within an exposure pathway equation will lead to highly precautionary estimates of exposure. As discussed below, precautionary estimates of exposure frequency and skin area are retained and thus the overall estimates of exposure are still expected to be precautionary. The proposed modification has been* ***retained*** *but as discussed in Section 6 the proposed framework includes an element of probabilistic modelling to ensure that the final set of parameter values used for derivation of C4SL is sufficiently precautionary.*

2.5.3.4 Exposure Frequency

The exposure frequency is a key uncertainty highlighted by the sensitivity analysis. The number of days per year that children have appreciable dermal contact with soils in their own garden will be highly variable. In general, in the UK exposure frequency is expected to be higher in summer than winter as a result of more favourable weather conditions, longer days and extended school holidays. Whilst a small proportion of children may spend most days of the year in their garden this is likely to be rare. A child playing in the garden for one or two hours, two or three days per week during summer months and one day or less per week during winter months is more likely to be representative of central tendency behaviour for UK children.

For the residential scenario, the CLEA model assumes that a child will be exposed to garden soil outdoors for 365 days a year. Based on the above rationale it is reasonable to conclude that this assumption will tend towards an over-estimation of exposure in the vast majority of cases. An average exposure frequency of approximately 3.5 days per week (170 days per year) may be a reasonable conservative estimate of central tendency for UK children living in properties with gardens.

> Suggested C4SL CLEA Modification 5: Reduce exposure frequency for dermal contact outdoors for residential land-use from 365 to 170 days per year, to better reflect "central tendency".
>
> *Whilst there was general support for this proposed modification from the steering group, there was mixed support from stakeholders. However, most agreed that the reduction to 170 d* yr^{-1} *was still likely to be a precautionary estimate and therefore this proposed modification has been* ***retained****. As discussed in Section 6 the proposed framework includes an element of probabilistic modelling to ensure that the final set of parameter values used for derivation of C4SL is sufficiently precautionary.*

2.5.3.5 Exposed Skin Area

The fraction of exposed skin area is a key uncertainty highlighted by the sensitivity analysis. The CLEA model assumes that children in both the residential and allotments scenarios have face, hands, lower arms and lower legs exposed whilst outdoors for 365 days per year. This implies that the child wears shoes, long shorts and T-shirt for 365 days per year. The CLEA model also makes the (relatively arbitrary) assumption that one third of the exposed area has adhered soil. This amounts to approximately 9% of total body area, roughly equivalent to the hands and lower arms having contact with soil. Whilst children are likely to get the hands and lower arms dirty with garden soil on occasion, it is unlikely to be a daily occurrence, 365 days per year. Consideration could be given to reducing the maximum fraction of exposed skin, however, this should not be done independently of consideration of the exposure frequency. The current values for exposed skin fraction may not be unreasonable if an exposure frequency of 170 days is assumed.

2.5.3.6 Dermal Absorption Factor

The dermal absorption factor (ABS_d) is a key uncertainty highlighted by the sensitivity analysis. It is the proportion of contaminant mass in the adhered soil that enters the blood stream. It is a contaminant specific property and is a key parameter for contaminants where dermal contact is a key pathway, such as benzo(a)pyrene. The Environment Agency SR3 guidance (EA, 2009c) provides recommended dermal absorption factors for some contaminants/groups of contaminants, which are based on USEPA recommended values. These have generally been derived from experimental studies on animals or humans involving one exposure event over a 24 hour period (US EPA, 2004). The uncertainty in the values used will be considered on a substance by substance basis in work packages 2 and 3.

2.5.4 DUST INHALATION INDOORS

Dust inhalation indoors is a key exposure pathway for chromium (VI) for residential and commercial land-uses. The ADE from dust inhalation is actually relatively small compared to other pathways, but of the six focus contaminants, chromium (VI) has the greatest ratio of the HCV_{oral} to $HCV_{inhation}$, with the latter being three orders of magnitude lower than the former. This large contrast in HCVs for the oral and inhalation pathways results in dust inhalation being a key route of exposure, despite the relatively low ADE.

The CLEA model uses the following equation to assess the exposure from the inhalation of indoor dust.

$$IR_{dust\_inhal\_in} = C_s \cdot \left[\frac{1}{PEF} + TF.DL \right] V_{inh} \frac{T_{site}}{24}$$

Where

$IR_{dust\_inhal\_in}$ = chemical intake rate from inhalation of dust from indoor air (mg d^{-1})
C_s = concentration in soil (mg g^{-1})
TF = soil to dust transport factor according to soil type (g g^{-1})
PEF = particulate emission factor (m^3 kg^{-1})
DL = indoor dust loading factor (g m^{-3})
V_{inh} = daily inhalation rate (m^3 d^{-1})
T_{site} = indoor site occupancy period (hr d^{-1})

In simplified terms, the exposure rate via inhalation of dust indoors is equal to the volume of indoor air inhaled in a day multiplied by the concentration of suspended soil particles less than 10 um in diameter (PM10) multiplied by the concentration of the contaminant in the suspended soil PM10. The terms in the square bracket in

the equation estimate the concentration of soil particles as PM10 in indoor air. The first term (1/PEF) is the estimated PM10 concentration outdoors arising from exposed soil at the property. This outdoor PM10 is assumed to enter the house and be available for indoor inhalation. The second term (TF.DL) is the estimated PM10 concentration indoors arising from re-suspension of soil derived floor dust. It is equal to the assumed indoor PM10 concentration (the dust loading factor, DL) and the fraction of indoor dust that is composed of soil from the property (TF).

There are a number of uncertainties associated with this equation that may have a bearing on the prediction of exposure:

- Firstly, there may be an element of double counting, as the dust loading factor should already account for the outdoor PM10 contribution to indoor PM10. However, as discussed below, the effect of this double counting is negligible, as the predicted outdoor PM10 arising from soils (1/PEF) is minimal relative to the second term (TF.DL);
- Secondly, not all PM10 will be inhaled. The majority of PM10 are deposited in the nose or throat and later ingested rather than inhaled. Indeed it is believed that PM2.5 (i.e. particles less than 2.5 um diameter) are responsible for much of the health effects attributable to PM10 (HPA, 2010). Thus, use of PM10 concentration could over-estimate exposure via inhalation of dust. However, the appropriateness of the PM10 size fraction should also be considered in the context of the critical study that the HCV for inhalation exposure is based on.

2.5.4.1 Soil Concentration

As previously discussed, soil concentration is an output and not an input in the CLEA model when used to derive GAC. When applying GAC it should be recognised that airborne dust is likely to be derived from the finer particles of soil, rather than the coarser fractions. Thus, as with the soil/dust and dermal contact pathways it is the concentration of contaminant in the finer particles that is important when predicting exposure via dust inhalation.

2.5.4.2 Daily Inhalation Rate

Inhalation rate (V_{inh}) is a key uncertainty highlighted by the sensitivity analysis. The inhalation rates used in CLEA are based on mean inhalation rates from Lordo *et al.* (2006) that had previously been recommended by the USEPA (2006). USEPA has since updated its recommendations for inhalation rates (USEPA, 2011) and their most recent recommended mean and 95th percentile values for long-term inhalation are compared to previous recommended mean values in Table 2.2 below. Given that the CLEA values are based on a now outdated USEPA draft report, it may be advisable to use the recommended mean inhalation rates from USEPA (2011) for derivation of C4SLs for residential and commercial land-uses. These are lower for the 0 to 6 year old child, which would result in slightly higher GAC for residential land-use and higher for adults, which would result in slightly lower GAC for commercial land-use.

Table 2.2: Comparison of inhalation rates from USEPA, 2006 and USEPA, 2011

CLEA Age Class	Inhalation rate (m^3 day^{-1})		
	USEPA, 2006	Recommended mean value from USEPA, 2011	Recommended 95th percentile value from USEPA, 2011
1	8.5	5.4	9.2
2	13.3	8.0	12.8
3	12.7	8.9	13.7
4-6	12.2	10.1	13.8
7-11	12.4	12.0	16.6
12-16	13.4	15.2	21.9
17	14.8 [1]	15.7 [1]	21.3 [1]
18	12.0 [2]	13.6 [2]	17.4 [2]

Notes
1. Average value for 16 to <65 year old
2. Average value for 65 to <75 year old

Suggested C4SL CLEA Modification 6: Update vapour inhalation rates to the mean values recommended in USEPA, 2011.

*There was widespread support for this modification from the steering group and stakeholders and therefore this proposed modification has been **retained**. As discussed in Section 6 the proposed framework includes an element of probabilistic modelling to ensure that the final set of parameter values used for derivation of C4SL is sufficiently precautionary.*

2.5.4.3 Time Indoors

For residential land-use CLEA assumes that 0 to <4 year old children spend 23 hours per day in the property and that 5 to < 12 year olds spend 19 hours per day in the property. This is based on the assumptions that 0 to <4 year old children spend all their time at home (with 1 hour per day outdoors) and that primary school age children spend all their time at the property (with 1 hour per day outdoors) whilst not at school. Whilst this may be the case for some children it is likely to be an over-estimate of central tendency, as many children will spend time away from the home, e.g. at the playpark, shopping with parents, at friends and in child care. Nevertheless, whilst the assumed times indoors are likely over-estimates of central tendency, the sensitivity analysis has shown that uncertainty in this parameter does not have a significant bearing on the derived GAC for residential land-use, i.e. use of values more likely to represent central tendency do not result in appreciably higher GAC.

For commercial land-use CLEA assumes that working adults spend an average of 8.3 hours per day indoors on working days. Whilst time indoors will be related to the type of work conducted and length of shift, this value is likely to be a reasonable estimate of central tendency.

2.5.4.4 Dust Loading Factor

The Dust Loading (DL) factor is a key uncertainty highlighted by the sensitivity analyses. It is effectively the assumed concentration of PM10 concentration indoors. The CLEA assumed values of 50 $\mu g\ m^{-3}$ for residential land-use & 100 $\mu g\ m^{-3}$ for commercial land-use are based on indoor PM10 estimates presented by Oatway & Mobbs (2003), Oomen & Lijzen (2004) and Simmonds *et al.* (1995).

PM10 indoors is related to physical activity in the house with increased activity generally leading to increased PM10. Figure 2.8 shows monitored dust concentrations in a terraced residential property in Bristol. The concentrations of PM10 are lowest during the night when the occupants are in bed and portions of the day when the house is vacated. Note that for this monitoring event, the concentration of PM2.5 indoors was, on average, 40% of the PM10 concentration. As discussed in Section 2.5.4, depending on the basis of the inhalation HCV, consideration could be given to the use of the concentration of PM2.5 to predict inhalation exposure. Values of 25 $\mu g\ m^{-3}$ and 50 $\mu g\ m^{-3}$ may be reasonable estimates of indoor PM2.5 concentrations for residential and commercial land-uses, respectively based on available data.

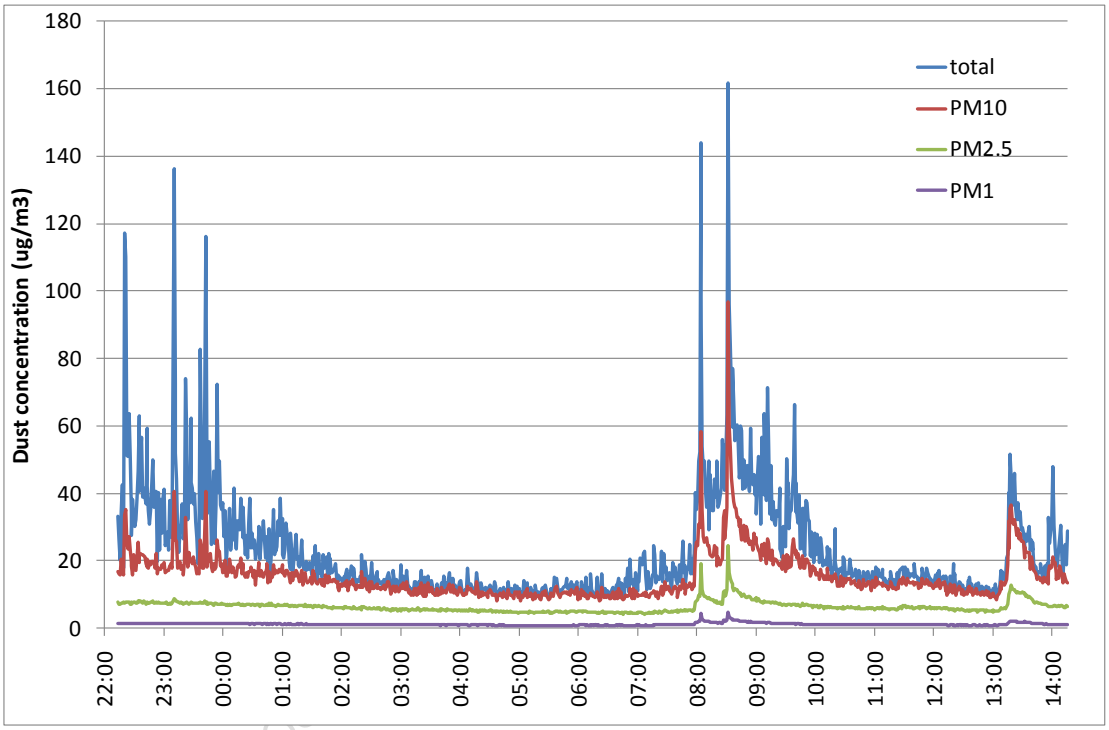


Figure 2.8: Monitored dust concentrations in terraced residential property in Bristol (Firth Consultants, 2010).

Suggested C4SL CLEA Modification 7: Depending on the basis of the HCV_{inhal} consider reducing indoor dust loading factors to 50 and 25 ug m^{-3} for residential and commercial land-uses, respectively, to better reflect likely concentration of respirable (PM2.5) particles.

There was mixed support for this modification from the steering group and stakeholders. Whilst there is increasing recognition that the majority of health effects are associated with PM2.5 there was concern that the toxicological data were unlikely to relate to PM2.5, and thus this proposal has been ***rejected.*** *The more precautionary approach of using estimated indoor air concentrations of PM10 for estimating exposure has been retained.*

2.5.4.5 Transport Factor

The transport factor (TF) is a key uncertainty highlighted by the sensitivity analyses. It is the fraction of indoor PM10 derived from soil. In practice, estimates of the mass fraction of soil in indoor dust (i.e. not just PM10) are generally used as a surrogate for this parameter. Various studies have attempted to correlate indoor dust concentration with soil concentration (see for example, USEPA 1998; Trowbridge & Burmaster, 1997; Oomen & Lijzen, 2004). The mass fraction of soil in indoor dust can be highly variable between houses, dependent on factors such as the number of children and pets that may track in soil, environmental factors such as climate, the extent of vegetative cover in gardens and the deposition of soils transported from neighbouring properties (USEPA, 1998). Estimates of average mass fraction have typically ranged from 0.3 and 0.7 and the midpoint of 0.5 has been assumed as a default in the CLEA model. Based on the available data this is considered a reasonable estimate of central tendency.

2.5.4.6 Exposure Frequency

For residential land-use CLEA assumes that children are at home 365 day a year, which is a worst case assumption. Central tendency for the UK population is more likely to be between 350 and 365 days per year, but as shown by the sensitivity analysis, use of these values results has negligible effect on the GAC.

CLEA assumes an exposure frequency of 230 days per year for commercial land-use. As discussed in Section 2.5.2.4, this is likely to be a reasonable estimate of central tendency for the UK workforce.

2.5.5 CONSUMPTION OF HOMEGROWN PRODUCE

The consumption of homegrown produce is a key exposure pathway for all six focus contaminants for allotments land-use. Its contribution to overall exposure is less significant for residential land-use, with greatest significance for benzene, cadmium and lead.

CLEA models exposure from consumption of homegrown produce via two pathways: 1) ingestion of soil attached to produce; and 2) uptake of contaminants into produce which are then consumed. The sensitivity analysis has shown that the greatest uncertainty arises from the latter and therefore this section focuses on that pathway.

The exposure from uptake of contaminants into homegrown produce that is consumed is calculated using the following equation:

$$IR_{plant\_uptake} = \sum_{all\_produce\_groups} C_s.CF_x CR_x.BW.HF_x$$

Where

IR_{plant_uptake} = chemical intake rate from uptake of contaminants into homegrown produce that is then consumed (mg d^{-1})
C_s = concentration in soil (mg g^{-1})
CF_x = soil to plant concentration factor for each produce group (mg g^{-1} fw per mg g^{-1} dw)
CR_x = food consumption rate per unit body weight for each produce group (g fw kg^{-1} bw d^{-1})
BW = body weight (kg)
HF_x = homegrown fraction for each produce group (dimensionless)

This equation uses simple mass balance to calculate the average mass of contaminant ingested each day for a range of produce types. The exposure rate for each produce type is equal to the estimated concentration of contaminant in the

produce, multiplied by the average amount of homegrown produce consumed in a day. One source of uncertainty with this equation relates to the assumption that there is a linear relationship between the concentrations of contaminant in soil and within the plant. This may not be the case, especially where solubility limits are exceeded in soil, which will tend to limit the transfer of contaminants to the plant via passive uptake, which is a more likely pathway for organic contaminants.

However, the majority of uncertainty associated with estimation of exposure for this pathway likely relates to the parameter values and is discussed further below.

2.5.5.1 Soil Concentration

As previously discussed, when deriving GAC, soil concentration is solved iteratively and is therefore an output and not an input in the CLEA model. In CLEA, the soil concentration is multiplied by the soil to plant concentration factor to estimate the concentration of contaminant in the portion of the plant that is consumed. As discussed further below, the concentration factor is either estimated from empirical data relating plant concentration to soil concentration or via uptake algorithms which attempt to model the partitioning between contaminants sorbed to soil, in soil pore water and within various parts of the plant. Either way, unlike the other pathways described above, the total concentration of contaminant in soil (as opposed to the concentration in the finer particles) is likely to be more appropriate for estimating exposure from this pathway.

2.5.5.2 Soil to Plant Concentration Factor

The value of the soil to plant concentration factor is a key uncertainty highlighted by the sensitivity analyses. It is the ratio of the concentration of contaminant in the portion of plant consumed to the concentration of contaminant in soil in contact with the plant. CLEA allows contaminant specific soil to plant concentration factors to be set for each plant-type. These can be either empirical based estimates entered directly by the user (e.g. from studies where soil and plant concentrations have been correlated) or modelled using a series of plant uptake algorithms within CLEA. Irrespective of which method is used, there will generally be a high degree of uncertainty associated with the estimates, for the following reasons:

- There is generally a high degree of variability in the contaminant specific soil to plant concentration factors reported in the literature. This is likely due to a variety of factors such as variability in soil characteristics (such as clay content, pH and organic matter content), differences in plant uptake between species and differences in experimental design;
- In addition, for organic contaminants, experimentally derived soil to plant concentration factors are often based on the uptake of radio-labelled carbon (rather than speciated analysis of organics within the plant material). This method ignores metabolic degradation of the contaminant within the plant and can therefore over-estimate uptake;
- Equations used to predict soil to plant concentration factors generally have a poor predictive capacity, i.e. there is often a large discrepancy between modelled and empirically based estimates;
- In particular, the equations used by CLEA for predicting uptake for inorganic contaminants are heavily reliant on the value of the soil to water partition coefficient for the contaminant. This parameter can be highly variable depending on soil type and mineralisation. Literature values typically range over several orders of magnitude.

Despite the high variability in empirical estimates, where available, these are generally preferred to modelled estimates.

The Environment Agency SGV addendum reports for arsenic and cadmium summarise available literature values of contaminant specific soil to plant concentration factors for each plant type (EA, 2009 d & e). These typically range

across two or three orders of magnitude. A lognormal distribution in values is considered a reasonable assumption and on this basis the Environment Agency has used geomean values as an estimate of central tendency for derivation of the SGVs for these contaminants.

The Environment Agency considered there to be insufficient empirical data reported in the literature to derive empirical soil to plant concentration factors for benzene (EA, 2009f). The SGVs for benzene are therefore based on modelled estimates of the soil to plant concentration factors. As discussed above, there is a large degree of uncertainty associated with these modelled estimates. In particular, the equations used have largely been derived from empirical correlations based on studies of plant uptake of pesticides and to a lesser extent, polycyclic aromatic hydrocarbons and their use for different classes of compound has not been validated. Soil organic matter is a key input in these equations and as illustrated by the sensitivity analyses this parameter can have a large influence on exposure estimates.

There are a number of further uncertainties that should also be considered when applying the estimated soil to plant concentration factors for predicting exposure concentrations in produce consumed:

- A key assumption in the use of these factors is that there is a linear relationship between soil concentration and plant uptake. However, for some contaminants aqueous solubility will limit plant uptake at relatively low concentrations. For example, the CLEA model predicts that the soil pore water concentration will become fully saturated with benzo(a)pyrene at a soil concentration of 2.8 mg kg^{-1} in a sandy loam soil containing 1% soil organic matter. In theory, plant uptake is unlikely to increase appreciably above this soil concentration;
- Another key assumption is that the predicted concentrations in raw produce are representative of the concentrations in ingested produce. Direct partitioning from soil pore water to skin can be the key uptake mechanism for root and tuber vegetables such as carrots and potatoes. For these vegetables, whether or not the skin is peeled or ingested can have a significant bearing on exposure. Cooking may also reduce contaminant concentrations, with contaminants being volatilised or leached into cooking water that is later discarded.

Overall, it is concluded that the soil to plant concentration factors used to derive SGVs are based on best estimates of central tendency where experimental data are available[6], but that there is a high degree of uncertainty in these estimates and there is a potentially greater uncertainty associated with the algorithms used to predict uptake of organic chemicals.

2.5.5.3 Consumption Rates

Produce type Consumption Rate (CR) is another key uncertainty identified in the sensitivity analyses. Consumption rate is the average amount of each produce type consumed daily. The consumption rates used in CLEA are the 90th percentile estimates for those who consume each produce type derived from UK surveys conducted in 1992, 1997 and 2000 (EA, 2009c). Consideration could be given to use of central tendency estimates for consumption rate.

[6] Where direct measurements of plant uptake are available the geometric mean is calculated from a review of the experimental data

Suggested C4SL CLEA Modification 8: Consider the use of central tendency estimates of fruit and vegetable ingestion rates rather than 90th percentiles.

There was some support for this modification from the steering group but there was a mixed response from stakeholders due to concerns that central tendency values would not be sufficiently protective of the increasing proportion of people growing their own fruit and vegetables. This modification has been ***retained*** *on the basis that it would be unlikely for any individual to have 90th percentile consumption rates across all types of fruits and vegetables. Further work will be undertaken to incorporate the most recent data from food survey studies and use central tendency values for consumption rates of all, or the vast majority, of fruit and vegetables.*

2.5.5.4 Homegrown Fraction

The Homegrown Fraction (HF) is the fraction of consumed produce that is grown in the home or allotment and is another key uncertainty identified by the sensitivity analyses. The homegrown fractions used in CLEA are based on results from a 2004/5 Expenditure and Food Survey where 6798 households provided data on the amount of fruit and vegetables purchased and obtained for free, with the latter presumed to include homegrown produce (EA, 2009c). The survey is conducted over a one year period with each household keeping a diary of food purchased/obtained over a two week period (Defra, 2010b) This survey indicated that 85% of people did not obtain food for free during their two week food diary and thus were assumed not to consume homegrown produce in that time. The remaining 15% did obtain varying proportions of food for free and thus potentially did consume homegrown produce (albeit not necessarily grown in their own garden or allotment). It is possible that the percentage of people consuming homegrown produce has been under-estimated as some people who occasionally eat homegrown produce may not have done so on the particular fortnight in which they kept their food diary.

The average proportion of free produce obtained across all respondents was 2 to 9%, depending on produce type and these percentages have been used in CLEA for residential land-use. However, it is doubtful whether these “average” values are truly representative of residents. For the 85% of residents who don’t grow produce, these average values are over-estimates of the amount of homegrown produce they consume. Of the 15% of residents who do grown produce, some of these will presumably be allotment holders who grow a relatively large proportion of the produce they consume and some will grow a relatively modest amount of produce in their own gardens. It is interesting to note that the most recent Defra survey from 2009 (Defra, 2011a) indicates that, on average, about 3% of fruit and vegetables entering the household in 2009 came from free sources, considered to be mainly gardens and allotments. This survey concluded that the fraction of home-grown produce had remained the same over the last four yearly surveys (i.e. since 2006).

The default homegrown fractions used in CLEA for residential land-use equate to an estimated yearly yield of 43 kg of produce grown in the garden for a family of two adults and two children (EA, 2009c). Theoretically, this yield could be produced from a 4 x 5 m vegetable plot (EA, 2009c). Whilst some gardeners in the UK no doubt fulfil this yield, it is probable that the homegrown fractions assumed in CLEA for residential land-use are over-estimates for the vast majority of residential properties where soil contamination is a potential concern. Consideration could be given to reducing the homegrown fractions used for deriving C4SLs, but this may be un-protective of a relatively small subgroup of the population.

The average homegrown fractions assumed for allotments land-use are judged not to be unreasonable estimates of central tendency for allotment holders.

> Suggested C4SL CLEA Modification 9: Consider reducing the fraction of homegrown produce for residential land-use to better reflect likely central tendency behaviour for residents with gardens.
>
> *This proposal received only limited support from the steering committee and was rejected by a majority of stakeholders and has been **rejected** on the basis that any reduction in the homegrown fraction would not be sufficiently protective of the increasing proportion of people growing their own fruit and vegetables.*
>
> *Use of central tendency values for consumption rates in conjunction with precautionary values for homegrown fraction is considered to appropriately represent a reasonable worst case scenario.*

2.5.5.5 Body Weight

Body Weight (BW) is a parameter used in the consumption of homegrown produce algorithm. However, when combined with the general equation for predicting ADE, body weight appears on both the top and bottom of the equation for this pathway and thus is effectively cancelled out. Thus body weight is not a key parameter in the prediction of ADE from consumption of homegrown produce.

2.5.5.6 Exposure Frequency

Exposure frequency (EF) is assumed to be 365 days per year for the consumption of homegrown produce with the exception of the 0 to 1 year old, where a value of 180 days is assumed. Whilst it is unlikely that homegrown produce will actually be consumed every day of the year in most cases, it is important to recognise that the consumption rates assumed for this pathway are based on estimated average annual consumption and thus an exposure frequency of 365 days per year is appropriate in this instance.

2.5.6 VAPOUR INHALATION INDOORS

The inhalation of vapours that have intruded through the foundation into buildings is a key exposure pathway for benzene for residential and commercial land-uses. The CLEA model uses the following equation to assess exposure from the inhalation of contaminant vapour indoors:

$$IR_{vap\_indoor} = C_{indoor\_air} . V_{inh} . \left(\frac{T_{site}}{24} \right)$$

Where

$IR_{vap\ indoor}$ = chemical intake rate from inhalation of vapour from indoor air (mg d^{-1})
$C_{indoor\ air}$ = contaminant conc. in indoor (mg m^{-3})
V_{inh} = daily inhalation rate (m^3 d^{-1})
T_{site} = occupancy period (hr d^{-1})

This equation is considered robust, although more recent inhalation rate (V_{inh}) parameter values than those used in CLEA v1.06 are available from USEPA (2011; see Section 2.5.4.2 and Table 2.2).

2.5.6.1 Modelling of indoor air concentration

Calculation of the contaminant concentration in indoor air is complex and involves multiple steps, starting with the estimation of a soil gas concentration based on simplified equilibrium partitioning, as follows:

$$C_{vap} = \frac{K_{aw}.C_s}{K_{sw}}$$

Where:

C_{vap} = soil gas concentration (mg m^{-3})
C_s = total concentration of contaminant in soil (mg kg^{-1})
K_{aw} = air-water partition coefficient at ambient temperature (cm^3 cm^{-3})
K_{sw} = total soil-water partition coefficient (cm^3 g^{-1})

Calculation of the indoor air concentration is then achieved by the application of an attenuation factor (α) to the soil gas concentration, as follows:

$$C_{indoor\_air} = \alpha.C_{vap}$$

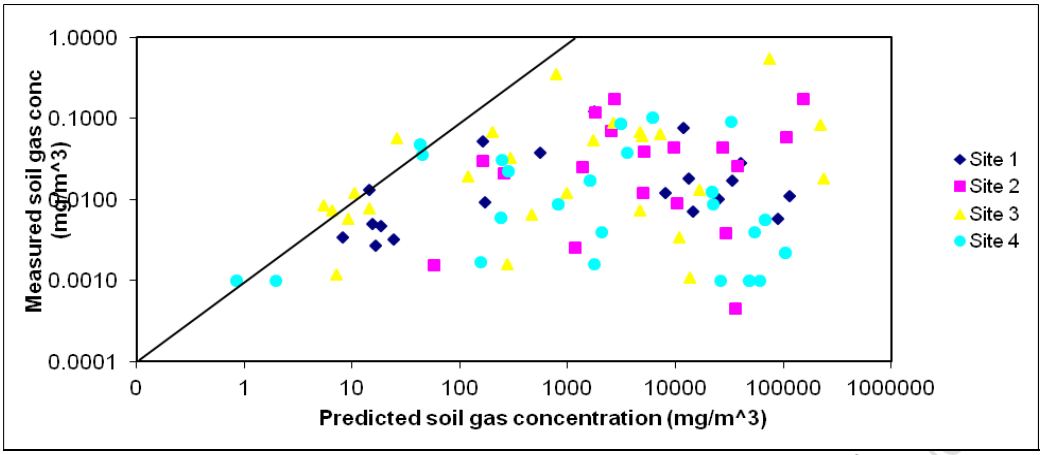
2.5.6.2 Equilibrium partitioning to estimate soil gas concentrations

Hartman (2002) states that the equilibrium partitioning assumption is the major source of over-estimation when using the Johnson-Ettinger model and the CLEA Report (EA, 2009c) acknowledges that the solid, aqueous and vapour phases are unlikely to achieve equilibrium in an open soil system. The CIRIA VOC Handbook (CIRIA, 2009) attributes over-prediction of soil gas concentrations to the use of Henry's Law constant[7] and a failure to take account of the influence of biodegradation on relatively biodegradable compounds such as the BTEX[8] and other low-medium molecular weight hydrocarbons.

Figure 2.9 (taken from CIRIA, 2009) plots measured soil gas concentration of a range of volatile and semi-volatile petroleum hydrocarbons against the predicted soil gas concentration estimated using equilibrium partitioning. This demonstrates that calculation of soil vapour based on equilibrium partitioning from measured contaminant concentrations in soil and groundwater results tends to produce overestimates of several orders of magnitude (the solid line plotted on the graph indicates a thousand-fold over-estimation of soil gas concentrations).

[7] Henry's Law constants for medium-low volatility compounds are commonly estimated based on vapour pressure and aqueous solubility; the very low solubility of these compounds leads to high estimated value for H^c which is not observed in reality.

[8] Benzene, toluene, ethylbenzene and xylenes.



Ref. CIRIA, 2009

Figure 2.9: Comparison of measured and predicted gas concentrations

2.5.6.3 Estimation of the soil to indoor air attenuation factor

In CLEA, the attenuation factor (α) is calculated using the Johnson and Ettinger model (Johnson and Ettinger, 1991), as shown below:

$$\alpha = \frac{\left[\left(\frac{D_{eff}.A_B}{Q_b.L_T}\right)\exp\left(\frac{Q_s.L_{crack}}{D_{crack}.A_{crack}}\right)\right]}{\left[\exp\left(\frac{Q_s L_{crack}}{D_{crack}.A_{crack}}\right)+\left(\frac{D_{eff}.A_B}{Q_b.L_T}\right)+\left(\frac{D_{eff}.A_B}{Q_s.L_T}\right)\left[\exp\left(\frac{Q_s L_{crack}}{D_{crack}.A_{crack}}\right)-1\right]\right]}$$

Where,

α = steady-state attenuation coefficient between soil and indoor air (dimensionless)
D_{eff} = effective diffusion coefficient for unsaturated soils ($cm^2\ s^{-1}$)
A_B = area of enclosed floor and walls below ground (cm^2)
Q_b = building ventilation rate ($cm^3\ s^{-1}$)
L_T = source-building separation (cm)
Q_s = volumetric flow rate of soil gas into the enclosed space ($cm^3\ s^{-1}$)
L_{crack} = foundation slab thickness (cm)
A_{crack} = floor crack area (cm^2)
D_{crack} = effective diffusion coefficient through the cracks (assumed equal to D_{eff} in CLEA) ($cm^2\ s^{-1}$)

This equation is based on the integration of equations that attempt to model three processes:

1. The upwards flux of contaminants from the soil source zone into the advective zone beneath the building foundation;
2. The advective flow of atmospheric air into the soil surrounding the building, beneath the foundations and into the building via cracks in the foundations/floor. This flow occurs due to reduced air pressure in the building relative to outdoors as a result of stack and wind effects; and
3. Dilution within the building caused by air flow through windows, doors, ventilation vents etc.

Although the Johnson and Ettinger model is widely used, it is acknowledged to over-predict indoor vapour concentrations in some circumstances and for certain contaminants such as petroleum hydrocarbons (Wilson 2008; EA, 2009c). It has

also been demonstrated to sometimes under-predict indoor vapour levels, including those of chlorinated solvents (EA, 2009c).
The Johnson and Ettinger model is based on the assumption that the building has a solid slab foundation or basement-type structure. While this type of housing is common in the USA, many UK houses have a suspended floor over a void meaning that the bottom of the floor slab may be at or above the external ground level. In this circumstance the Johnson and Ettinger model is likely to significantly overestimate vapour ingress to the building (EA, 2009c; Wilson, 2008).

CLEA assumes a contaminant source that is less than one metre beneath the surface (i.e. 0.5m below the bottom of the floor). This is relatively shallow and it therefore assumes only a limited potential for biodegradation to occur as vapour migrates towards a building. An indoor air correction factor is currently applied in CLEA to petroleum hydrocarbons, to take account of some of the acknowledged over-prediction for this class of compounds when using equilibrium partitioning and the Johnson and Ettinger model (see SGV reports for BTEX compounds; e.g. EA, 2009f). This could be increased on a substance or site-specific basis where this is evidence that a compound is highly biodegradable or that the use of equilibrium partitioning significantly over-estimates vapour phases concentrations in soil.

Although the Johnson and Ettinger model has a number of acknowledged deficiencies and leads to overestimates for certain types of housing construction and for certain classes of contaminants (specifically petroleum hydrocarbons), it is considered appropriate as a screening tool that will give protective estimates of the potential indoor air concentrations of volatile contaminants across all types of housing. However, the Johnson and Ettinger model is unlikely to be suitable for the assessment of vapour risk for UK new build housing and alternative approaches such as that proposed by Wilson (2008) may be more suitable in this instance.

It is considered that alternative approaches to the assessment of the vapour inhalation pathway should be incorporated at the level of site-specific assessment, rather than for the development of C4SLs. On actual sites, the verification of any risk posed by volatile contaminants can be achieved by direct gas or vapour measurement either in the ground or in buildings and recent guidance has been published detailing how this can undertaken when assessing the vapour risk from contaminated land (CIRIA, 2009).

2.5.7 SUMMARY

Pathway and sensitivity analyses have been used to identify key pathways and parameters that lead to uncertainty in the exposure modelling performed by CLEA. The equations and associated assumptions and parameter values for these key pathways and parameters have been critically reviewed to qualitatively assess the level of precaution they represent and, where appropriate, to make suggestions regarding modifications which could be made to CLEA to enable the development of C4SLs. The key findings for each pathway are summarised below:

Soil and Dust Ingestion

- Soil and dust ingestion is a key exposure pathway for one or more contaminants for all three generic land-uses. Key parameters are soil and dust ingestion rate, exposure frequency and relative bioavailability.
- There is a relatively high level of uncertainty associated with the input parameters for this pathway due to limited data. Nevertheless, from the available data it is reasonable to conclude that the combination of the soil and dust ingestion rates and exposure frequencies used for residential and commercial land-uses are more likely to over-estimate than under-estimate exposure for a random, typical individual living/working on the property[9].

[9] High levels of soil ingestion resulting from pica behaviour or geophagia (considered psychopathological conditions) are not considered in our proposed approach or the CLEA framework on which it is based and should be assessed on an individual basis, where relevant.

Consideration could be given to use of reduced soil ingestion rates based on weighted indoor and outdoor exposure to more accurately reflect central tendency for residential and commercial land-uses. However, this proposed modification has not been retained.

- The assumption of a RBA of 100% is likely to be conservative for some contaminants (e.g. arsenic, lead and benzo(a)pyrene) for the majority of sites investigated in the UK. However, bioavailability is often highly dependent on the characteristics of the soil and speciation of the contaminant and thus can be highly variable between sites. Thus, in most cases consideration of bioavailability will be more appropriate on a site by site basis rather than within the derivation of generic screening levels. Nevertheless, consideration could be given to reducing the RBA below 100% for derivation of C4SLs for contaminants where there is strong evidence that the bioavailability of the soil bound contamination is significantly lower than that associated with the critical toxicological studies.

Dermal Contact Outdoors

- Dermal contact outdoors is a key exposure pathway for benzo(a)pyrene and arsenic for the residential land-use. Key parameters are the soil to skin adherence factor, the area of skin with adhered soil, the dermal absorption factor and exposure frequency.
- Upper percentile values are currently used in CLEA for each of these parameters and the combined effect likely results in an over-estimation of exposure in the vast majority of cases. The uncertainty in the input parameters is high due to limited data, but not appreciably greater than the soil and dust ingestion pathway. Consideration could therefore be given to use of values closer to central tendency, consistent with the approach used for the soil and dust ingestion pathway.

Dust Inhalation Indoors

- Dust inhalation indoors results in a relatively low contribution to overall ADE but can be a key exposure pathway for the residential and commercial land-uses for contaminants with a HCV for inhalation orders of magnitude lower than the HCV for oral exposure such as hexavalent chromium. Key parameters are the concentration of airborne respirable dust particles indoors (the dust loading factor), the proportion of airborne indoor dust derived from soil at the property (the transport factor), time spent indoors and the respiration rate indoors.
- Best estimates of central tendency values have been used for these parameters, but consideration could be given to updating the respiration rates to more recent values recommended by the USEPA.

Consumption of Homegrown Produce

- The uptake of contaminants into the edible portions of fruit and vegetables followed by their consumption is a key pathway for five of the six focus contaminants for allotments land-use and for benzene and cadmium for residential land-use. Key parameters are the soil to plant concentration factor, consumption rates of fruit and vegetables and the fractions of these that are for homegrown produce.
- In general, the values for the soil to plant concentration factors used for derivation of published SGVs can be regarded as best estimates of central tendency, but it should be recognised that there is a high degree of uncertainty associated with these estimates.
- The consumption rates are based on the 90th percentile estimates for consumers of each fruit and vegetable type from various UK surveys. Consideration could be given to use of central tendency estimates for the purposes of derivation of C4SLs.

- The homegrown fractions likely represent upper percentiles for the UK population. However, whilst the values likely over-estimate homegrown fraction for the vast majority of the UK population, they are not unreasonable estimates of central tendency for the sub-group of the population who are keen fruit and vegetable growers.

Vapour Inhalation Indoors

- Calculation of the contaminant concentration in indoor air is complex and involves multiple steps, including the estimation of a soil gas concentration, based on simplified equilibrium partitioning, and an attenuation factor, based on the Johnson and Ettinger model.
- Although the Johnson and Ettinger model has a number of acknowledged deficiencies, which can lead to considerable overestimates of indoor air concentrations, it is considered appropriate as a screening tool that will give protective estimates of the potential indoor air concentrations of volatile contaminants in all types of housing.

3. TOXICOLOGICAL ASSESSMENT

The toxicological assessment of contaminants is a key part of land contamination risk assessment. Such assessments are typically complex evaluations involving a significant amount of data to be evaluated, with different types of toxicity, endpoints and study designs needing to be considered. As a consequence, toxicological assessments and reviews should only be performed by suitably qualified individuals who understand the nature of the raw toxicological data.

This section outlines the process of toxicological assessment for the purposes of land contamination risk assessment. It begins with a summary of the requirements of such assessments under Part 2A (in terms of the toxicological effects that are potentially relevant) and continues with a review of existing guidance to derive Health Criteria Values (HCVs) under the CLEA framework that represent minimal risk (namely that outlined in SR2). It concludes with suggestions on how this framework could be adapted for the purpose of the development of C4SLs, presenting decisions on how default minimal risk values could be refined with further chemical-specific knowledge to generate a new guidance value that can still be regarded as sufficiently low as to meet the requirements of the C4SLs. In relation to the latter, it is suggested that a new term is defined – a Low Level of Toxicological Concern (LLTC) – which would correspond to a pragmatic intake level that remains sufficiently protective of health but represents a level of risk slightly above minimal.

3.1 SIGNIFICANT HARM

Toxicological studies can be used to investigate a wide range of endpoints. When selecting critical endpoints on which to base toxicological risk assessment for land contamination, it is important to consider whether such endpoints are relevant to assessing significant harm under Part 2A. The new Part 2A statutory guidance (April 2012) describes what types of harm to human health should be considered "significant" in relation to land contamination, as summarised in Table 3.1 below.

Table 3.1 Part 2A Statutory Guidance Definition of Harm to Human Health

	Part 2A Environmental Protection Act 1990 Old Statutory Guidance 2006	Part 2A Environmental Protection Act 1990 New Statutory Guidance 2012
Always considered as significant harm	Significant harm or significant possibility of significant harm	Significant harm or significant possibility of significant harm
	Death	Death
	Disease taken to mean an unhealthy condition of the body or a part of it and can include, for example, cancer, liver dysfunction or extensive skin ailments. Mental dysfunction is included only insofar as it is attributable to the effects of a pollutant on the body of the person concerned.	Life threatening diseases (cancers)
	Serious injury	Serious injury caused by the chemical or biochemical properties of the substance, such as injury resulting from explosive or asphyxiating properties of gases.
	Birth defects	Birth defects
	Impairment of reproductive functions	Impairment of reproductive functions
	Genetic mutation	
		Other diseases likely to have serious impacts on health
May or may not constitute significant harm		Physical injury
		Gastrointestinal disturbances
		Respiratory tract effects
		Cardiovascular effects
		Central nervous system effects
		Skin ailments
		Effects on organs such as kidney or liver
		Wide range of other health impacts

3.2 EXISTING GUIDANCE ON DERIVING HEALTH-BASED GUIDANCE VALUES

This section describes the current guidance on deriving Health-Based Guidance Values (HBGV) that are defined as the estimated dose in humans that is without appreciable risk over a lifetime. Examples of HBGVs include a tolerable daily intake (TDI) used for environmental contaminants or an acceptable daily intake (ADI) used for additives or residues in food.

Similarly, the term HCVs has been used to describe the level of long-term human exposure to chemicals *in soil* that are tolerable or pose a minimal risk to health. It is an umbrella term that encompasses a TDI for threshold compounds and index dose (ID) for non-thresholded chemicals. HCVs represent a baseline and health protective position to minimise risks of significant harm for all people exposed (including children); *they do not represent thresholds above which an intake would be unacceptable* (EA, 2009b).

The methods used to derive HBGVs differ depending on, amongst other things, whether or not a given chemical exhibits a threshold for its critical toxicological effects. The remainder of this section describes the derivation of HBGVs for both threshold and non-threshold chemicals and identifies areas of high uncertainty and where conservative assumptions are made.

3.2.1 SELECTION OF THE PIVOTAL STUDY AND IDENTIFICATION OF CRITICAL ENDPOINT

The first step in the derivation of a HBGV is the selection of the pivotal study and identification of the critical endpoint from an array of toxicity studies. This is done by reviewing all available toxicology data and identifying suitable Points of Departure (PODs) in the form of No Observed Adverse Effect Levels (NOAELs), Lowest Observed Adverse Effect Levels (LOAELs) and BenchMark Doses (BMDs). The NOAEL is the highest dose at which no adverse effects are seen in the toxicity

study. If a NOAEL cannot be determined from the data, due to effects being seen at even the lowest dose tested, a LOAEL is determined i.e. the lowest dose at which some adverse effects are seen. A NOAEL (or LOAEL) is determined for all good quality studies and for all endpoints, and the study with the lowest (most sensitive) value is considered the pivotal study for the most sensitive effect. If there is more than one good study for the most sensitive effect, the highest NOAEL (or lowest LOAEL) is selected. This NOAEL represents the most sensitive endpoint of toxicity. This can be used as a POD to form the basis of the HBGV derivation.

It should be noted that the magnitude of a NOAEL or LOAEL is highly dependent on the dosage regime used and endpoints measured in the original toxicity study. As a consequence, the true "no effect level" could conceivably be higher or lower than the experimental NOAEL, depending on the sensitivity of the study and the choice of endpoint. Similarly, the true "lowest effect level" could be lower than the experimental LOAEL. This makes a NOAEL a highly uncertain value in some studies.

As an alternative approach to qualifying hazard, a BMD may be derived. This is the dose that produces a predetermined change in response, or Bench Mark Response (BMR), for a given toxicological effect. For risk assessment purposes, the 95% lower confidence limit of the BMD (BMDL) is often used as the POD.

The concept of the benchmark dose is illustrated below in Figure 3.1.

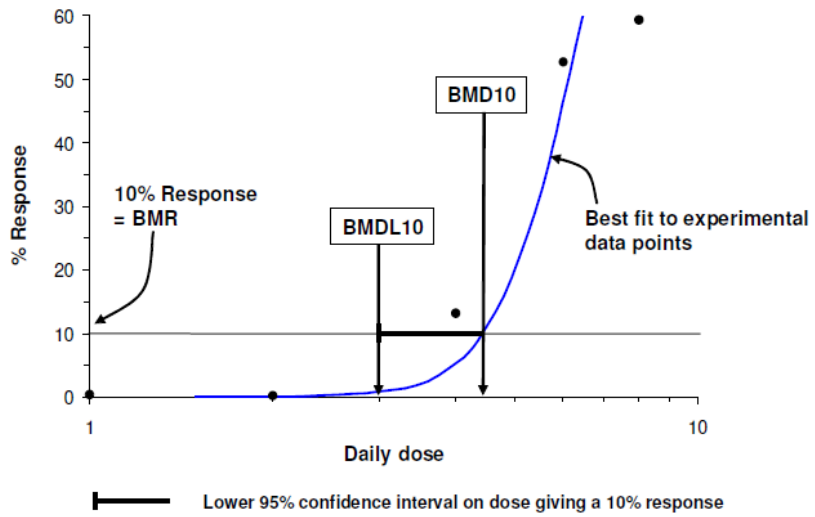


Figure 3.1: Hypothetical dose-response curve to illustrate the concepts of BMR, BMD and BMDL, for a 10% incidence response above control (taken from EFSA 2005).

The use of the BMD is beneficial as it is based on all available data of the dose response, and is on the scale of observable effects, rather than being based on one uncertain data point e.g. a NOAEL (EFSA, 2005, 2009a). However, there may be some endpoints not amenable for BMD modeling (e.g. in a study where no response is seen at any dose) for which a NOAEL approach should still be used (USEPA, 2012).

BMD modelling is being used more widely for dose-response modelling (USEPA, 1995 & 1996). In the EU, EFSA (2005) recommended the use of BMD modelling for genotoxic carcinogens, as well as other toxicity endpoints, as the modelling of choice in order to derive a quantitative POD. A quote from EFSA (2005) indicates the main scientific rationale as to why a BMD is considered a better choice than a NOAEL for quantitative risk assessment, as follows:

> *"…..the Scientific Committee concludes that the BMD approach is a scientifically more advanced method to the NOAEL …..it makes extended*

use of available dose-response data and it provides a quantification of the uncertainties in the dose-response data."

The UK COC also advise using the BMD approach for the interpretation of dose-carcinogenicity response data (COC, 2012). The BMD refers to central estimates for continuous and dichotomous endpoints, based on a predefined level of response above background (the BMR). For dichotomous endpoints (e.g. incidence data such as carcinogenic endpoints, an incidence of 10% is commonly used largely due to the 10% response being at or near the limit of sensitivity in most cancer bioassays (Benford *et al*., 2010). A default BMR of 5% is recommended by EFSA for continuous data (EFSA, 2009) A lower BMR for either dichotomous or quantal data could be used if the study has greater sensitivity or is considered biologically relevant (eg., for lead, a BMR of 1% has been selected by EFSA, 2010). It is also possible to calculate a value that represents a higher incidence rate of effect than 10%. Therefore, a quantitative selection for the incidence rate that represents minimal risk is a scientific judgement based on the data.

To date, toxicology data for only a few land contaminants have been interpreted using BMD modeling, and this approach has not formed the basis of any published HCVs (although the HPA's Contaminated Land Information Sheet publication on benzo[a]pyrene/PAHs does use this approach). Its wider adoption could reduce some of the uncertainty inherent within risk assessments which utilise NOAEL or LOAEL-based HCVs (or their equivalents). Having better defined information about the nature of the dose response curve, rather than just providing a single screening number, it may also help in the future to inform the further substance specific discussions around where the C4SL sits in relation to the category 1,2,3 and 4 boundaries described in the revised statutory guidance.

Suggested C4SL CLEA Modification 10: Use BMD modelling rather than NOAELs and LOAELS to derive toxicological criteria, where possible.

The use of Benchmark Dose Modelling approaches for interpreting toxicology study data, as the best scientific approach, received widespread support from the steering group and stakeholders. Therefore this modification will be ***retained*** *and used where data allows.*

3.2.2 DEALING WITH UNCERTAINTY

In order to derive a HBGV for a given substance, the selected POD is divided by a measure of uncertainty to derive an estimated intake for humans that is judged to be protective of public health. The Uncertainty Factors (UFs) or margin (i.e. the difference between the POD and exposure intake) selected will depend on the quality and type of toxicity study, the species used in the study and the critical endpoint. The incorporated uncertainty aims to account for potential differences in the human response to the chemical compared to the species used in the toxicity study, and also variability in human responses due to age, genetic factors and health status.

Threshold chemicals

For all thresholded chemicals, an UF approach is recommended (COT, 2007). For thresholded carcinogens, the COC (2012) guidance advocates the use of an UF approach. This has not changed from the COC guidance of 2004 on which SR2 is based. The choice of UFs used for non-genotoxic carcinogens depends on the quality of the animal data and the uncertainties in the evaluation of the toxicological data (COT, 2007; COC, 2012).

When basing a HBGV on a NOAEL from a chronic animal study, a default UF of 100 is typically used, consisting of a factor of 10 for interspecies variability (4 for toxicokinetics and 2.5 for toxicodynamics[10]) and 10 to account for intraspecies differences (3.2 for toxicokinetics and 3.2 for toxicodynamics) (EFSA, 2012a). Put another way, the first factor of 10 is assumed to move the dose response curve in the test species to an exposure value for the average human (taking account of the fact that the true no effect level in average humans could actually be 10-fold less than the animal NOAEL, given toxicokinetic and toxicodynamic differences); and the second factor of 10 is assumed to move an exposure value in the average human to a value that will cover the whole population, including sensitive sub-groups (Walton *et al*., 2001).

In many cases, the use of default UFs that are not chemical- or species-specific will result in conservative HBGVs, as the underlying data supporting them are generic and show wide variability. Default UFs do not take into consideration the sensitivity of the animal used in the toxicity study, the number of doses used, the interval between doses, the number of animals per dose group and the choice of toxicological endpoint (Health Council of the Netherlands, 2008). An alternative approach may therefore be to define chemical specific adjustment factors (CSAFs) on a case by case basis, making each uncertainty and its associated factor transparent. As indicated above, evidence suggests that a distinction should be made between toxicokinetic and toxicodynamic components as variations between animals and humans are largely due to absorption, distribution, metabolism and excretion (toxicokinetic factors) (Health Council of the Netherlands, 2008).

SR2 already supports the use of CSAFs for thresholded substances and states the following in relation to this issue:

Box 2.4 Uncertainty factors

Uncertainty factor is the generic term used in the UK for the numerical factors applied to toxicity data (points of departure) to take into account the uncertainty in extrapolating the data to derive HCVs for humans. Various terms are used by different organisations to denote such factors, including **safety factor**, **variability factor**, **assessment factor** and others. These terms are generally interchangeable. In some cases, however, it may not be uncertainty that dictates the application of the factor, but rather evidence that humans or a human subpopulation are more sensitive than the subjects (either animal or human) of the critical study. Similarly, there may be evidence of decreased sensitivity of the target population relative to the test population, in which case a smaller than usual factor may be applied. Where the difference in sensitivity of the test and target populations to a particular chemical is known and can be quantified or estimated, a **chemical-specific adjustment factor** is applied (see IPCS, 2005).

Moreover, for non-genotoxic carcinogens, the COC also advocates that default factors could be replaced in part or in full by CSAFs if the available data provide adequate information on interspecies or human variability (COC, 2012; Meek *et al.*, 2002).

Suggested C4SL CLEA Modification 11: Use chemical-specific adjustment factors (CSAFs), rather than default uncertainty factors, to derive toxicological criteria, where possible.

The steering group and stakeholders were in general agreement with this. It should be noted that this is not a 'modification' as such but a retention of practices that have already been mentioned in recent guidance.

[10] Toxicokinetics - the rates that chemicals pass into, through and out of the body's organs. Toxicodynamics - the interactions the chemicals have with molecules, cells and organs of the body.

Non-threshold chemicals

Some chemicals exhibit an effect that does not have an observable threshold (i.e. there is no dose that shows no effects) in experimental studies. This is often a cancer related effect but not always (e.g. neurobehavioural toxicity for lead also shows no threshold in human epidemiological studies). Specifically, 'genotoxic carcinogens' that are seen to damage DNA in genotoxicity assays, are chemicals that are considered to have no threshold dose. For these substances, all doses, however small carry a risk of effect, even at the level of minimal risk described in SR2.

SR2 is based on guidance from the COC in 2004. This has now been superseded as of October 2012, as the Committee on Carcinogenicity (COC) published a new guidance document (G06) for the risk assessment of chemical carcinogens (COC, 2012). However, the basic principles for defining 'minimal risk' as described in SR2 remain valid and hence that document can still be referred to for 'minimal risk' guidance. For circumstances where exposure to non-thresholded chemicals is unavoidable, COC (2012) states:

> 'For carcinogens which do not show a threshold for effect, exposure should be as low as reasonably practicable (ALARP). In addition, the Committee recommends that the Margin of Exposure (MOE) approach be adopted as a tool *to indicate the level of concern* in situations where exposure is unavoidable. When it is necessary to set a standard or guideline value for a genotoxic contaminant, identification of a minimal risk level may be appropriate.'
>
> It continues: 'The derivation of a minimal risk level for a genotoxic and carcinogenic contaminant or impurity involves assessment of all available dose-response data for carcinogenicity to determine an appropriate point of departure and *use of expert judgement to identify a suitable margin between this point of departure and a level of exposure which would result in a minimal risk*. One proposal is that a suitable margin might be 10,000 (Gaylor, 1994; Gold *et al*, 2003), which parallels the margin of exposure approach, where an MOE of 10,000 is considered to be *unlikely to be of concern* when based on a BMDL10 from an animal study. For a genotoxic and carcinogenic contaminant or impurity, a comparison of the minimal risk level with estimated exposure can be informative to risk managers.'

The classical way of implementing a 'margin of exposure' approach is to divide the POD by an exposure intake value estimated using a model of the exposure scenario (e.g. that would mean to use CLEA in 'forward mode' to derive an average daily exposure (ADE) for each site assessed and compare with the POD to arrive at an MOE). One would then decide in the context of risk management as to whether the MoE was 'acceptable' or 'unacceptable'. MoE approaches to risk characterisation are being used more widely, and in particular for the risk characterisation of genotoxic carcinogens in foods (EFSA, 2005; IPCS-WHO, 2009; EFSA, 2009a & USEPA, 1995). A joint EFSA, ILSI and WHO workshop was held in 2005, and a comprehensive list of the advantages and limitations of adopting an MOE approach was produced afterwards. This is provided in Appendix 3.

EFSA (2005 & 2012b) have indicated that for genotoxic and carcinogenic contaminants, in general, an MOE of >10,000 is of low public health concern when based on an $BMDL_{10}$ from an animal study. The exact recommendations from the EFSA statement in 2012 are as follows:

> *'In the 2005 opinion, the Scientific Committee gave some guidance on how to interpret the MOE. It was stated that "The Scientific Committee is of the view that in general a margin of exposure of 10,000 or higher, if it is based on the BMDL10 from an animal carcinogenicity study, and taking into account overall uncertainties in the interpretation, would be of low concern from a public health point of view and might be reasonably considered as a low priority for risk management actions. However, such a judgment is ultimately a matter for the risk managers. Moreover an MOE of that magnitude should not preclude the application of risk management measures to reduce human exposure".*

The Scientific Committee is aware that the magnitude of an MOE only indicates a level of concern and does not quantify risk. Moreover, the implications of any MOE need to be considered case-by-case, looking at both its magnitude and the uncertainties regarding its derivation. The Scientific Committee reiterates that an MOE of 10,000 or higher is considered of low concern from a public health point of view with respect to the carcinogenic effect. As a small MOE represents a higher risk than a larger MOE, it follows that a very high MOE would be very unlikely to be of safety concern.

However, there is at present no international consensus on banding of MOEs and corresponding descriptive terminology. When using the MOE approach for assessing impurities, EFSA Scientific Committee and Panels should describe the derivation of the MOE, its magnitude, and the associated uncertainties regarding its derivation. They should also give their view on whether the MOE is of high concern, low concern, or unlikely to be of safety concern. It will then be the role of the risk managers to decide whether the substance containing the impurities should be authorised.'

The UK Committee on Carcinogenicity (2007) have agreed MOE bandings for genotoxic carcinogens, for use in risk management and communication, as follows:

Table 3.2. MOE bands (as agreed by COC, 2007)

MOE band	Interpretation
< 10,000	May be a concern
10,000 – 1,000,000	Unlikely to be a concern
>1,000,000	Highly unlikely to be a concern

An MOE of 10,000 represents a default 100-fold difference between the point of departure and human exposures to allow for general differences between species and for human variability and an additional 100-fold difference is considered appropriate to allow for the additional uncertainties due to using a BMDL and due to the inter-individual variability in carcinogenic processes. Therefore, a MOE of 10,000 or higher when used with a $BMDL_{10}$ would be of low concern from a public health point of view, whereas a MOE of less than 10,000 indicates that exposure 'may be of concern' (EFSA, 2005). Proposals on interpreting the magnitude of the MOE were adopted and expanded by COC and a system for banding MOE values was proposed, as above.

However, it should be noted for our purposes here, that whilst MOE is a usefully flexible approach to risk characterisation, the MOE approach *per se* does not lead to a health-based guideline value, which is what is needed to derive a C4SL. The conceptual difference between use of guideline values vs margin of exposure approaches in risk characterization is well described in Figure 2 of the IGHRC CR9 (2003) document on use of uncertainty factors in risk assessment.

We describe below in section 3.2.4 how a 'margin' approach, which parallels the MOE approach, can be implemented when setting guideline values.

Suggested C4SL CLEA Modification 12: Adopt the wider use of Margin of Exposure (MOE) approaches and recommend target substance-specific margins for each substance.

All agencies agreed with this approach as it is in line with COC (2012). Hence this modification will be ***retained****. At the workshop, stakeholders did not show a good understanding of this approach and needed further explanation about what it means and how it would be implemented.*

3.2.3 HCVs FOR THRESHOLD SUBSTANCES

As mentioned above, according to SR2, HCVs for threshold substances (i.e. those chemicals whose toxic effects exhibit a threshold) are typically referred to as Tolerable Daily Intake (TDI) values in the UK. A TDI is defined as 'the estimated amount of a chemical (expressed on a body weight basis) that can be ingested daily over a lifetime without appreciable risk to health' and it is typically calculated by dividing a POD by a UF. For inhalation exposure, a tolerable concentration in air (TCA) can instead be defined, as the estimated amount of a chemical (expressed as an atmospheric concentration) that can be inhaled over a lifetime without appreciable risk. The HCVs, TDIs and TCAs used in the UK are equivalent to many of the toxicological criteria used in other countries, such as JECFA provisional tolerable weekly intakes (PTWIs) and USEPA Reference Doses (RfDs), Reference Concentrations (RfCs) and US ATSDR Minimum Risk Levels (MRLs). All of these criteria take data from a pivotal toxicology study (often the same one) and incorporate a value (an uncertainty or assessment factor) to account for uncertainties in the data. Differences in the choice of pivotal toxicology study and POD should be appreciated when comparing HCVs from different jurisdictions and some may have been relatively conservative, and some may be less so, in their choice of uncertainty factors (EA, 2009b)(see Appendix 2).

3.2.4 HCVs FOR NON-THRESHOLD SUBSTANCES

According to SR2, HCVs for non-threshold effects (i.e. those chemicals whose toxic effects do not exhibit a threshold) should take the form of Index Doses (IDs). An ID is defined as 'a daily dose, derived for a non-threshold carcinogen, which is expected to be associated with a minimum excess risk of cancer'. IDs can be derived using two approaches, referred to in SR2 as "quantitative dose-response modeling" and "non-quantitative extrapolation". The selection of the approach to use should be largely dependent on the extent and quality of data available (EA, 2009b).

Non-quantitative extrapolation has been used in SR2 to set HCVs for non-threshold carcinogens using an approach which is similar to that used for threshold chemicals (i.e. a POD divided by a default UF). The POD is identified from relevant carcinogenicity data as the dose without discernible carcinogenic effect, or the dose where effects are seen, in the form of a BMD. As with threshold effects, the consideration of uncertainty needs to account for potential inter and intraspecies differences, but additional factors are also added to reflect the additional uncertainties for substances that are genotoxic and carcinogenic, due to human variability in cell cycle control and DNA repair, as well as the uncertainties surrounding using a reference point that is not equivalent to a NOAEL, as effects could occur at lower doses.

The EFSA Scientific Committee considered the application of additional measures of uncertainty to allow for the severity of an effect. Whilst this is not routinely used, it should be considered on a case by case basis as there are some examples where the toxicological effects are judged to be irreversible or particularly severe (EFSA, 2012a). The Guidelines for Drinking Water Quality (WHO, 2011), suggested that additional uncertainty may be needed for endpoints such as foetal malformations, or carcinogenicity with a thresholded mode of action.

For deriving guideline values for non-thresholded carcinogens, there is now strong support in COC (2012) for adopting an approach that parallels the 'margin of exposure' approach described above in section 3.2.2. The 'margin' applied to the POD is a value derived to represent a specified level of concern and is arrived at by reviewing the toxicological evidence, reviewing the uncertainties in the data (similar in approach to that above for thresholded chemicals), using expert judgment (the basis for which should be well documented) and also with good knowledge of the exposure model context and uncertainties within the exposure parameters.

The default margin of 10,000 between human exposure and a $BMDL_{10}$ from an animal study is considered to be 'unlikely to be a concern' (COC, 2007 & 2012), and echoes the way of defining minimal risk as per SR2 (EA, 2009b), DEFRA

(2008) and COC (2004). Using a $BMDL_{10}$ for non-threshold carcinogenic effects divided by a default UF of 10,000 achieves the minimal risk level of 1 in 100,000 (EA, 2009b). A recent publication EFSA 2012b, reiterated its 2005 opinion that a default MOE of 10,000 when used in conjunction with a $BMDL_{10}$ from an animal study, represented a generic default low level of public health concern. If scientific evidence is available to refine the degree of uncertainty required in a chemical specific manner, lower margins than 10,000 may describe 'low' concern scenarios.

In *quantitative dose-response modelling*, numerical approaches are used to derive a numerical estimate of dose that corresponds to an excess lifetime cancer risk (ELCR) of 1 in 100,000 (10^{-5}) (EA, 2009b; DEFRA, 2008). Although this approach is used in some parts of the world (e.g. US EPA) with data obtained from high dose animal studies, the Committee on Carcinogenicity does not recommend its use for routine risk assessment, as the models used to extrapolate data do not adequately simulate carcinogenic processes and can lead to highly variable outcomes (COC, 2004; COC, 2012). As a consequence, it is recommended for use in the UK only where there are human data. Defra has considered that an ELCR of 1 in 100,000 based on suitable human cancer data is appropriate to represent "minimal risk" (DEFRA, 2008). Given that C4SLs are designed to represent risks which are 'low', consideration should be given to defining an ELCR that represents a 'low level of concern' in the derivation of toxicological criteria using this approach.

Suggested C4SL CLEA Modification 13: Use a higher ELCR than 1 in 100,000 (eg, a maximal 1 in 10,000) when setting toxicological criteria for non-threshold carcinogenic effects using quantitative dose-response modelling (based on human data).

There is general discomfort from all stakeholders in using an ELCR of 1 in 10,000 to derive a C4SL value as it was thought to be more akin to the 2/3 boundary. This modification will only be ***retained*** *if considering only modest changes above 1 in 100,000.*

3.2.5 LIFE-TIME AVERAGING

CLEA does not allow the user to select an averaging time greater than exposure duration but the user is able to select the age classes considered in the ADE calculations and thus can base the ADE calculations on exposure over a lifetime. As indicated in Section 2.5.1.2, averaging exposure over a lifetime can have a large influence on the ADE estimates derived by CLEA and, therefore, any SGVs or other criteria that are derived using it.

Lifetime averaging as a concept arises from Haber's rule in the context of acute inhalation toxicity and is described as the concentration/dose x time of exposure = toxic effect (C x t = k). The USEPA (and others) assume that the lifetime cumulative dose (LCD) is appropriate for cancer risk assessment. When assessing less than lifetime exposure periods, it is assumed that a high dose over a shorter periods is equivalent to a low dose over a longer (lifetime) period. However, for shorter exposure periods a dose rate correction factor may be needed to correct for dose-related toxic effects and it is important that toxicokinetic factors are also taken into account (Felter *et al.*, 2011). Other authors have suggested that the risk attributable to early-life exposure often appears modest compared with the risk from lifetime exposure, but it can be about 10-fold higher than the risk from an exposure of similar duration occurring later in life (Ginsberg, 2003).

A key consideration in regards to lifetime averaging is whether there are differences in susceptibility to the chemical between children and adults. As mentioned in Section 3.2.2, the default UF of 10 for intraspecies differences already allows for variation within the human population, including specific subgroups such as children (COT, 2007). The US Food Quality Protection Act (USA, 1996) proposed the need for additional UFs to calculate health based guidance values of pesticides for infants and children. Such a need is based on

whether the 10-fold intraspecies UF is sufficiently protective of pregnant women, embryo/foetuses, infants and children. It has been proposed that elimination/clearance of some xenobiotics is higher in children than in adults hence in that instance children could be less sensitive as they could have lower body burden than adults for the same daily intake, when expressed on a body weight basis, and in fact, the higher elimination of the chemical may in part compensate for increased organ sensitivities during child development (Renwick, 1998). Therefore it has been suggested that an additional UF to account for infants and children is not required in relation to age-related toxicokinetics (Renwick, 1998; Renwick *et al*., 2000). Moreover, Renwick *et al*. (2003) also suggested that additional UFs would not be required if age-related differences are tested for in animal toxicology studies. The scientific evidence for making these arguments in risk assessment is not extensive however.

The current understanding of the biological processes of carcinogenesis is that young animals or children are more susceptible to many carcinogens compared to mature animals or adults (McConnell, 1992; Anderson *et al*., 2000; Birnbaum and Fenton, 2003; Ginsberg, 2003; Miller *et al*., 2002; Scheuplein *et al*., 2002). Studies in rodents with chemicals with a mutagenic mode of action suggest a decline in cancer risk with age at exposure, as the earliest two or three postnatal weeks in rodents appear to be most susceptible (USEPA, 2005 a & b). This is due to a variety of biological mechanisms:

- There can be differences in the capacity to metabolize and eliminate chemicals, resulting in different internal doses of the active agent(s), depending on whether the parent compound or metabolite is the active agent.
- More frequent cell division during development can result in enhanced expression of mutations due to the reduced time available for DNA repair (Slikker *et al*., 2004).
- More frequent cell division during development can result in clonal expansion of cells with mutations from prior unrepaired DNA damage (Slikker *et al*., 2004).
- Key DNA repair enzymes are sometimes lacking in embryonic cells, such as brain cells.
- Some components of the immune system are not fully functional during development (Holladay and Smialowicz, 2000; Holsapple *et al*., 2003).
- Hormonal systems operate at different levels during different lifestages.
- Induction of developmental abnormalities can result in a predisposition to carcinogenic effects later in life (Anderson *et al*., 2000; Birnbaum and Fenton, 2003; Fenton and Davis, 2002).

Understanding the mode of action of the compound where a key event is likely to occur in children, as well as understanding the toxicokinetics in different life stages that may predict a sufficiently large internal dose in children, are critical in the understanding of whether children are in fact more susceptible than adults. For example, pro-carcinogens may require metabolic activation by hepatic enzymes (cytochrome P450) to exert their carcinogenic effect. The expression and activity of some cytochrome P450 isoforms in some cases has been shown to be lower in neonates and children compared to adults (Faustmann *et al.*, 2000). Therefore, in terms of pro-carcinogens, children may effectively be protected against carcinogenic metabolites due to their lower metabolic capacity. Conversely, if the parent compound exerts the toxicological effects then a reduced metabolism and elimination could result in higher body burden. Moreover, exposures to chemicals acting through a mutagenic, as well as through other modes of action can result in a greater susceptibility for the development of tumours when the exposures occur in early life stages (USEPA 2005 a & b).

The decision to perform lifetime averaging when using CLEA is therefore not trivial, and it should be taken at the toxicology-exposure interface, with the question being asked on a chemical-by-chemical basis, where evidence permits. If there is evidence to suggest that a child could be more susceptible than an adult to a chemical's toxic effect, based on the mode of action of the chemical for the critical

toxicity endpoint and child specific toxicokinetic/toxicodynamic factors, then averaging exposure over a lifetime would not be considered appropriate. Where there is an absence of evidence either way regarding the mode of action and the sensitivity of children, a precautionary position could be adopted i.e. that a child *could* be more sensitive and therefore lifetime averaging is not applied, or alternatively, lifetime averaging is adopted as there is no evidence to suggest children are more sensitive than adults. Within CLEA, the current position is the former conservative position for most chemicals, with the exception of cadmium where lifetime averaging was considered to be appropriate, and the details of this will be discussed in WP2.

It should be noted that the fact that children can have higher exposure to soil than adults, due to their assumed behaviour and lower body weight, is accounted for in the parameters and modeling of the CLEA model.

Suggested C4SL CLEA Modification 14: Use lifetime averaging when deriving C4SLs using CLEA, if judged to be appropriate on the basis of the toxicological assessment.

This proposed modification received a mixed response from both the steering committee and stakeholders. Concerns over possible implementation of lifetime averaging focussed on whether there would be adequate protection of children who have higher levels of exposure at what may be a more sensitive life-stage. However, as lifetime averaging is still deemed appropriate for some contaminants i.e. cadmium this modification will be ***retained*** *and used when appropriate for the derivation of C4SLs.*

3.2.6 USE OF DEFAULT VALUES FOR PHYSIOLOGICAL PARAMETERS

During the derivation of toxicological criteria, it is sometimes necessary to calculate human dose estimates from chemical concentrations in water or air (e.g. drinking water standards and air quality objectives). Default values for physiological parameters such as body weight, inhalation rate and drinking water consumption are used for this purpose. The bodyweight parameter used for derivation of a HCV in the UK is based on an adult of 70 kg drinking 2 litres per day (EA, 2009b). This correlates with new guidance recently published by EFSA who stated that a body weight of 70 kg should be used as a default for the European adult population. Moreover, a 2L default value for chronic daily total liquid intake was also recommended (EFSA, 2012a).

The inhalation rate is also based on a 70 kg adult breathing 20 cubic metres of air per day (EA, 2009b).

There are deviations from these values in other parts of the world. For example, other authoritative bodies such as the World Health Organisation (WHO) use a default body weight of 60 kg and volume of water drunk is 2 litres water per day (WHO, 2011).

There is no reason to change the above assumptions in the context of risk assessment for UK contaminated land (unless new data becomes available that more accurately reflects the average for the UK population in terms of body weight), they are, however, highly relevant to the derivation and use of toxicological criteria in CLEA, to avoid possible over-conservatism if lifetime averaging is not used (see above). For example, inhalation HCVs (HCV_{inh}) for volatile contaminants are recommended as intake values (mg kg^{-1} bw day^{-1}) based on airborne contaminant concentrations such as reference concentrations taken from toxicology studies (e.g. USEPA RfCs) and Air Quality Objectives (AQOs, $mg.m^{-3}$). AQOs and RfCs are generally recommended for long-term or lifetime exposure with minimal risk.

The conversion from an airborne concentration to a HCV_{inh} is based on adult receptor characteristics (i.e. daily inhalation rate of 20 m^3 and 70 kg bodyweight) whereas the calculation of exposure for the residential land use scenario is for a 0-6 year old child (with the default lower inhalation rate and significantly lower bodyweight). This approach is considered to introduce an unnecessary level of conservatism as a child's exposure relative to bodyweight is approximately 2-3 times higher than that for adult. A similar situation can arise where ingestion HCVs are based on drinking water standards.

If lifetime averaging is not used, it is therefore considered appropriate to derive receptor-specific $LLTC_{inh}$ and $LLTC_{oral}$, in the form of values for a residential land use scenario, based on the average inhalation or ingestion rate and bodyweight for a 0 - 6 year old child (13.3 kg, 1 litre day^{-1} and 8.8 m^3). Separate $LLTC_{inh}$ and $LLTC_{oral}$ for commercial land use would be recommended based on adult receptor characteristics.

Suggested C4SL CLEA Modification 15: Use child-specific exposure assumptions to convert media concentrations to toxicological criteria for residential land-use, as appropriate, if lifetime averaging is not employed.

This modification had strong support from the steering committee and those stakeholders that fully understood the nature of the proposal. This modification has been ***retained*** *and appropriate receptor characteristics for an average child (covering CLEA age classes 1-6) will be used to derive LLTC for the residential land use scenario. LLTC for commercial land use will be based on typical adult receptor characteristics.*

3.3 DEFINITION OF A LOW LEVEL OF TOXICOLOGICAL CONCERN (LLTC)

As indicated above, for the purposes of defining a C4SL, it is suggested that a new term is defined – a Low Level of Toxicological Concern (LLTC) – which would correspond to a pragmatic intake level that remains sufficiently protective of health but represents a level of risk slightly above minimal. The units of the LLTC will be the same as those of the HCVs - mg kg^{-1} bw day^{-1} (unless judged otherwise) and they will be used to provide information on the toxicological aspects of a substance, as part of a range of factors to be considered in deriving a C4SL.

It could be argued that it might be simple and effective to adopt a policy decision to derive LLTCs and simply multiply the minimal risk HCVs by a factor of, say, 10. The advantage of this approach is that it would, in theory, be easy to implement, as risk assessors would simply multiply the existing HCVs/GACs by a fold factor (assuming linearity). However, there are serious downsides with this approach. A generic fold increase could be used but for one substance this may still lie within a low risk/low level of concern range and for another substance it may lead to a level of concern that could be SPOSH i.e. if the dose-effects curve is steep. Also, if the uncertainty used in deriving a HCV has not been a high value, eroding the uncertainty by allowing increases in exposure of a fold factor, may lead to a number that includes little or no aspect of uncertainty. Also, in setting the HCV, the most sensitive effect has been looked at quantitatively. Multiplying the HCV by a fold factor may then encroach on a different health effect where the dose-response curves overlap. Hence, there could be a risk of significant harm occurring, if this purely numerical approach to raising the HCV to a LLTC were taken. Hence, it is important to use toxicological interpretations of dose response information, particularly if increases above minimal risk are to be proposed. Reflecting the above, a chemical-specific, scientific approach to defining LLTCs is recommended, as described below in Section 3.4.

Suggested C4SL CLEA Modification 16: Adopt the term "low level of toxicological concern" (LLTC) to describe toxicological criteria derived for the purposes of developing C4SLs.

This modification was supported by the steering group but some stakeholders, although they agreed with the need for new terminology, had some concern over the word 'low' and its definition. However, this modification will be ***retained*** *but will require careful communication with practitioners.*

3.4 SUGGESTED FRAMEWORK FOR DEFINING A LOW LEVEL OF TOXICOLOGICAL CONCERN (LLTC)

A framework for evaluating chemical-specific toxicology data for the purposes of C4SL derivation is presented in the form of a flowchart in Figure 3.2. The remainder of this section is structured to guide the reader through the flowchart by referring to, and providing further information on, its numbered elements.

3.4.1 FLOWCHART ELEMENT 1: REVIEW & COLLATE THE MINIMAL RISK EVALUATIONS FOR THE SUBSTANCE (AS PER SR2)

The general principles described in the section above, together with the detailed methods published in SR2 and the COC guidance (2012), form the basis of defining minimal risk. Since the purpose of LLTCs is to define a level above minimal risk which can be considered "more pragmatic but still strongly precautionary", it is recommended that, for any substance, the minimal risk position is understood and mapped, before attempting to derive a LLTC. This is the purpose of flowchart element 1.

As an example of this element, Appendix 2 presents relevant information for the six substances of interest to this project - arsenic, benzene, benzo[a]pyrene/PAHs, cadmium, chromium VI and lead. The information is presented in spreadsheet form and provides an overview of the various minimal risk criteria for each substance. All of the identified human health hazards by the oral and inhalation routes are presented, and where possible a POD given from the pivotal study for the endpoint and exposure route. All of the authoritative evaluations of the substance, by worldwide organisations (as mentioned in SR2) are tabulated in descending order of the HCV derived. It should be noted that the HCVs have not necessarily been calculated for the purposes of assessing land contamination and that they may have been derived in the context of the accompanying exposure scenarios.

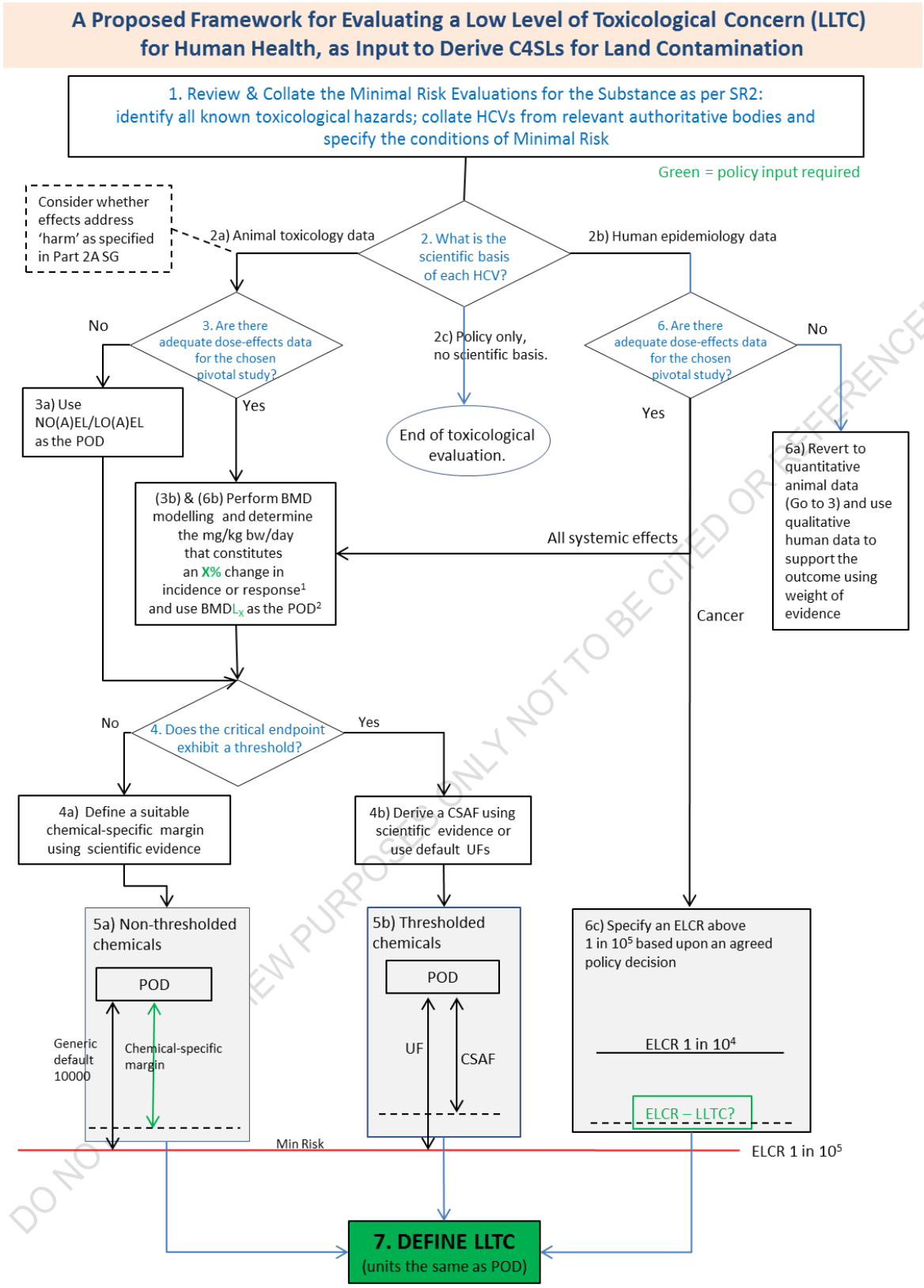


Figure 3.2: Toxicological Framework for Defining LLTCs

3.4.2 FLOWCHART ELEMENT 2: WHAT IS THE SCIENTIFIC BASIS OF EACH HCV?

Flowchart element 2 requires the assessor to identify the scientific basis of all existing HCVs. Three possible options are provided, in the form of: 1) animal toxicology data; 2) human epidemiology data; and 3) policy (i.e. no scientific basis). Each of these is described below.

2a) Animal Toxicology Data

Many *in vivo* toxicological studies are available to study the effects of chemicals, including acute, sub-acute, sub-chronic and chronic toxicity tests, as well as one- and two-generational reproductive studies. For the purposes of deriving HCVs, data from chronic toxicity tests, carcinogenicity tests, as well as reproductive studies are predominantly used, if available, as these better simulate the chronic exposure of humans to contaminants in soil. In general, *in vivo* studies should be performed in accordance with internationally accepted guidelines (e.g. OECD guidelines).

Chronic toxicity studies are used to characterise the profile of the chemical in a mammalian species (usually rodents), and to determine the dose-response relationships, following prolonged and repeated exposure to defined doses of chemical. Carcinogenicity studies are carried out to observe test animals for the majority of their life span for the development of neoplastic lesions during or after exposure to a chemical via various routes of exposure.

One-generation studies are designed to evaluate the reproductive and developmental effects that may occur following pre- and postnatal chemical exposure, as well as to assess systemic toxicity in pregnant and lactating females, and young and adult offspring. Pups are assessed for reproductive and developmental effects, developmental neurotoxicity and developmental immunotoxicity (OECD, 2012).

Two-generation studies are designed to provide general information on the effects of a chemical on the integrity and performance of male and female reproductive systems, as well as on the growth and development of offspring. Data from such a study should provide an estimation of the no-effect level and an understanding of the adverse effects on reproduction, parturition, lactation, postnatal development, growth and sexual development (OECD, 2001).

The protocol used for all toxicity tests is broadly similar. Both sexes of animals should be used for each dose group, and at least three doses should be applied, as well as zero for the control, non-treated group. Twenty or fifty animals should be used per sex, per dose group for chronic and reproductive studies, or carcinogenicity studies, respectively. Daily exposure is usually carried out for 12 (chronic study) or 24 (carcinogenicity studies) months, after which time general toxicological effects are observed and reported and the detection of neoplastic (new cancer causing) effects and the determination of carcinogenic potential can be carried out (OECD, 2009 a & b). For reproductive tests, dosing occurs two weeks prior to mating and continuously through the gestation and weaning of the pups.

2b) Human Epidemiology Data

Epidemiology studies consist of studies of populations of humans exposed to a chemical in order to identify any adverse health effects. Most epidemiological data is obtained from observational studies, such as cohort and case-control studies, in an occupational setting.

A cohort study looks at the effects that arise following exposure to a chemical. Subjects are defined according to their exposure status and followed over a period of time to assess the prevalence of health outcomes. In contrast, case-control studies select subjects on the basis of their disease status. Their potential chemical exposures are then compared with a control, non diseased group. Data from both types of study may be used as the basis of a LLTC, although in most cases, cohort studies are most relevant. If epidemiology or other human data are available, they will often take precedence over animal data, although this is largely dependent on the quality of the human data (EA, 2009b).

2c) Policy only, no scientific basis

In very rare cases, if there is not a scientific basis on which to base the derivation of a LLTC, it can be based on policy decisions alone. An instance where this might occur is when there are substances that do not have any toxicity data that are considered scientifically robust enough to derive a POD and therefore a HCV cannot be derived. In such cases it would be a policy decision how to go forward with the risk assessment.

3.4.3 FLOWCHART ELEMENT 3: ARE THERE ADEQUATE DOSE-EFFECTS DATA FOR THE CHOSEN PIVOTAL STUDY – ANIMAL DATA?

This element of the flowchart relates to the use of animal toxicology data to derive a LLTC. More specifically, it requires the assessor to assess whether there are adequate data from the chosen pivotal study to perform BMD modelling.

If the answer is "no", then the assessor should use a NO(A)EL/LO(A)EL as the POD (3a). In this case, the process would be the same as described in SR2 and COC guidance (2012), as the information provided in the study would be considered too weak to draw good quantitative conclusions about the dose response, to provide robust scientific evidence of the level of risk/concern at doses higher than a single POD. Depending upon the substance and the nature of the data in the pivotal toxicology study, it may be possible to use a NOAEL to define minimal risk, and a LOAEL to define the LLTC. However, this would need to be judged on a substance by substance basis, looking at the dosing regimen used in the study. One could also consider using an arbitrary value in between the NOAEL and the LOAEL (e.g. the median point).

If the answer is "yes", then BMD modelling should be performed (3b). As explained above, BMD modelling provides a more quantitative way of interpreting toxicology data, such that incremental increases in exposure can be aligned to an increase or decrease in continuous data as well as to an increased incidence of an effect. Therefore, if data are available, that are suitable for BMD modelling, then such modelling should indeed be carried out, in order to provide a more quantitative interpretation of the data. As discussed in Section 3.2.1, a chemical-specific decision regarding what % increased incidence of effect i.e. the BMR and subsequently the BMDL is necessary, based on limit of sensitivity, as the BMR should be in the observed range, hence 10% is proposed for carcinogenicity studies and 5% as a default for continuous data, although this could be smaller for incidence data in epidemiology studies with large populations.

Benchmark dose software (BMDS) is freely available from the USEPA, as well as PROAST software developed by the Netherlands National Institute for Public Health and the Environment (RIVM) (EFSA, 2011; USEPA, 2012). Additional commercially available resources include the Excel-based Wizard and DRAGON software products developed by ICF international (USEPA, 2012). Whilst it is mathematically straight forward to use the software, accompanying technical guidance should be closely followed and care taken in modelling the data appropriately and transparently.

3.4.4 FLOWCHART ELEMENT 4: DOES THE CRITICAL ENDPOINT EXHIBIT A THRESHOLD?

The identification of whether the chemical in question exhibits a threshold for the critical toxicity endpoint is a key decision in the framework.

(4a) If the answer is "no", i.e. for non-thresholded chemicals, then the assessor should look to define a chemical-specific margin based on a scientifically defensible rationale around the uncertainties in the toxicological data and with the use of expert judgement (4a). For example, the use of toxicokinetic and toxicodynamic data in choosing an appropriate margin would be akin to the considerations used in the derivation of CSAFs described below. Chemical-specific margins from the point of departure would represent a LLTC for the purposes of defining a C4SL.

As mentioned above in section 3.2.2, the COC (2012) propose that a suitable margin might be 10,000 for minimum risk. Similarly, SR2 mentioned the application of a factor of 10,000 to a BMDL10 (EA, 2009b). An example of other factors

accounting for specified uncertainties that have been used in UK Government chemical risk assessment are shown in table 3.3, as presented by the Interdepartmental Group on Health Risks from Chemicals (IGHRC, CR9, 2003). As shown in the table, various factors in considering the toxicology data could be amended and used to derive chemical-specific margins.

Table 3.3. Default factors used in UK Government risk assessment (IGHRC, 2003)

Chemical sector	Animal to human factor	Human variability factor	Quality or quantity of data factor	Severity of effect factor
Food additives and contaminants	10	10	2-10	2-10
Agricultural pesticides	10	10	2-10	2-10
Veterinary products	10	10	2-5	2-10
Air pollutants	10	10	-	-
Consumer products	10	10	2 or greater	2 or greater
Drinking water contaminants	1-10	1-10	1-10	1-10
Soil contaminants	1-10	1-10	1-10	1-10
Human medicines	1-10	1-10	1-100	-

Interspecies fate and behaviour differences (between animals and human) could be amended if there are toxicokinetics/ dynamic data that show there is <10-fold difference between animals and humans. This could be applied to all endpoints from animals studies. Similarly, toxicokinetics/ dynamic data may indicate that there is <10-fold different between individuals. In term of the quality or quantity of data that indicate the adequacy of the study or database, if the quality of the study is high, the UF could be less than 10, in terms of reliability of data points and NOAEL/BMD etc. To account for the nature and severity (irreversibility of effect e.g. use for carcinogens, reproductive toxins etc) an additional factor may be used, but again, could be modified based on expert judgment.

The EFSA Scientific Committee (2005) considered the figure of 10,000 for a MOE (which parallels the COC-proposed margin approach). As such a MOE adequately allowed for various uncertainties, namely:

- Species difference and human variability in toxicokinetic and toxicodynamics
- Inter-individual human variability in cell cycle control and DNA repair, which influence the carcinogenic process
- The use of a point of departure that is not a NOAEL, such as a BMDL, as effects could occur at lower doses. This dose effect relationship below the reference point, and the dose level below which cancer incidence is not increased are unknown, representing additional uncertainties.

In summary, a 100-fold difference between the reference point and human exposures would allow only for general species differences and human variability described in the first bullet point above. An additional 100-fold difference would allow for the additional uncertainties covered in the latter bullet points.

If robust data are not available on which to make an informed decision on how to derive a chemical-specific margin, then the default margin of 10,000 should still be used.

(4b) If the answer is “yes” i.e. for thresholded chemicals, then the assessor should look to derive a CSAF, if robust data are available. Chemical specific toxicokinetic or toxicodynamic data may be used, if available, to help identify more specifically the differences in sensitivity between humans and the animals used in the toxicity

study, and between different human populations (i.e. adults and children). Hence more specific factors for toxicokinetics and toxicodynamics could be used rather than the default factors of 10.

This is not a new concept as it was described in SR2 as a potential methodology for deriving HCVs and has also been used by other authoritative bodies. For example, the European Food Safety Authority (EFSA) used a CSAF of 3.9 to a $BMDL_5$ to derive a urinary cadmium concentration that represents an internal dose below which 95 % of the population would not show kidney effects i.e. would not have urinary β_2-microglobulin greater than 1 μg Cd g^{-1} creatinine. In this case, the CSAF of 3.9 was derived by dividing the 95th percentile BMD by the medium BMD using the standard formula for lognormal percentiles (EA, 2009e; EFSA, 2009b).

If there is no additional information available that could be used, or if the available data are not considered to be robust and scientifically defensible, then default UFs should be used.

For both threshold and non-threshold chemicals, factors for all of the individual uncertainties are simply multiplied together to contribute to an overall value for a chemical-specific margin (for non-threshold chemicals) or a CSAF (for threshold chemicals), that is then applied to the POD.

3.4.5 FLOWCHART ELEMENT 5: CALCULATING THE LLTC

Flowchart element 5 requires the risk assessor to perform the calculation using the derived POD and the appropriate measure of uncertainty.

(5a) For non-thresholded chemicals, the POD is divided by the 'margin' to yield a guidance value and the calculation is

POD/(chemical-specific margin or default 10000 margin) = LLTC (units as per POD)

(5b) For thresholded chemicals, the POD is divided by a CSAF the calculation is

POD/(CSAF or UF) = LLTC (units as per POD)

These calculations yield a fixed value (which we define here for the purposes of deriving a C4SL, as a LLTC) based upon the uncertainties in the toxicology data for the pivotal study on which the POD is based.

3.4.6 FLOWCHART ELEMENT 6: ARE THERE ADEQUATE DOSE-EFFECTS DATA FOR THE CHOSEN PIVOTAL STUDY – HUMAN DATA?

This element of the flowchart relates to the use of human epidemiological data to derive a LLTC. More specifically, it requires the assessor to assess whether there are adequate quantitative data from the chosen pivotal human study. If "no", then the assessor should revert to quantitative data from animal studies (6a). If the answer is "yes" then BMD modelling can be performed on the human data (6b) or an excess lifetime cancer risk (ELCR) can be defined.

Since it is not ethical to perform toxicology studies in humans, human dose-response data comes from epidemiology studies. Epidemiology is the study of the distribution of disease in human populations and the factors that may influence that distribution. Such studies are often in worker populations, where exposure to a substance has occurred within a given exposure scenario, and in population studies where people were exposed to chemicals inadvertently or in an unregulated context. It can be difficult to gain good quantitative dose-effects information from human data, but evidence of effects in man can corroborate the findings from animal studies in a weight-of-evidence approach.

In circumstances where there are good dose-effects relationships in human epidemiology data, they can be modelled using BMD approaches, as with animal data (see above). In such cases, as with animal data, a CSAF may also be derived, which conceivably may be lower as interspecies differences does not need to be

accounted for, and an LLTC may be derived. Good human data tend to carry more weight than animal data, where both are available.

As indicated above, quantitative dose-response modelling of cancer data involves the concept of ELCR, defined as:

> *'Potential carcinogenic effects that are characterized by estimating the probability of cancer incidence in a population of individuals for a specific lifetime from projected intakes (and exposures) and chemical-specific dose-response data (i.e., slope factors). By multiplying the intake by the slope factor, the ELCR result is a probability.'*

From such quantitative risk estimations, it has been the position of UK government that an excess lifetime cancer risk (ELCR) of 1 in 100,000 (10^{-5}) should constitute minimal risk (EA, 2009a; DEFRA, 2008). For the purposes of C4SL derivation, a risk estimate slightly higher than this could be specified as 'low risk', which may be substance specific. However, it is recommended that this should not approach a suggested maximum permissible risk level of 1 in 10^4.

3.4.7 FLOWCHART ELEMENT 7: DERIVE LLTC

The definition of the LLTC has been described previously. Overall, there are 3 routes to deriving a LLTC:

- For thresholded chemicals: derivation of a human intake using POD divided by CSAFs (or default UFs). The POD can be derived from animal or human data
- For non-thresholded chemicals: derivation of a human intake using POD divided by a recommended chemical-specific margin (or default margin of 10000). The POD can be derived from animal or human data.
- For human carcinogens: Recommendation of an intake dose based on human data that equals a specified ELCR that is considered low risk (to be agreed with policy input)

4. BACKGROUND EXPOSURE

Background exposure to a contaminant from non-soil sources can be an important consideration in the evaluation of risks from soil contamination and in the derivation of generic screening criteria. Consideration of background is discussed in the context of the existing CLEA methodology and the derivation of C4SLs below.

4.1 APPROACH USED FOR THE DERIVATION OF SGVs AND GACs

In the existing CLEA model, background exposure is accounted for in the derivation of SGVs and GACs for threshold substances using the following approach:

1. The MDI from non-soil sources (water, food and air) is estimated for the critical receptor.
2. CLEA uses the above information to calculate the ADE from non-soil sources and adds this to the ADE from soil to calculate a total ADE for the critical receptor.
3. The total ADE is then compared to the HCV to calculate the assessment criteria.

This method is based on the principle that total exposure to a contaminant (whether from soil or non-soil sources or both) should ideally not exceed the TDI. However, for contaminants where the MDI accounts for a large proportion of, or exceeds the TDI, the allowable exposure from soil can be disproportionately low. As a consequence of this, government policy (Defra, 2008) allows CLEA to limit the ADE from non-soil sources to 50% of the TDI. This policy allows for the modelled total combined exposure from soil and non-soil sources to exceed the TDI, in some cases.

Note that CLEA does not include background exposure in the calculation of ADE when deriving GAC for non threshold compounds.

4.2 BACKGROUND EXPOSURE IN THE REVISED STATUTORY GUIDANCE

Paragraph 4.21 of the revised Statutory Guidance describes the type of land that should be placed into Category 4 for Human Health. This includes:

> *"(d) Land where estimated levels of exposure to contaminants in soil are likely to form only a small proportion of what a receptor might be exposed to anyway through other sources of environmental exposure (e.g. in relation to average estimated national levels of exposure to substances commonly found in the environment, to which receptors are likely to be exposed in the normal course of their lives)."*

This suggests that a different approach could be used for the consideration of background when deriving C4SLs compared to that used for the derivation of the SGVs and GACs. Firstly, unlike the derivation of SGVs and GACs, in the SG no distinction is made between threshold and non threshold compounds. Secondly, rather than limiting the ADE from soils to some proportion of the HCV, the statement above implies that exposure from soils is of low concern where it is a small proportion of typical exposure from non-soil sources, irrespective of the health effects (presumably the rationale for this policy is that there is unlikely to be an appreciable benefit to human health from managing risks from soil contamination if the major source of exposure of a particular contaminant is from non-soil sources such as food, water or air).

The potential significance of soil contamination in the context of background exposure is illustrated in Table 4.1, below. This table shows the estimated contribution of soil to the total ADE for the residential scenario for a selection of the focus contaminants, assuming the CLEA-derived SGV or GAC as the representative soil concentration. The ADE estimates for background exposure are based on the Environment Agency's estimated MDIs for UK children, whilst the ADE estimates from soil have been calculated using the current configuration of CLEA for the generic residential scenario (and the SGV).

Table 4.1: Estimated ratio of soil ADE to total ADE (soil + non-soil sources) for a residential land-use with soil concentrations equal to the SGV

	Ratio of soil ADE to total ADE	
	Oral/dermal exposure	**Inhalation exposure**
Arsenic	61 %	60 %
Benzene	64 %	6 %
Benzo(a)pyrene	71 %	13 %
Cadmium	40 %	25 %
Chromium (VI)	15 %	9 %

As discussed in Section 2, the current configuration of CLEA is likely to over-estimate central tendency exposure from soil and thus, the true ratios are likely to be lower than those shown in the table. As it stands, however, the table illustrates that remediation of soil contaminated with benzene, chromium (VI) or benzo(a)pyrene at their respective GACs/SGVs is unlikely to result in a significant (>20%) reduction in exposure via critical pathways.

4.3 SUGGESTED APPROACH TO CONSIDERING BACKGROUND IN THE C4SLs

4.3.1 CONSIDERATION OF BACKGROUND EXPOSURE WHEN SETTING LLTC

Based on the above, and given the requirements of the revised SG, it could be appropriate to consider background exposure within the derivation of the C4SLs. This could be done when setting the LLTC, by undertaking a check to ensure that the LLTC is not less than some "small proportion" (to be defined) of the MDI. The exact proportion used depends on how the word "small" is interpreted, but a value of 10 to 25% may not be unreasonable for the purposes of setting a C4SL. At present an ADE of up to 50% of the TDI from non-soil sources is allowed (Defra, 2008).

Suggested C4SL CLEA Modification 17: In order to meet the requirement of 4.21(d) of the revised SG, the toxicity criteria used to derive C4SLs should be not less than a "small proportion" (say 10-25%) of chemical-specific background exposure, as estimated via published MDIs.

There was mixed support for this modification from the steering committee and stakeholders. Review of their comments suggested that whilst background exposure from non soil sources was a consideration in deciding whether a site was in Category 4 for human health it should not be used to over-ride the toxicology when setting the LLTC. It is considered more appropriate to compare the estimated exposure (or MOEs) from soil at the C4SL with other exposures for that contaminant, such as exposure from soil at the Normal Background Concentration (NBC)[1] and non-soil sources (such as background air quality and dietary exposure). This comparison could be used as a line of evidence when setting the C4SL (See Section 6) and would assist assessors in deciding whether or not the land they were assessing was in Category 4. This modification has therefore been revised accordingly.

4.3.2 CONSIDERATION OF BACKGROUND EXPOSURE IN THE ESTIMATES OF ADE

Consideration should also be given as to whether exposure from non-soil sources should be included in the exposure estimates that are ultimately compared with the LLTC to derive a C4SL. In particular, the following points could be considered:

- As discussed in Section 4.1, current Defra policy allows for combined contaminant exposure from soil and non-soil sources to exceed the TDI in some cases; and
- Other countries (e.g. USA and Netherlands) do not generally account for exposure from non-soil sources in calculations used to derive generic soil screening criteria.

Given that the C4SLs are intended to describe a higher level of risk (albeit low) than the SGVs and GACs, and in the light of the points described above, it may be appropriate for the derivation of the C4SLs to exclude estimates of background exposure from the calculations of ADE.

> Suggested C4SL CLEA Modification 18: Exclude the quantitative consideration of background exposure (via MDIs) from the derivation of C4SLs but provide relevant data for information purposes (in the form of ratios of modelled soil-related exposure to estimated total exposure).
>
> *There was mixed support for this modification form steering committee members and stakeholders. There was concern that exclusion of MDI from the estimates of ADE would not be sufficiently precautionary for threshold compounds. This proposed modification has therefore been* **rejected.**

5. C4SLS FOR PUBLIC OPEN SPACE

This section presents preliminary information on the approach to be adopted for the development of C4SLs for public open space (POS).

5.1 EXISTING GUIDANCE

Although the Environment Agency's Contaminated Land Exposure Assessment (CLEA) model does not consider recreational land-use (or variations thereof), the 2002 overview document relating to the human health risk assessment of soil contaminants (and the SGVs), CLR 7, states the following (Environment Agency, 2002b; now withdrawn):

> *"As part of the forward programme of developing the CLEA model, a new land–use related to public open space such as parks and playing fields is being developed."*

More recently, one of the "frequently answered questions" about a previous version of CLEA which were answered on the Environment Agency's website in April 2005 was as follows (Environment Agency, 2005; now withdrawn):

> *"3. Why are there no Soil Guideline Values (SGVs) for recreational open spaces?*
>
> *Soil Guideline Values have been developed so far for three types of land-use: residential, allotments and commercial/industrial. These land-uses are fully described in CLR10 (Table 2.1 and Chapter 4). Soil Guideline Values for recreational open space has not been included at this stage for two reasons. Firstly, sufficient information to generate and document an acceptable conceptual exposure model for this standard land-use has not yet been compiled. For example, 'Who visits parks?', 'How long is an average visit to a local park?, 'Is there a difference between summer and winter visits?' and so on. Secondly, the diversity in leisure land-uses such as city parks, school-playing fields and golf courses may not be suited to the derivation of a single standard land-use scenario. The Agency has therefore undertaken to compile and review information on a wide variety of leisure land-uses (as part of the Environment Agency's on-going science programme) in order to develop a toolkit for developing conceptual exposure models. This technical guidance will be useful to assessors undertaking a detailed quantitative risk assessment and may form the basis of any subsequent Soil Guideline Values for this type of land-use."*

No documents or publications from the Environment Agency relating to the proposed research are available and neither a recent document on using SGVs (Environment Agency, 2009a) nor the current version of the Environment Agency's CLEA FAQs (Environment Agency, 2011) mentions this issue.

Although not a regulatory body, the Scottish and Northern Ireland Forum for Environmental Research published a "Framework for Deriving Numeric Targets to Minimise the Adverse Human Health Effects of Long-term Exposure to Contaminants in Soil" in 2000 (SNIFFER, 2000). Although it included a "parks, playing fields and open spaces" land-use, this has been removed in a more recent document, which states that (SNIFFER, 2003):

> *"CLR 10 and the SGVs do not consider the parks, playing fields or open spaces scenarios. This [SNIFFER] method may be used to derive Site-Specific Assessment Criteria for such land uses if sufficient robust data has been obtained. The Environment Agency is commissioning work to develop an understanding of how public open spaces are used."*

It is not clear from a review of the first edition of the SNIFFER document how the "parks, playing fields and open spaces" land-use was characterised, although it would appear to involve the use of similar assumptions to those used in modelling a residential land-use.

5.2 TYPES OF PUBLIC OPEN SPACE

There is a large variety of land uses that could be considered "public open space", with exposure characteristics varying significantly between them. For example, the following land-uses could be considered as examples of public open space with distinct exposure characteristics:

- Grassed area that is rarely used adjacent to residential housing
- Grassed area where children play on a regular basis adjacent to residential housing (potentially comparable to garden without home-grown produce)
- Play park in close proximity to housing where some children play regularly and others less so
- Public park with football pitch where children play or practice sport several times per week and teenagers/adults play once per week
- Dedicated sports grounds where exposure only occurs to players and groundworkers
- Nature reserves or open ground with a low-level of activity (e.g. dog walking)

It may therefore be necessary to model more than one exposure scenario to identify a set of exposure characteristics that delivers C4SLs that are suitable as screening levels for the vast majority of public open spaces that are likely to be assessed.

5.3 SUGGESTED APPROACH

Following the approach used for allotments it may be reasonable to assume that tracking back of soils from public open space into the place of residence or work will be negligible. As such, the key exposure pathways for public open space are likely to be:

- Ingestion of soil outdoors
- Dermal contact with soil outdoors
- Inhalation of dust outdoors
- Inhalation of vapours outdoors

The critical evaluation of the exposure parameters used for the residential, commercial and allotments land-uses (Section 2.5) provides a good base of information for setting exposure characteristics for the public open space land-use. A key exposure parameter will be exposure frequency and as far as possible the value(s) used will be based on available surveys (e.g. Natural England and Forestry Commission surveys[11]).

[11] http://www.naturalengland.org.uk/ourwork/research/mene.aspx

Suggested C4SL CLEA Modification 19: Develop C4SLs for public open space, based on exposure via ingestion of soil, dermal contact and inhalation of dusts and vapours outdoors only.

This is not actually a suggested modification as it was a designated task in the specification for this research project. The steering committee and stakeholders expressed a variety of views about the type of POS that should be considered for development of C4SL(s) and as to whether or not this land use scenario should include exposure pathways such as the tracking back of soil.

We propose to develop C4SLs for two types of POS – the scenario of green space close to housing (which includes tracking back of soil) and a park-type scenario where we consider the park to be at a sufficient distance that there is negligible tracking back of soil. We will also undertake sensitivity analysis to identify the most sensitive receptor.

6. CATEGORY 4 SCREENING LEVELS

As explained in Section 1.1, C4SLs are intended as "relevant technical tools" (in relation to Paragraph 4.21c of the Statutory Guidance) to help local authorities and others when deciding to stop assessing a site, on the grounds that it could not pose the level of risk to human health required for determination under Part 2A (i.e. SPOSH). Defra's intention is that the C4SLs should be higher than the current SGVs/GACs but still strongly precautionary (Defra, 2012b, para. 47(h)).

Our overall approach to the development of C4SLs consists of the retention and use of the CLEA framework of exposure modelling and toxicological assessment, with modifications that are designed to achieve Defra's policy objective. Section 3 proposes to modify the toxicological assessment by using 'Low Levels of Toxicological Concern' (LLTCs) in place of the Health Criteria Values (HCVs) on which SGVs/GACs are based. Section 2 proposes a series of modifications to the calculation of exposure using CLEA, while Sections 4 and 5 make proposals relating to background exposure and exposures in public open space. Each of these proposals will contribute to making C4SLs higher than the current SGVs/GACs. However, Defra's objective also requires that the C4SLs remain "strongly precautionary". This section describes the methodology we propose to use to achieve this part of Defra's objective.

The overall approach we propose is illustrated in Figure 6.1. Steps 1-3 comprise the proposals for modified toxicological assessment and exposure modelling, as set out in Sections 2-5. The modified exposure model is then used in step 4 to calculate the soil concentration that would result in an exposure equal to the LLTC: this soil concentration is the proposed C4SL. In step 5, a probabilistic version of CLEA is used to estimate the probability of an individual receptor exceeding the LLTC assuming a substance is present in soil at the C4SL. This is one of the factors that should be considered when deciding, in step 6, whether the level of precaution implied by the proposed C4SL is appropriate. However, other factors may also be considered, as indicated in Steps 6a-6d. First, it is necessary to consider additional sources of variability and uncertainty in exposure that are not quantified by the probabilistic version of CLEA, which may have caused under- or over-estimation of the probability of exceeding the LLTC in step 5. Second, it is important to consider the level of precaution associated with the LLTC, that is, the likelihood, nature and severity of harm if the LLTC is exceeded. Third, consideration should be given to other relevant scientific considerations (e.g. background concentrations in soil, exposure via routes other than soil and epidemiological evidence for or against health effects from the chemical under assessment). Finally, when the relevant authorities and stakeholders consider the appropriateness of the proposed C4SL, they may wish to take account of social and economic considerations such as the costs of further assessment or remediation or societal perceptions of risk.

If, taking account of all relevant considerations, the proposed C4SL is considered appropriately precautionary, then it may be judged suitable for use. If, however, the parties involved consider that the level of precaution associated with the proposed C4SL is too high or too low, it could be adjusted by reviewing and revising the modifications to the exposure model (as illustrated by the return to step 3 in Figure 6.1). Consideration could also be given to revising the toxicological assessment and changing the LLTC (return to steps 1 and 2), if appropriate. In either case, steps 4-6 would then be repeated, to derive a revised C4SL and reassess the level of precaution provided. This cycle of steps could be repeated until a C4SL with the appropriate degree of precaution is derived. Note that while the toxicological assessment (steps 1 and 2 in Figure 6.1) will be conducted only once for each chemical, steps 3-6 must be repeated for each land use scenario for which a C4SL is required.

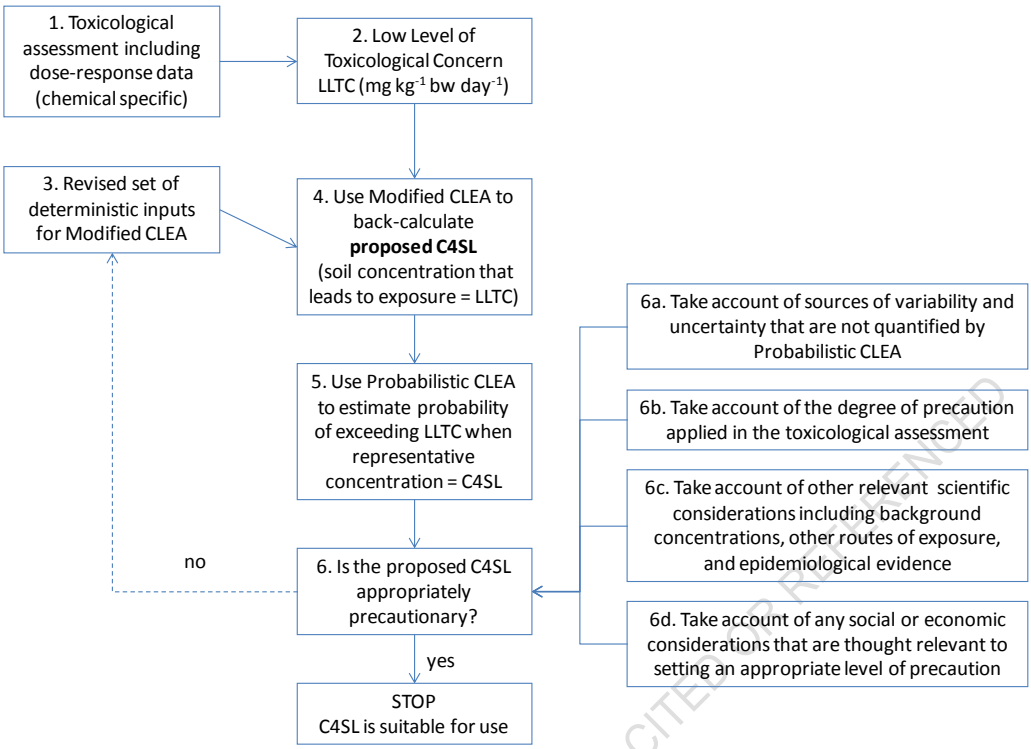


Figure 6.1. Overall approach proposed for developing C4SLs.

This proposed approach takes account of factors considered in the revised SG when describing the "possibility of significant harm". Although C4SLs are not "SPOSH levels", they are intended to be more precautionary than SPOSH and therefore need to take account of the same considerations. Paragraph 4.11 of the SG describes the "possibility of significant harm" as comprising the estimated likelihood that significant harm might occur to an identified receptor (this is addressed jointly by steps 5, 6a and 6b in Figure 6.1), and the estimated impact if the significant harm did occur i.e. the nature of the harm, the seriousness of the harm to any person who might suffer it (these are addressed by step 6b) and (where relevant) the extent of the harm in terms of how many people might suffer it (this is addressed by steps 5 and 6a). Paragraph 4.12 states that the estimated likelihood should take account of the estimated probability that the significant harm might occur, and the evidence, key assumptions and uncertainty underlying the risk estimate: these are also addressed by steps 5 and 6a-d.

Note that the use of probabilistic modelling in setting C4SLs does not imply a requirement for probabilistic modelling when using them. It will only be necessary to use the sample data to calculate the representative concentration (see section 7 for statistical method) and compare this with the C4SL. In cases where the representative concentration exceeds the C4SL, a refined (DQRA) assessment may be considered. Probabilistic modelling might be one option for conducting a DQRA, but a refined deterministic assessment is also possible.

The following sections provide more detail on the methodology proposed for step 5, and on some of the additional considerations in steps 6a-6d.

6.1 PROBABILITY OF EXCEEDING THE LLTC

Step 5 of the approach described in the preceding section requires the use of a probabilistic version of CLEA to estimate the probability of exceeding the LLTC, for a random individual receptor exposed to an estimated soil concentration equal to the proposed C4SL. The principles of the proposed methodology are illustrated in Figure 6.2. The main components of the approach are as follows:

- At the top of the figure: toxicological assessment, determining the LLTC.
- At the middle left side of the figure: a probabilistic version of CLEA. This is being developed by using sensitivity analysis to identify the assumptions and input parameters that contribute most to uncertainty in estimated exposures (section 2.4), and then replacing those assumptions and parameters with distributions that quantify their uncertainty.
- The probabilistic version of CLEA is used to produce an uncertainty distribution for the exposure of a random individual receptor, assuming that the true concentration is equal to the proposed C4SL. This distribution is illustrated by the bell-shaped curve at the middle right of Figure 6.2. Comparing this distribution to the LLTC, we obtain an estimate of the probability of the random receptor exceeding the LLTC (shaded grey in Figure 6.2). This is an estimate of the probability required at step 5 of the overall procedure for assessing the level of precaution associated with the proposed C4SL (Figure 6.1).
- If this process is repeated for a series of potential C4SL values, a graph may be plotted (lower right of Figure 6.2) showing the relationship between the choice of C4SL and the probability of a random receptor exceeding the LLTC when the measured representative concentration is equal to the C4SL. This graph may also be useful when the C4SL is exceeded at a particular site, because it indicates how much the probability of exceeding the LLTC rises as concentration increases.

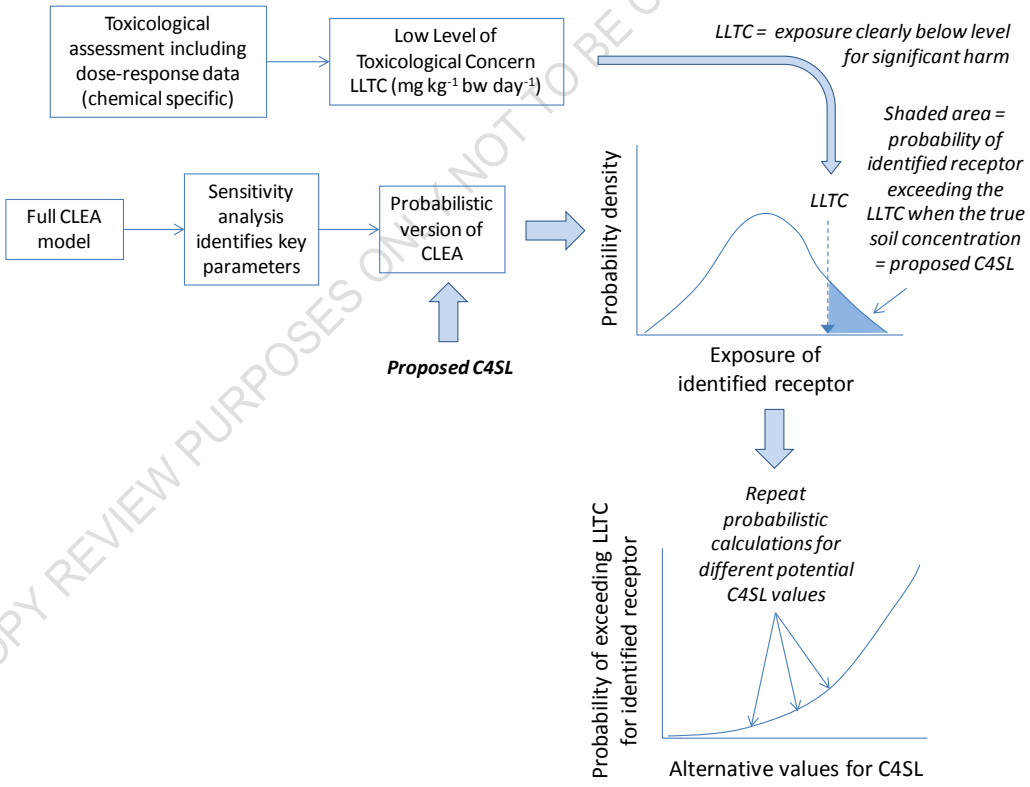


Figure 6.2: Outline of probabilistic methodology for estimating the probability of exceeding the LLTC.

Note that the probability estimated by this approach assumes that the *true* average soil concentration is equal to the C4SL. In practice, the probability of exceeding the LLTC at a particular site will also be influenced by the sampling and measurement uncertainty associated with the concentration data for that site. This will be taken into account in the next stage of this project (Work Package 2), when reviewing the methods for statistical treatment of site data (see Section 7.1).

The details of the probabilistic approach will be worked out in Work Package 2. For each chemical and land use scenario, alternative estimates of the probability of

exceeding the LLTC could be generated to show, for example, the separate contributions of the modifications proposed for the exposure and toxicology assessments, or the effect of alternative combinations of modifications. Such comparisons may be helpful when discussing the appropriateness of different levels of precaution in setting the C4SL.

Suggested C4SL CLEA Modification 20: Use uncertainty modelling (Monte Carlo etc) to inform decisions regarding the level of conservatism within C4SLs derived using a LLTC.

*This received some support from the steering committee and stakeholders, but it was evident that a clearer explanation was required. To provide this, the description and figures in section 6 have been extensively revised, and linked more explicitly to the content of preceding sections. This proposal has been **retained** but will require careful communication with practitioners.*

Some respondents inferred that probabilistic calculations would be required when using C4SLs. In fact probabilistic calculations are only required when setting the C4SL, not in its subsequent use. This is now explained in section 6.1 (above).

Suggested C4SL CLEA Modification 21: Use uncertainty modelling (Monte Carlo etc) to derive C4SLs when using a MOE approach.

*This is equivalent to Modification 20, when the LLTC is based on an MOE approach and is therefore no longer required, i.e. it has been **rejected**.*

6.2 QUALITATIVE EVALUATION OF C4SL UNCERTAINTY

The proposed approach for setting C4SLs includes probabilistic quantification of some uncertainties affecting exposure, and the use of chemical-specific adjustment factors in the toxicological assessment. Since it is never possible to quantify all uncertainties, additional assessment is needed to identify those uncertainties that remain unquantified and evaluate by expert judgement their potential impact on the estimated probabilities (approximately how much higher or lower they might be). Possible methods for this include the tabular scoring approach used by Fera (2009) or formal elicitation of expert judgements (O'Hagan *et al*., 2006). These approaches will be used to assess unquantified uncertainties affecting the probabilistic exposure assessment (step 6a in Figure 6.1). They may also be helpful in evaluating the level of precaution associated with the LLTC and the contribution of other scientific considerations when evaluating proposed C4SLs (steps 6b and 6c in Figure 6.1).

Suggested C4SL CLEA Modification 22: Use qualitative approaches to capture residual unquantified uncertainty within the C4SL derivation process.

There was little specific comment on this proposal but as discussed above, it is necessary to ensure that the C4SL represent an appropriate level of precaution. This proposed modification has been ***retained****.*

6.3 CONSIDERING OTHER LINES OF EVIDENCE

When it comes to pulling all the information together and making a weight-of-evidence decision on where the C4SL should be defined for a substance, all appropriate lines of evidence (qualitative and quantitative) should be brought into the final decision making process. This will provide a 'cross-check' that in the context of the normal course of people's daily exposure, the C4SL for soil exposures is *reasonable and pragmatic*.

The exposure modelling and the LLTC provide the main scientific backbone of the C4SL calculation as outlined in Sections 2 and 3. As described in step 6 of Figure 6.1, there may be scope for the resulting C4SL to be modified further by taking a scientifically informed policy-based decision on where it should sit, when put into context with other lines of evidence, including the following:

- Comparing intakes and MOEs from soil alone with current exposure levels and MOEs for environmental intakes of non-soil sources (it will be important to be transparent and explicit about the treatment of background sources from food and water in the initial C4SL derivation within CLEA, in order to take proper account of non-soil sources and consider an individual's total exposure). This provides information on whether soil is a major contributor to the total exposure of a contaminant, and ensures that focusing solely on the soil for exposure reduction would have a beneficial impact on a person's health.
- Evidence as to whether chronic exposures to soil contaminants have or have not led to observable health issues in a population living in a region with contaminants at the C4SL soil concentration or above. It may be worth noting that Defra and the Welsh Assembly Government stated that, to their knowledge, no site in England or Wales has been determined as contaminated due to it causing actual significant health effects (Defra, 2012b). Moreover, recent research has found limited evidence to support a link between adverse health effects and the level and type of and contamination found in England and Wales (Fera, 2009; Bull, 2012).
- Background soil concentrations in the British Geological Survey Report (Johnson *et al.,* 2012) to which people are exposed during normal daily life.
- Any social or economic considerations that authorities or stakeholders consider relevant to determining an appropriate level of precaution.

7. CONSIDERATIONS IN USE OF THE C4SL

This section outlines some considerations in the use of C4SLs. It will be developed further in WP2 and WP3.

7.1 STATISTICAL CONSIDERATIONS

The appropriate use of statistics is fundamental to ensuring that the risks associated with soil contamination are appropriately characterised and understood. There is a considerable amount of guidance available on this subject, including the following:

- Guidance from the Environment Agency (EA, 2000; EA, 2002b)
- Guidance from CIEH/CL:AIRE (2008);
- Relevant published articles (eg, Nathanail, 2004, Welch, 2011, CL:AIRE, 2006).

The above documents are being reviewed as part of Work Package 2 (WP2) of this research project, with a particular emphasis on the following:

- Appropriate use of the Chebyshev test for non parametric data;
- Problems arising from the use of lower confidence limits and small sample sizes;
- Alternative and simpler non-parametric and data-driven approaches for assessing uncertainty; and
- An improved methodology for consideration of non-detects in the statistical analysis of measured concentrations.

Recommendations will be made on whether the existing guidance represents best practice or whether alternative methods should be adopted (and, if so, what these are). This aspect of the C4SLs research project is being undertaken by Fera and has yet to be completed.

7.2 CONSIDERATION OF ACUTE EXPOSURE

Given the focus of the C4SLs will be on chronic exposure scenarios and statistical methods will be used to interpret site soil data, there is a possibility that land contamination risk assessment could be under-protective of potential acute exposure scenarios, especially in non-residential settings. As a result, it is suggested that this is flagged up as an issue to be addressed on a site-specific basis, as explained within the existing CLEA framework. The authors are aware of a recent Part 2A determination on the basis of acute risks (Macklin *et al.,* 2012) and some work is being undertaken on this aspect by a sub-group of the Society of Brownfield Risk Assessment (SoBRA).

Suggested C4SL CLEA Modification 23: Acute exposure scenarios should be considered on a site-specific basis, especially when C4SLs are used in combination with statistical approaches.

There was majority agreement with this modification although potentially it is not a 'modification' but a restatement of practice that can/should already be used under the existing CLEA framework. We will ***retain*** *this suggested modification for further discussion.*

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APPENDIX 1

SENSITIVITY ANALYSES

Table A2.1: Range in parameter values used for Sensitivity Analysis - Residential Land-Use

Parameter	Units	CLEA default	Minimum	Maximum	Justification
Ambient soil temperature	K	283	280	284	Minimum and maximum values taken from range given in Section 4.3.1 in SR3.
Building footprint	m^2	28	28	78	No change for minimum value. Maximum value assumes a bungalow building type, table 4.21 in SR3.
Living space air exchange rate	hr^{-1}	0.5	0.5	0.5	No change
Living space height (above ground)	m	4.8	2.4	4.8	No change for maximum value. Minimum value assumes a bungalow building type, table 4.21 in SR3.
Living space height (below ground)	m	0	0	0	No change
Pressure difference (soil to enclosed space)	Pa	3.1	2.6	3.1	No change for maximum value. Minimum value assumes a bungalow building type, table 4.21 in SR3.
Foundation thickness	m	0.15	0.075	0.3	Min and max values based on 0.5 x and 2 x CLEA value
Floor crack area	cm^2	423.3	423.3	706.5	No change for minimum value. Maximum value assumes a bungalow building type, table 4.21 in SR3.
Dust loading factor	$\mu g\ m^{-3}$	50	25	100	Min and max values based on 0.5 x and 2 x CLEA value
Mean annual windspeed (10 m)	$m\ s^{-1}$	5	4.1	9.3	Minimum and maximum values taken from range given in Section 9.2.2 in SR3.
Air dispersion factor at height of 0.8 m	$g\ m^{-2}\ s^{-1}$ per $kg\ m^{-3}$	2400	2200	3500	Minimum and maximum values taken from Table 9.1 in SR3.
Fraction of site with hard or vegetative cover	$m^2\ m^{-2}$	0.75	0.5	1	Minimum and maximum values considered to give a reasonable range to test uncertainty
Depth to top of source (beneath building)	cm	65	30	100	Minimum and maximum values considered to give a reasonable range to test uncertainty
Air-water partition coefficient (Kaw) benzene	cm3 cm-3	0.116	0.09	0.116	No change in the maximum value. Minimum value based on lowest henry's law constant value given in Table A4, SR7.
Air-water partition coefficient (Kaw) benzo(a)pyrene	cm3 cm-3	0.00000176	1.76E-06	1.91E-06	No change in the minimum value. Maximum value highest henry's law constant value given in Table A4, SR7.
Diffusion coefficient in air benzene	m2 s-1	0.00000877	7.98E-06	8.80E-06	Minimum value from table E1, SR7. Maximum value from J&E database
Diffusion coefficient in air benzo(a)pyrene	m2 s-1	0.00000438	4.16E-06	4.60E-06	Maximum value fromtable E1, SR7. Minimum value assumes that CLEA default value is a median based on max
Diffusion coefficient in water benzene	m2 s-1	6.64E-10	5.78E-10	7.5E-10	Average absolute error between calculateed and experimental values reported as 13%. Minimum and maximum values reflect this error.
Diffusion coefficient in water benzo(a)pyrene	m2 s-1	3.67E-10	3.19E-10	4.15E-10	Average absolute error between calculateed and experimental values reported as 13%. Minimum and maximum values reflect this error.
Koc benzene	Log (cm3 g-1)	1.83	1.8	1.85	Minimum and maximum values estimated by linear regression from log Kow ranges, using estimation method in Table 2.12, SR7
Koc benzo(a)pyrene	Log (cm3 g-1)	5.11	4.99	5.12	Minimum and maximum values estimated by linear regression from log Kow ranges, using estimation method in Table 2.12, SR8
Kow benzene	Log (dimensionless)	2.13	2.1	2.16	Minimum value from Table A7, SR7. Maximum value given assumes that CLEA default value is a median based on min
Kow benzo(a)pyrene	Log (dimensionless)	6.18	6.04	6.2	Minimum and maximum values from Table A7, SR7.
Dermal absorption fraction benzene	dimensionless	0.1	0.05	0.2	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction benzo(a)pyrene	dimensionless	0.13	0.065	0.26	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction arsenic	dimensionless	0.03	0.015	0.06	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction chromium (VI)	dimensionless	0.01	0.005	0.02	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction cadmium	dimensionless	0.001	0.0005	0.002	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction lead	dimensionless	0	0	0.001	No change in the minimum value. Reasonable maximum value given.
Relative Bioavailability soil	dimensionless	1	1.00E-01	1.00E+00	No change in maximum value. Reasonable minimum value given
Relative Bioavailability airborne dust	dimensionless	1	1.00E-01	1.00E+00	No change in maximum value. Reasonable minimum value given
Soil-to-plant concentration factor (green vegetables) BaP	mg g-1 FW plant / mg g-1 DW soil	0.000412	5.24E-05	3.90E-03	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (green vegetables) As	mg g-1 FW plant / mg g-1 DW soil	0.00043	1.60E-05	1.10E-02	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (green vegetables) Cd	mg g-1 FW plant / mg g-1 DW soil	0.052	1.10E-03	4.4	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (green vegetables) Pb	mg g-1 DW plant / mg g-1 DW soil	0.012	0.006	0.024	Min and max values based on 0.5 x and 2 x CLEA value
Soil-to-plant concentration factor (root vegetables) BaP	mg g-1 FW plant / mg g-1 DW soil	0.00178	2.73E-05	1.39E-02	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (root vegetables) As	mg g-1 FW plant / mg g-1 DW soil	0.0004	6.00E-05	3.60E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (root vegetables) Cd	mg g-1 FW plant / mg g-1 DW soil	0.029	5.40E-04	3.30E-01	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (root vegetables) Pb	mg g-1 DW plant / mg g-1 DW soil	0.008	0.004	0.016	Min and max values based on 0.5 x and 2 x CLEA value

Table A2.1: Range in parameter values used for Sensitivity Analysis - Residential Land-Use

Parameter	Units	CLEA default	Minimum	Maximum	Justification
Soil-to-plant concentration factor (tuber vegetables) BaP	mg g-1 FW plant / mg g-1 DW soil	0.000889	7.33E-06	4.57E-02	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (tuber vegetables) As	mg g-1 FW plant / mg g-1 DW soil	0.00023	2.80E-05	1.80E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (tuber vegetables) Cd	mg g-1 FW plant / mg g-1 DW soil	0.031	5.00E-03	1.10E-01	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (tuber vegetables) Pb	mg g-1 DW plant / mg g-1 DW soil	0.008	0.004	0.016	Min and max values based on 0.5 x and 2 x CLEA value
Soil-to-plant concentration factor (herbaceous fruit) BaP	mg g-1 FW plant / mg g-1 DW soil	0.000508	3.33E-06	2.07E-01	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (herbaceous fruit) As	mg g-1 FW plant / mg g-1 DW soil	0.00033	9.40E-05	2.60E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (herbaceous fruit) Cd	mg g-1 FW plant / mg g-1 DW soil	0.016	7.70E-04	1.00E+00	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (herbaceous fruit) Pb	mg g-1 DW plant / mg g-1 DW soil	0.012	0.006	0.024	Min and max values based on 0.5 x and 2 x CLEA value
Soil-to-plant concentration factor (shrub fruit) BaP	mg g-1 FW plant / mg g-1 DW soil	0.00000563	5.63E-07	5.63E-05	In absence of literature values, min and max values based on an order of magnitude below and above the default value. (This range is consistent with the range for BaP in tree fruit)
Soil-to-plant concentration factor (shrub fruit) As	mg g-1 FW plant / mg g-1 DW soil	0.0002	5.40E-05	9.10E-04	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (shrub fruit) Cd	mg g-1 FW plant / mg g-1 DW soil	0.0031	1.70E-03	5.60E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (shrub fruit) Pb	mg g-1 DW plant / mg g-1 DW soil	0.012	0.006	0.024	Min and max values based on 0.5 x and 2 x CLEA value
Soil-to-plant concentration factor (tree fruit) BaP	mg g-1 FW plant / mg g-1 DW soil	0.0000469	5.21E-06	4.22E-04	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (tree fruit) As	mg g-1 FW plant / mg g-1 DW soil	0.0011	7.10E-04	1.80E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (tree fruit) Cd	mg g-1 FW plant / mg g-1 DW soil	0.0014	3.20E-04	3.20E-02	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (tree fruit) Pb	mg g-1 DW plant / mg g-1 DW soil	0.012	0.006	0.024	Min and max values based on 0.5 x and 2 x CLEA value
Sub-surface soil to indoor air correction factor benzene	dimensionless	10	1.00E+00	1.00E+03	Minumum and maximum values based on Fig A2.1 in VOC handbook, CIRIA C682, 2009
Soil-to-dust transport factor	g g-1 DW	0.5	2.50E-01	8.00E-01	Minimum and maximum values considered to give a reasonable range to test uncertainty
Exposure duration / averaging time	years	6	6.00E+00	7.50E+01	6 years = Average ADE calculated for age classes 1 to 6. 75 years = Average ADE calcuated for age classes 1 to 18. Note: no change for cadmium as lifetime averaging used for derivation of SGV.

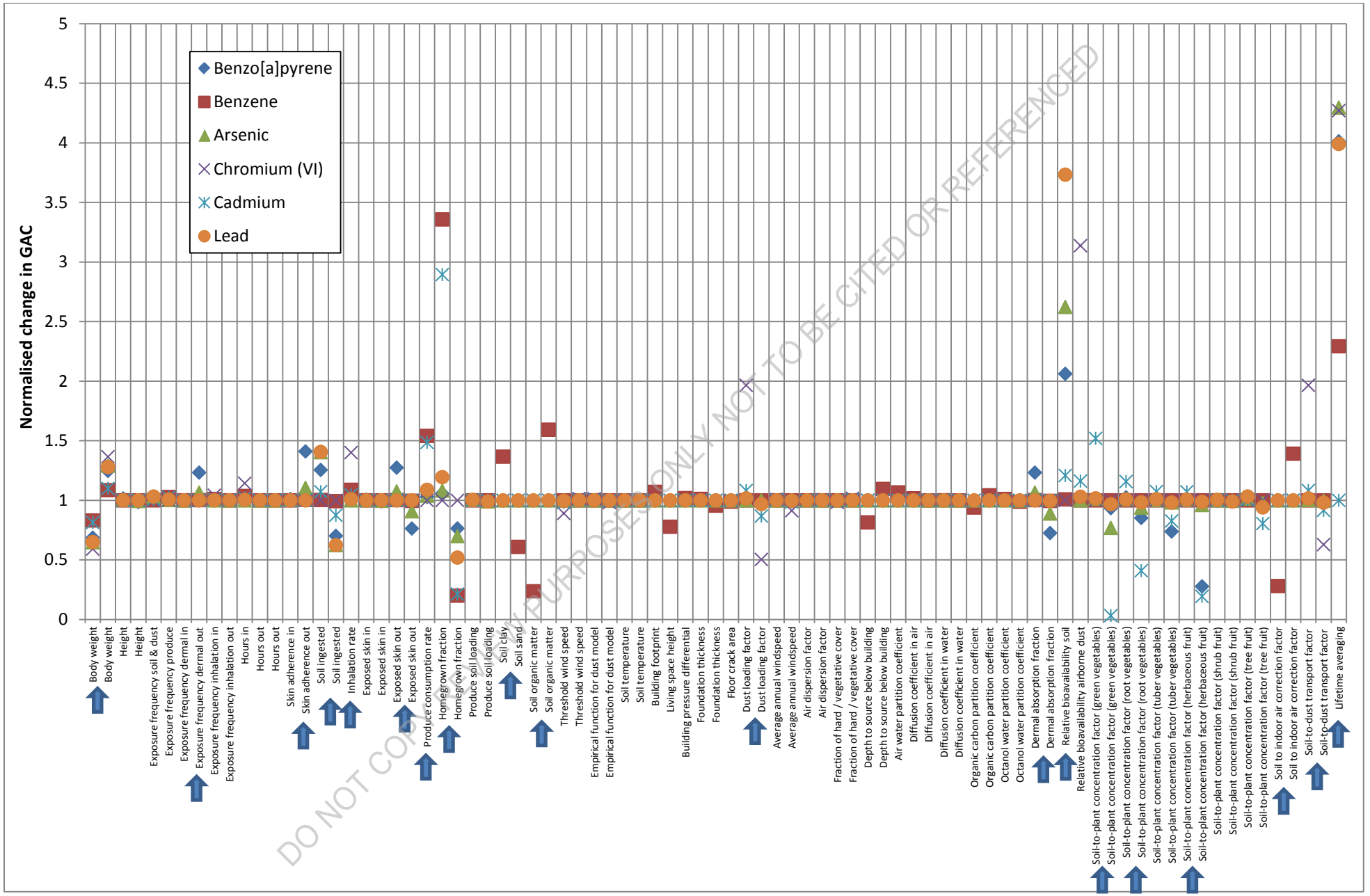


Figure A2.1: Results of sensitivity analysis for residential land-use

Table A2.2: Range in parameter values used for Sensitivity Analysis - Allotments Land-Use

Parameter	Units	CLEA default	Minimum	Maximum	Justification
Body weight age classes 1-6	kg	5.6 - 19.7	2.4 - 12.1	8.8-28.7	Minimum values calculated assuming 2 standard deviations below mean weight, thus inclusive of approximately 5% of population. Maximum values Calculated assuming 2 standard deviations above mean weight, thus inclusive of approximately 95% of population. Taken from Jeffries 2009.
Body height age classes 1-6	m	0.7-1.1	0.62-1	0.78-1.2	Minimum values calculated assuming 2 standard deviations below mean weight, thus inclusive of approximately 5% of population. Maximum values Calculated assuming 2 standard deviations above mean weight, thus inclusive of approximately 95% of population. Taken from Jeffries 2009. Needed to calculate non-CLEA total skin area.
EF (soil and dust ingestion) age class 1	day yr^{-1}	25	13	52	Original values based on Table 3.5 in SR3. Minimum and maximum values are based on 0.5 x and 2 x CLEA values.
EF (soil and dust ingestion) age classes 2-4	day yr^{-1}	130	65	258	
EF (soil and dust ingestion) age classes 5-6	day yr^{-1}	65	32	130	
EF (consumption of homegrown produce) age class 1	day yr^{-1}	180	175	180	No change for maximum values. Minimum values assume child is away from home for 2 weeks of the year, such as holidays and a 0-1 year old child does not have solids for first 6 months of year.
EF (consumption of homegrown produce) age classes 2-6	day yr^{-1}	365	350	365	
EF (skin contact, indoor) age classes 1-6	day yr^{-1}	0	0	0	No change for maximum values. Minimum values assume child is away from home for 2 weeks of the year, such as holidays and a 0-1 year old child does not come into contact with surfaces for first 6 months of year.
EF (skin contact, outdoor) age class 1	day yr^{-1}	25	13	52	Original values based on Table 3.5 in SR3. Minimum and maximum values are based on 0.5 x and 2 x CLEA values.
EF (skin contact, outdoor) age classes 2-4	day yr^{-1}	130	65	258	
EF (skin contact, outdoor) age classes 5-6	day yr^{-1}	65	32	130	
EF (inhalation of dust and vapour, indoor) age classes 1-6	day yr^{-1}	0	0	0	No change for maximum values. Minimum values assume child is away from home for 2 weeks of the year, such as holidays
EF (inhalation of dust and vapour, outdoor) age class 1	day yr^{-1}	25	13	52	Original values based on Table 3.5 in SR3. Minimum and maximum values are based on 0.5 x and 2 x CLEA values.
EF (inhalation of dust and vapour, outdoor) age classes 2-4	day yr^{-1}	130	65	258	
EF (inhalation of dust and vapour, outdoor) age classes 5-6	day yr^{-1}	65	32	130	
Occupancy Period (indoor) age classes 1-6	hr day^{-1}	0	0	0	No change for maximum values. Minimum values are reasonable for representing majority of 0 to 6 year old children
Occupancy Period (outdoor) age classes 1-6	hr day^{-1}	3	1.5	4	Min and max is a reasonable range for representing majority of 0 to 6 year old children
Soil to skin adherence factor (indoor) age classes 1-6	mg cm^{-2} day^{-1}	0	0	0	No change for maximum value. Minimum value taken from US EPA (2004) for 1-13 year old children for indoor play . Based on the geometric mean of experimental studies.
Soil to skin adherence factor (outdoor) age classes 1-6	mg cm^{-2} day^{-1}	1	0.2	1	No change for maximum value. Minimum value taken from US EPA (2004) for 8-12 year old children for wet soil (the more conservative scenario). Based on the geometric mean of experimental studies.
Soil and dust ingestion rate age classes 1-6	g day^{-1}	0.1	0.04	0.175	Minimum value based on 70% of mean values in USEPA, 2008 (assumes that 30% of 100 mg soil ingested is from off-site sources). Maximum value based on SR3 which notes that a reasonable worst-case estimate is 150-200mg/day.
Inhalation rate age classes 1-6	m^3 day^{-1}	10.3-24.9	4.32-6.72	20.16-30.72	Minimum values based on mean inhalation rates for a sedentary and passive activity, maximum values based on a moderate intensity activity, Table 4.13 in SR3.
Max exposed skin fraction (indoor) age classes 1-6	m^2 m^{-2}	0.32-0.35	0.17-0.18	0.52-0.59	Minimum values assume face, hands and feet exposed. Maximum values assume face, hands, arms, legs and feet exposed (Values taken from USEPA, 2008 for age classes 1 to 6)
Max exposed skin fraction (outdoor) age classes 1-6	m^2 m^{-2}	0.25-0.28	0.1-0.11	0.45-0.52	Minimum values assume face and hands exposed. Maximum values assume face, hands, arms and legs exposed (Values taken from USEPA, 2008 for age classes 1 to 6)
Produce consumption rate	g FW kg-1 BW day-1	1	5.00E-01	1.00E+00	No change in maximum values, i.e.90th percentile rates. Minimum values are half the maximum values.
Homegrown fraction	dimensionless	high	average	high	No change in maximum value. Minimum value assumes that an allotment produces average produce for consumption.
Produce soil loading	g g-1 DW	0.001	5.00E-04	2.00E-03	Min and max values based on 0.5 x and 2 x CLEA value
Porosity, air-filled	cm^3 cm^{-3}	0.2	0.12	0.3	Minimum values assume clay type soil. Maximum values assume sand type soil. Values used taken from Table 4.4 in SR3.
Porosity, water-filled	cm^3 cm^{-3}	0.33	0.47	0.24	
Residual soil water Content	cm^3 cm^{-3}	0.12	0.24	0.07	
Saturated hydraulic conductivity	cm s^{-1}	0.00356	9.93E-04	7.36E-03	
van Genuchten shape parameter (m)	dimensionless	0.3201	0.2972	0.3509	

Table A2.2: Range in parameter values used for Sensitivity Analysis - Allotments Land-Use

Parameter	Units	CLEA default	Minimum	Maximum	Justification
Bulk density	g cm^{-3}	1.21	1.07	1.18	
Soil organic matter	%	6	1.00E+00	1.00E+01	Minimum and maximum values considered to give a reasonable range to test uncertainty
Threshold value of wind speed at 10m	m s^{-1}	7.2	3.6	14.4	Min and max values based on 0.5 x and 2 x CLEA value
Empirical function (Fx) for dust model	dimensionless	1.22	0.26	2.55	Minimum and maximum values calculated using minimum and maximum threshold values of wind speed at 10m and Equation 9.4 in SR3.
Ambient soil temperature	K	283	280	284	Minimum and maximum values taken from range given in Section 4.3.1 in SR3.
Mean annual windspeed (10 m)	m s^{-1}	5	4.1	9.3	Minimum and maximum values taken from range given in Section 9.2.2 in SR3.
Air dispersion factor at height of 0.8 m	g m^{-2} s^{-1} per kg m^{-3}	120	120	270	Minimum and maximum values taken from Table 9.1 in SR3.
Fraction of site with hard or vegetative cover	m^2 m^{-2}	0.5	0	0.75	Minimum and maximum values considered to give a reasonable range to test uncertainty
Default soil gas ingress rate	cm^3 s^{-1}	0	0	0	No change
Depth to top of source (beneath building)	cm	50	30	100	Minimum and maximum values considered to give a reasonable range to test uncertainty
Air-water partition coefficient (Kaw) benzene	cm3 cm-3	0.116	0.09	0.116	No change in the maximum value. Minimum value based on lowest henry's law constant value given in Table A4, SR7.
Air-water partition coefficient (Kaw) benzo(a)pyrene	cm3 cm-3	0.00000176	1.76E-06	1.91E-06	No change in the minimum value. Maximum value highest henry's law constant value given in Table A4, SR7.
Diffusion coefficient in air benzene	m2 s-1	0.00000877	7.98E-06	8.80E-06	Minimum value from table E1, SR7. Maximum value from J&E database
Diffusion coefficient in air benzo(a)pyrene	m2 s-1	0.00000438	4.16E-06	4.60E-06	Maximum value fromtable E1, SR7. Minimum value assumes that CLEA default value is a median based on max
Diffusion coefficient in water benzene	m2 s-1	6.64E-10	5.78E-10	7.5E-10	Average absolute error between calculateed and experimental values reported as 13%. Minimum and maximum values reflect this error.
Diffusion coefficient in water benzo(a)pyrene	m2 s-1	3.67E-10	3.19E-10	4.15E-10	Average absolute error between calculateed and experimental values reported as 13%. Minimum and maximum values reflect this error.
Koc benzene	Log (cm3 g-1)	1.83	1.8	1.85	Minimum and maximum values estimated by linear regression from log Kow ranges, using estimation method in Table 2.12, SR7
Koc benzo(a)pyrene	Log (cm3 g-1)	5.11	4.99	5.12	Minimum and maximum values estimated by linear regression from log Kow ranges, using estimation method in Table 2.12, SR8
Kow benzene	Log (dimensionless)	2.13	2.1	2.16	Minimum value from Table A7, SR7. Maximum value given assumes that CLEA default value is a median based on min
Kow benzo(a)pyrene	Log (dimensionless)	6.16	6.04	6.2	Minimum and maximum values from Table A7, SR7.
Dermal absorption fraction benzene	dimensionless	0.1	0.05	0.2	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction benzo(a)pyrene	dimensionless	0.13	0.065	0.26	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction arsenic	dimensionless	0.03	0.015	0.06	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction chromium (VI)	dimensionless	0.01	0.005	0.02	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction cadmium	dimensionless	0.001	0.0005	0.002	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction lead	dimensionless	0	0	0.001	No change in the minimum value. Reasonable maximum value given.
Soil-to-plant concentration factor (green vegetables) BaP	mg g-1 FW plant / mg g-1 DW soil	0.000412	5.24E-05	3.90E-03	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (green vegetables) As	mg g-1 FW plant / mg g-1 DW soil	0.00043	1.60E-05	1.10E-02	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (green vegetables) Cd	mg g-1 FW plant / mg g-1 DW soil	0.052	1.10E-03	4.4	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (green vegetables) Pb	mg g-1 DW plant / mg g-1 DW soil	0.012	0.006	0.024	Min and max values based on 0.5 x and 2 x CLEA value
Soil-to-plant concentration factor (root vegetables) BaP	mg g-1 FW plant / mg g-1 DW soil	0.00178	2.73E-05	1.39E-02	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (root vegetables) As	mg g-1 FW plant / mg g-1 DW soil	0.0004	6.00E-05	3.60E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (root vegetables) Cd	mg g-1 FW plant / mg g-1 DW soil	0.029	5.40E-04	3.30E-01	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (root vegetables) Pb	mg g-1 DW plant / mg g-1 DW soil	0.008	0.004	0.016	Min and max values based on 0.5 x and 2 x CLEA value
Soil-to-plant concentration factor (tuber vegetables) BaP	mg g-1 FW plant / mg g-1 DW soil	0.000889	7.33E-06	4.57E-02	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (tuber vegetables) As	mg g-1 FW plant / mg g-1 DW soil	0.00023	2.80E-05	1.80E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (tuber vegetables) Cd	mg g-1 FW plant / mg g-1 DW soil	0.031	5.00E-03	1.10E-01	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (tuber vegetables) Pb	mg g-1 DW plant / mg g-1 DW soil	0.008	0.004	0.016	Min and max values based on 0.5 x and 2 x CLEA value
Soil-to-plant concentration factor (herbaceous fruit) BaP	mg g-1 FW plant / mg g-1 DW soil	0.000508	3.33E-06	2.07E-01	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (herbaceous fruit) As	mg g-1 FW plant / mg g-1 DW soil	0.00033	9.40E-05	2.60E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (herbaceous fruit) Cd	mg g-1 FW plant / mg g-1 DW soil	0.016	7.70E-04	1.00E+00	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (herbaceous fruit) Pb	mg g-1 DW plant / mg g-1 DW soil	0.012	0.006	0.024	Min and max values based on 0.5 x and 2 x CLEA value

Table A2.2: Range in parameter values used for Sensitivity Analysis - Allotments Land-Use

Parameter	Units	CLEA default	Minimum	Maximum	Justification
Soil-to-plant concentration factor (shrub fruit) BaP	mg g-1 FW plant / mg g-1 DW soil	0.00000563	5.63E-07	5.63E-05	In absence of literature values, min and max values based on an order of magnitude below and above the default value. (This range is consistent with the range for BaP in tree fruit)
Soil-to-plant concentration factor (shrub fruit) As	mg g-1 FW plant / mg g-1 DW soil	0.0002	5.40E-05	9.10E-04	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (shrub fruit) Cd	mg g-1 FW plant / mg g-1 DW soil	0.0031	1.70E-03	5.60E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (shrub fruit) Pb	mg g-1 DW plant / mg g-1 DW soil	0.012	0.006	0.024	Min and max values based on 0.5 x and 2 x CLEA value
Soil-to-plant concentration factor (tree fruit) BaP	mg g-1 FW plant / mg g-1 DW soil	0.0000469	5.21E-06	4.22E-04	Minimum and maximum ranges taken from Table 2.7 of EA, unpublished info on PAHs
Soil-to-plant concentration factor (tree fruit) As	mg g-1 FW plant / mg g-1 DW soil	0.0011	7.10E-04	1.80E-03	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on As
Soil-to-plant concentration factor (tree fruit) Cd	mg g-1 FW plant / mg g-1 DW soil	0.0014	3.20E-04	3.20E-02	Minimum and maximum ranges taken from Table 3.1 of EA, 2009 - Supp SGV info on Cd
Soil-to-plant concentration factor (tree fruit) Pb	mg g-1 DW plant / mg g-1 DW soil	0.012	0.006	0.024	Min and max values based on 0.5 x and 2 x CLEA value
Relative Bioavailability soil	dimensionless	1	1.00E-01	1.00E+00	No change in maximum value. Reasonable minimum value given
Relative Bioavailability airborne dust	dimensionless	1	1.00E-01	1.00E+00	No change in maximum value. Reasonable minimum value given
Exposure duration / averaging time	years	6	6.00E+00	7.50E+01	6 years = Average ADE calculated for age classes 1 to 6. 75 years = Average ADE calcuated for age classes 1 to 18. Note: no change for cadmium as lifetime averaging used for derivation of SGV.

Table A2.1: Range in parameter values used for Sensitivity Analysis - Residential Land-Use

Parameter	Units	CLEA default	Minimum	Maximum	Justification
Body weight age classes 1-6	kg	5.6 - 19.7	2.4 - 12.1	8.8-28.7	Minimum values calculated assuming 2 standard deviations below mean weight, thus inclusive of approximately 5% of population. Maximum values Calculated assuming 2 standard deviations above mean weight, thus inclusive of approximately 95% of population. Taken from Jeffries 2009.
Body height age classes 1-6	m	0.7-1.1	0.62-1	0.78-1.2	Minimum values calculated assuming 2 standard deviations below mean weight, thus inclusive of approximately 5% of population. Maximum values Calculated assuming 2 standard deviations above mean weight, thus inclusive of approximately 95% of population. Taken from Jeffries 2009. Needed to calculate non-CLEA total skin area.
EF (soil and dust ingestion) age class 1	day yr^{-1}	180	175	180	No change for maximum values. Minimum values assume child is away from home for 2 weeks of the year, such as holidays and a 0-1 year old child does not come into contact with surfaces for first 6 months of
EF (soil and dust ingestion) age classes 2-6	day yr^{-1}	365	350	365	
EF (consumption of homegrown produce) age class 1	day yr^{-1}	180	175	180	No change for maximum values. Minimum values assume child is away from home for 2 weeks of the year, such as holidays and a 0-1 year old child does not come into contact with surfaces for first 6 months of
EF (consumption of homegrown produce) age classes 2-6	day yr^{-1}	365	350	365	
EF (skin contact, indoor) age class 1	day yr^{-1}	180	175	180	No change for maximum values. Minimum values assume child is away from home for 2 weeks of the year, such as holidays and a 0-1 year old child does not come into contact with surfaces for first 6 months of
EF (skin contact, indoor) age classes 2-6	day yr^{-1}	365	350	365	
EF (skin contact, outdoor) age class 1	day yr^{-1}	180	88	180	No change for maximum values. Minimum values assume child comes into dermal contact with soil outdoors at property 50% of days at property
EF (skin contact, outdoor) age classes 2-6	day yr^{-1}	365	175	365	
EF (inhalation of dust and vapour, indoor) age classes 1-6	day yr^{-1}	365	350	365	No change for maximum values. Minimum values assume child is away from home for 2 weeks of the year, such as holidays
EF (inhalation of dust and vapour, outdoor) age classes 1-6	day yr^{-1}	365	175	365	No change for maximum values. Minimum values assume child is outside (1hr per day) at property 50% of days at property
Occupancy Period (indoor) age classes 1-4	hr day^{-1}	23	20	23	No change for maximum values. Minimum values are reasonable for representing majority of 0 to 6 year old children
Occupancy Period (indoor) age classes 5-6	hr day^{-1}	19	17	19	
Occupancy Period (outdoor) age classes 1-6	hr day^{-1}	1	0.5	2	Min and max is a reasonable range for representing majority of 0 to 6 year old children
Soil to skin adherence factor (indoor) age classes 1-6	mg cm^{-2} day^{-1}	0.06	0.01	0.06	No change for maximum value. Minimum value taken from US EPA (2004) for 1-13 year old children for indoor play . Based on the geometric mean of experimental studies.
Soil to skin adherence factor (outdoor) age classes 1-6	mg cm^{-2} day^{-1}	1	0.2	1	No change for maximum value. Minimum value taken from US EPA (2004) for 8-12 year old children for wet soil (the more conservative scenario). Based on the geometric mean of experimental studies.
Soil and dust ingestion rate age classes 1-6	g day^{-1}	0.1	0.04	0.175	Minimum value based on 70% of mean values in USEPA, 2008 (assumes that 30% of 100 mg soil ingested is from off-site sources). Maximum value based on SR3 which notes that a reasonable worst-case estimate is 150-200mg/day.
Inhalation rate age classes 1-6	m^3 day^{-1}	8.5-13.3	4.8-10.9	8.5-13.3	No change for maximum values. Minimum values are recommended mean inhalation rates from USEPA, 2008.
Max exposed skin fraction (indoor) age classes 1-6	m^2 m^{-2}	0.32-0.35	0.17-0.18	0.52-0.59	Minimum values assume face, hands and feet exposed. Maximum values assume face, hands, arms, legs and feet exposed (Values taken from USEPA, 2008 for age classes 1 to 6)
Max exposed skin fraction (outdoor) age classes 1-6	m^2 m^{-2}	0.25-0.28	0.1-0.11	0.45-0.52	Minimum values assume face and hands exposed. Maximum values assume face, hands, arms and legs exposed (Values taken from USEPA, 2008 for age classes 1 to 6)
Produce consumption rate	g FW kg-1 BW day-1	1	5.00E-01	1.00E+00	No change in maximum values, i.e.90th percentile rates. Minimum values are half the maximum values.
Homegrown fraction	dimensionless	average	none	high	Minimum and maximum values reflect other two options available in CLEA model
Produce soil loading	g g-1 DW	0.001	5.00E-04	2.00E-03	Min and max values based on 0.5 x and 2 x CLEA value
Porosity, air-filled	cm^3 cm^{-3}	0.2	0.12	0.3	Minimum values assume clay type soil. Maximum values assume sand type soil. Values used taken from Table 4.4 in SR3.
Porosity, water-filled	cm^3 cm^{-3}	0.33	0.47	0.24	
Residual soil water Content	cm^3 cm^{-3}	0.12	0.24	0.07	
Saturated hydraulic conductivity	cm s^{-1}	0.00356	9.93E-04	7.36E-03	
van Genuchten shape parameter (m)	dimensionless	0.3201	0.2972	0.3509	
Bulk density	g cm^{-3}	1.21	1.07	1.18	
Soil organic matter	%	6	1.00E+00	1.00E+01	Minimum and maximum values considered to give a reasonable range to test uncertainty
Threshold value of wind speed at 10m	m s^{-1}	7.2	3.6	14.4	Min and max values based on 0.5 x and 2 x CLEA value
Empirical function (Fx) for dust model	dimensionless	1.22	0.26	2.55	Minimum and maximum values calculated using minimum and maximum threshold values of wind speed at 10m and Equation 9.4 in SR3.

Human Toxicological Data Sheet for C4SL derivation: Toxicological Evidence, HBGVs, MDIs and LLTC derivation

Chemical: **Benzo(a)pyrene**

I) Human Health Hazard Profile - Toxicological Evidence

Type of Evidence	POD type	POD value	Units	Species	Study Type	Comments/Study Quality	Reference
1. Toxicokinetics							EFSA 2008
Oral							
Inhalation							
Dermal							
2. Acute Toxicity							
Oral							Defra & EA 2002; EFSA 2008
Inhalation							
Dermal							
3. Irritation and Corrosivity							
Dermal							Defra & EA 2002
Eye							
4. Sensitisation							
Dermal							Defra & EA 2002
Respiratory							
5. Repeat-dose Toxicity							
Oral							EFSA 2008
Inhalation							IPCS 1998
Dermal							ATSDR 1995
6. Genetic Toxicology							EFSA 2008
In vitro							
In vivo							
7. Carcinogenicity							IARC 2010
Oral							EFSA 2008; Culp et al 1998
Inhalation							
Dermal							
8. Reproduction							
Reproductive							EFSA 2008
Developmental							
Teratogenicity							
9. Human epidemiology data							
Oral							EFSA 2008
Inhalation							
Dermal							ATSDR 1995

Most Sensitive Health Effect:

Table A2.3: Range in parameter values used for Sensitivity Analysis - Commercial Land-Use

Parameter	Units	CLEA default	Minimum	Maximum	Justification
Body weight age class 17	kg	70	39	101	Minimum values calculated assuming 2 standard deviations below mean weight, thus inclusive of approximately 5% of population. Maximum values Calculated assuming 2 standard deviations above mean weight, thus inclusive of approximately 95% of population. Taken from Jeffries 2009.
Body height age class 17	m	1.6	1.48	1.72	Minimum values calculated assuming 2 standard deviations below mean weight, thus inclusive of approximately 5% of population. Maximum values Calculated assuming 2 standard deviations above mean weight, thus inclusive of approximately 95% of population. Taken from Jeffries 2009. Needed to calculate non-CLEA total skin area.
EF (soil and dust ingestion) age class 17	day yr^{-1}	230	178	282	Minimum value assumes employees works for 4 days a week at workplace (with 6 weeks annual leave). Maximum value assumes that employee works 6 days a week at workplace (with 6 weeks annual leave).
EF (consumption of homegrown produce) age class 17	day yr^{-1}	0	0	0	No change
EF (skin contact, indoor) age class 17	day yr^{-1}	230	178	282	Minimum value assumes employees works for 4 days a week at workplace (with 6 weeks annual leave). Maximum value assumes that employee works 6 days a week at workplace (with 6 weeks annual leave).
EF (skin contact, outdoor) age class 17	day yr^{-1}	170	89	282	Minimum value assumes half of minimum days at workplace. Maximum value assumes maximum days at workplace
EF (inhalation of dust and vapour, indoor) age class 17	day yr^{-1}	230	178	282	Minimum value assumes employees works for 4 days a week at workplace (with 6 weeks annual leave). Maximum value assumes that employee works 6 days a week at workplace (with 6 weeks annual leave).
EF (inhalation of dust and vapour, outdoor) age class 17	day yr^{-1}	170	89	282	Minimum value assumes half of minimum days at workplace. Maximum value assumes maximum days at workplace
Occupancy Period (indoor) age class 17	hr day^{-1}	8.3	6	12	Minimum and maximum values considered to give a reasonable range to test uncertainty
Occupancy Period (outdoor) age class 17	hr day^{-1}	0.7	0	3	Minimum and maximum values considered to give a reasonable range to test uncertainty
Soil to skin adherence factor (indoor) age class 17	mg cm^{-2} day^{-1}	0.14	0.06	0.3	Minimum value based on indoor residential adult (Table 8.1, SR3). Maximum value based on outdoor residential adult.
Soil to skin adherence factor (outdoor) age class 17	mg cm^{-2} day^{-1}	0.14	0.06	0.3	Minimum value based on indoor residential adult (Table 8.1, SR3). Maximum value based on outdoor residential adult.
Soil and dust ingestion rate age class 17	g day^{-1}	0.05	0.025	0.1	Min and max values based on 0.5 x and 2 x CLEA value
Inhalation rate age class 17	m^3 day^{-1}	14.8	6.72	34.08	Minimum values based on mean inhalation rate for a sedentary and passive activity, maximum values based on a moderate intensity activity, Table 4.13 in SR3.
Max exposed skin fraction (indoor) age class 17	m^2 m^{-2}	0.08	0.026	0.27	Minimum values assume face exposed (US EPA, 2004, exhibit C1). Maximum values assume face, hands, forearms and lower legs exposed (Table 4.8, SR3)
Max exposed skin fraction (outdoor) age class 17	m^2 m^{-2}	0.08	0.026	0.27	Minimum values assume face exposed (US EPA, 2004, exhibit C1). Maximum values assume face, hands, forearms and lower legs exposed (Table 4.8, SR3)
Porosity, air-filled	cm^3 cm^{-3}	0.2	0.12	0.3	Minimum values assume clay type soil. Maximum values assume sand type soil. Values used taken from Table 4.4 in SR3.
Porosity, water-filled	cm^3 cm^{-3}	0.33	0.47	0.24	
Residual soil water Content	cm^3 cm^{-3}	0.12	0.24	0.07	
Saturated hydraulic conductivity	cm s^{-1}	0.00356	9.93E-04	7.36E-03	
van Genuchten shape parameter (m)	dimensionless	0.3201	0.2972	0.3509	
Bulk density	g cm^{-3}	1.21	1.07	1.18	
Soil organic matter	%	6	1.00E+00	1.00E+01	Minimum and maximum values considered to give a reasonable range to test uncertainty
Threshold value of wind speed at 10m	m s^{-1}	7.2	3.6	14.4	Min and max values based on 0.5 x and 2 x CLEA value
Empirical function (Fx) for dust model	dimensionless	1.22	0.26	2.55	Minimum and maximum values calculated using minimum and maximum threshold values of wind speed at 10m and Equation 9.4 in SR3.
Ambient soil temperature	K	283	280	284	Minimum and maximum values taken from range given in Section 4.3.1 in SR3.
Building footprint	m^2	424	424	1914	No change for minimum value. Maximum value assumes post 1970 warehouse building type, table 4.21 in SR3.
Living space air exchange rate	hr^{-1}	1	1	1	No change
Living space height (above ground)	m	9.6	4.6	12.8	Minimum value assumes pre 1970 warehouse building type and maximum value assumes post 1970 office building type, table 4.21 in SR3.

Table A2.3: Range in parameter values used for Sensitivity Analysis - Commercial Land-Use

Parameter	Units	CLEA default	Minimum	Maximum	Justification
Living space height (below ground)	m	0	0	0	No change
Pressure difference (soil to enclosed space)	Pa	4.4	3.2	5.1	Minimum value assumes pre 1970 warehouse building type and maximum value assumes post 1970 office building type, table 4.21 in SR3.
Foundation thickness	m	0.15	0.075	0.3	Min and max values based on 0.5 x and 2 x CLEA value
Floor crack area	cm^2	1647.3	1647.3	3499.9	No change for minimum value. Maximum value assumes a post 1970 warehouse building type, table 4.21 in SR3.
Dust loading factor	$\mu g\ m^{-3}$	100	50	200	Min and max values based on 0.5 x and 2 x CLEA value
Mean annual windspeed (10 m)	$m\ s^{-1}$	5	4.1	9.3	Minimum and maximum values taken from range given in Section 9.2.2 in SR3.
Air dispersion factor at height of 0.8 m	$g\ m^{-2}\ s^{-1}$ per $kg\ m^{-3}$	68	68	170	No change in minimum value. Maximum value taken from Table 9.1 in SR3.
Air dispersion factor at height of 1.6 m	$g\ m^{-2}\ s^{-1}$ per $kg\ m^{-3}$	120	120	270	No change in minimum value. Maximum value taken from Table 9.1 in SR3.
Fraction of site with hard or vegetative cover	$m^2\ m^{-2}$	0.8	0.5	1	Minimum and maximum values considered to give a reasonable range to test uncertainty
Depth to top of source (beneath building)	cm	65	30	100	Minimum and maximum values considered to give a reasonable range to test uncertainty
Air-water partition coefficient (Kaw) benzene	cm3 cm-3	0.116	0.09	0.116	No change in the maximum value. Minimum value based on lowest henry's law constant value given in Table A4, SR7.
Air-water partition coefficient (Kaw) benzo(a)pyrene	cm3 cm-3	0.00000176	1.76E-06	1.91E-06	No change in the minimum value. Maximum value highest henry's law constant value given in Table A4, SR7.
Diffusion coefficient in air benzene	m2 s-1	0.00000877	7.98E-06	8.80E-06	Minimum value from table E1, SR7. Maximum value from J&E database
Diffusion coefficient in air benzo(a)pyrene	m2 s-1	0.00000438	4.16E-06	4.60E-06	Maximum value fromtable E1, SR7. Minimum value assumes that CLEA default value is a median based on max
Diffusion coefficient in water benzene	m2 s-1	6.64E-10	5.78E-10	7.5E-10	Average absolute error between calculateed and experimental values reported as 13%. Minimum and maximum values reflect this error.
Diffusion coefficient in water benzo(a)pyrene	m2 s-1	3.67E-10	3.19E-10	4.15E-10	Average absolute error between calculateed and experimental values reported as 13%. Minimum and maximum values reflect this error.
Koc benzene	Log (cm3 g-1)	1.83	1.8	1.85	Minimum and maximum values estimated by linear regression from log Kow ranges, using estimation method in Table 2.12, SR7
Koc benzo(a)pyrene	Log (cm3 g-1)	5.11	4.99	5.12	Minimum and maximum values estimated by linear regression from log Kow ranges, using estimation method in Table 2.12, SR8
Kow benzene	Log (dimensionless)	2.13	2.1	2.16	Minimum value from Table A7, SR7. Maximum value given assumes that CLEA default value is a median based on min
Kow benzo(a)pyrene	Log (dimensionless)	6.18	6.04	6.2	Minimum and maximum values from Table A7, SR7.
Dermal absorption fraction benzene	dimensionless	0.1	0.05	0.2	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction benzo(a)pyrene	dimensionless	0.13	0.065	0.26	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction arsenic	dimensionless	0.03	0.015	0.06	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction chromium (VI)	dimensionless	0.01	0.005	0.02	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction cadmium	dimensionless	0.001	0.0005	0.002	Minimum and maximum values are half and double the CLEA default value.
Dermal absorption fraction lead	dimensionless	0	0	0.001	No change in the minimum value. Reasonable maximum value given.
Sub-surface soil to indoor air correction factor benzene	dimensionless	10	1.00E+00	1.00E+03	Minumum and maximum values based on Fig A2.1 in VOC handbook, CIRIA C682, 2009
Soil-to-dust transport factor	g g-1 DW	0.5	2.50E-01	8.00E-01	Minimum and maximum values considered to give a reasonable range to test uncertainty
Relative Bioavailability soil	dimensionless	1	1.00E-01	1.00E+00	No change in maximum value. Reasonable minimum value given
Relative Bioavailability airborne dust	dimensionless	1	1.00E-01	1.00E+00	No change in maximum value. Reasonable minimum value given

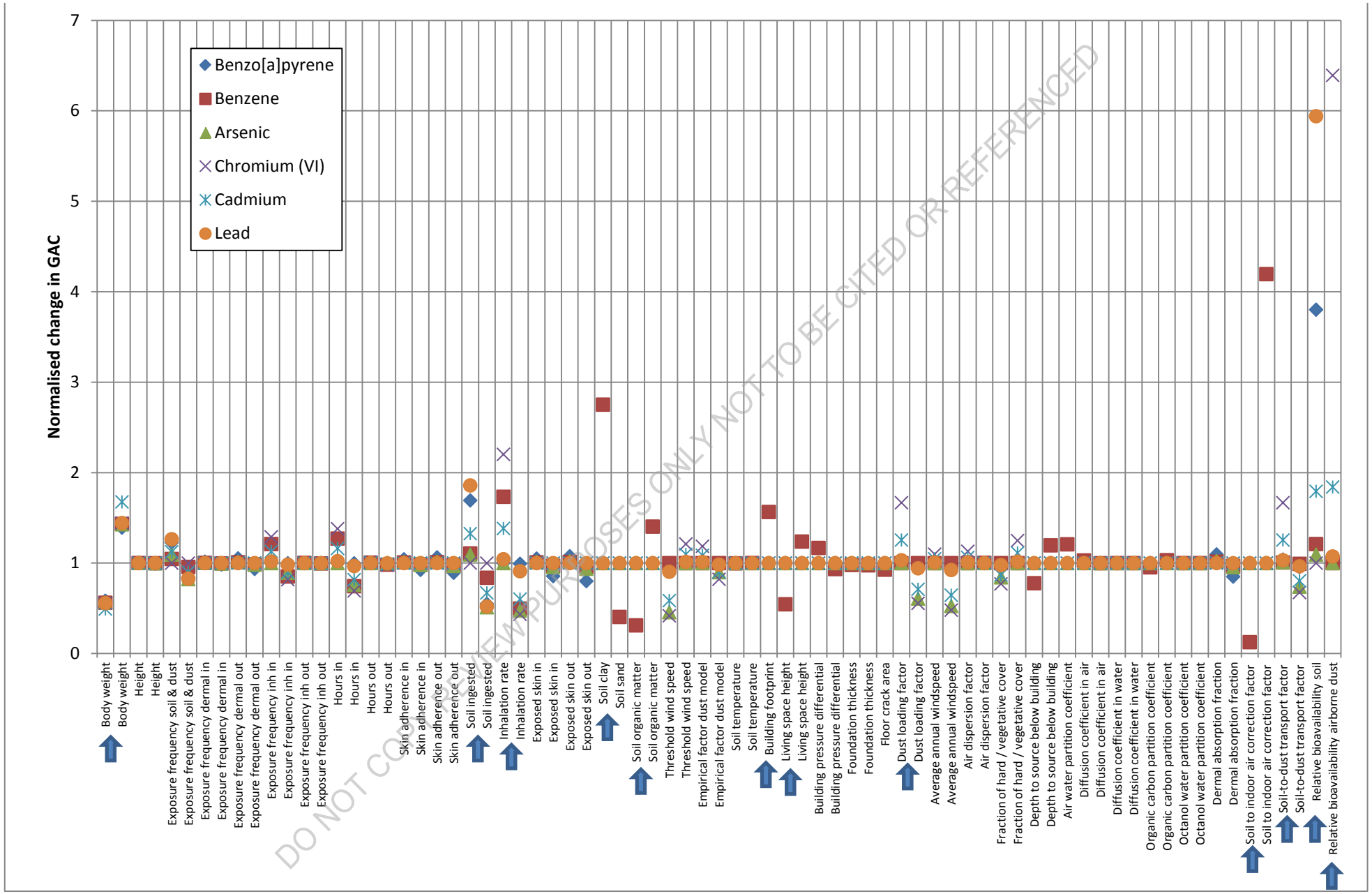


Figure A2.3: Results of sensitivity analysis for commercial land-use

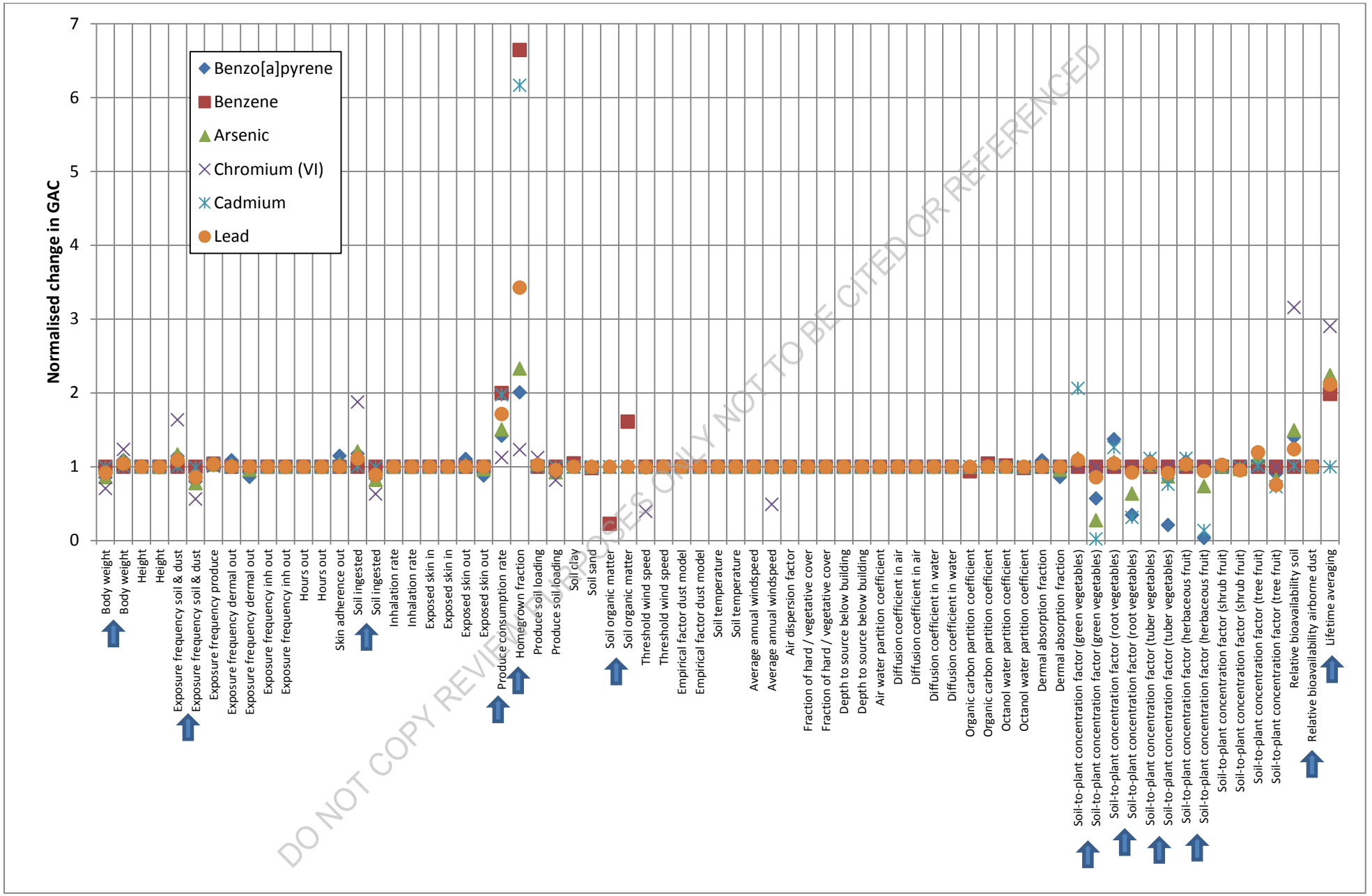


Figure A2.2: Results of sensitivity analysis for allotments land-use

APPENDIX 2

HUMAN TOXICOLOGICAL DATA SHEETS

II) Health Based Guidance Values (HBGVs) from Authoritative Bodies (in descending order of magnitude)							
A) Oral Route	HBGVoral	Unit	UF used	PoD	Endpoint	Pivotal data used & Comments	Reference

Comment:

Current UK oral HCV

B) Inhalation Route	Converted HBGVinh	ng kg^{-1} bw day^{-1}	HBGVinh	ng m^{-3}	UF used	PoD	Endpoint	Pivotal Study used & Comments	Reference

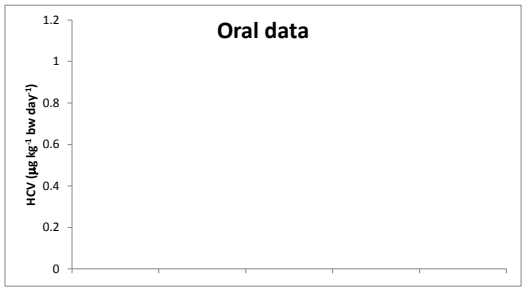
Comment:

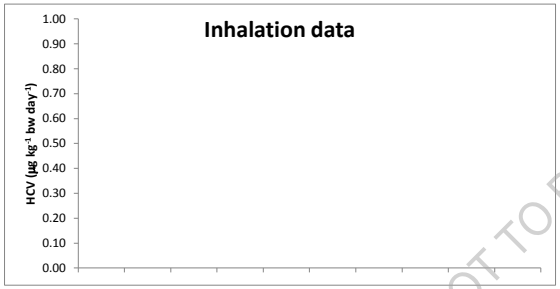
UK inhalation HCV

C) Dermal Route	HBGVderm	Units	UF used	POD	Endpoint	Pivotal Study used & Comments	Reference

COT/COC Opinion:

Positioning of UK Minimal Risk HCV vs other HBGV from authoritative bodies





III) Mean Daily Intakes from Other Sources (e.g. Diet)

	Pathways	Units	Adults	Children	Refs
Food (average)	Oral	µg kg^{-1} bw day^{-1}			
Water	Oral	µg kg^{-1} bw day^{-1}			
Air	Inhalation	ng kg^{-1} bw day^{-1}			
Smoking	Inhalation	ng kg^{-1} bw day^{-1}			

Comment:

IV) LLTC derivation

A) ORAL

Choice of Pivotal Data	Dosing vehicle	Doses	Units	Species	Study Type	Comments	Reference
							Culp et al 1998. A A comparison of the tumors induced by coal tar and benzo[a]pyrene in a two-year bioassay.

BMD Modelling (if relevant)

Software used: US EPA BMDS 2.3.1

	BMD1	BMD5	BMD10	BMD15	BMD20
BMD modelling (value) (mg kg^{-1} bw day^{-1})					
	BMDL1	BMDL5	BMDL10	BMDL15	BMDL20
BMD modelling (value) (mg kg^{-1} bw day^{-1})					

Comments: Modelling carried out for 10, 15 and 20 % tumour incidence. BMDL15 has been selected as the PoD to be sufficiently protective of health but slightly above minimum risk. Alternatively, BMDL20 or BMD10 could be selected.

Point of Departure for ORAL LLTC:	Value	Units
Type of PoD		mg kg^{-1} bw day^{-1}
Description of PoD		
Value selected		mg kg^{-1} bw day^{-1}

Chemical Specific Adjustment Factor to account for uncertainties in the data		
	Range	Selected value
Intraspecies	1 - 10	
Interspecies	1 - 10	
Quality of study	1 - 10	
Severity of effect	1 - 50	

Thresholded chemical?

If yes - calculate CSAF
If no - calculate CSM

CSAF = (for thresholded chemical)

CSM = 0 (for non-thresholded chemical)

ELCR =

Lifetime averaging to be applied in CLEA

Oral LLTC calculation:

	Units
LLTC (Thresholded chemical)	
LLTC (Non Thresholded chemical)	#DIV/0! µg kg^{-1} bw day^{-1}
LLTC (Human carcinogen)	

Comments:

B) INHALATION

Choice of Pivotal Data	Dosing vehicle	Doses	Units	Species	Study Type	Comments	Reference
							UK Air Quality Standards Regulation (2010)

BMD Modelling (if relevant)

Software used

	BMD1	BMD5	BMD10	BMD15	BMD20
BMD modelling (value)					
	BMDL1	BMDL5	BMDL10	BMDL15	BMDL20
BMD modelling (value)					

Comments:

Paste BMDL graph here

Point of Departure for INHALATION LLTC:	Value	Units
Type of PoD		ng m^{-3}
Description of PoD		
Value selected		ng m^{-3}

Chemical Specific Adjustment Factor to account for uncertainties in the data		
	Range	Selected value
Intraspecies	1 - 10	
Interspecies	1 - 10	
Quality of study	1 - 10	
Severity of Effect	1 - 50	

Thresholded chemical?
If yes - calculate CSAF
If no - calculate CSM

CSAF = 0 **(for thresholded chemical)**

CSM = 0 **(for non-thresholded chemical)**

ELCR = 10000

Lifetime averaging to be applied in CLEA

Inhalation LLTC calculation:

	Units
LLTC (Thresholded chemical)	
LLTC (Non Thresholded chemical)	0.0 ng kg^{-1} bw day^{-1}
LLTC (Human carcinogen)	

Comments:

Physiological conversion factors		
	Value	Units
Body weight	70	kg
Inhalation rate	20	m^3

Human Toxicological Data Sheet for C4SL derivation: Reference checklist

Chemical: **Benzo(a)pyrene**

Human Health Hazard Profile - References

Authoratative bodies	Website	Checked (Y/N)	References
EA	http://www.environment-agency.gov.uk/		
FSA	http://www.food.gov.uk/		
COC	http://www.iacoc.org.uk/		
COM	http://www.iacom.org.uk/		
COT	http://cot.food.gov.uk/		
EFSA	http://www.efsa.europa.eu/		
JECFA	http://www.who.int/foodsafety/chem/jecfa/publications/en/index.html		
WHO	http://www.who.int/en/		
RIVM	http://www.rivm.nl/English		
ATDSR	http://www.atsdr.cdc.gov/		
USEPA	http://www.epa.gov/		
Health Canada	http://www.hc-sc.gc.ca/index-eng.php		
Other references			
IOM			
SCF			

APPENDIX 3

MARGIN OF EXPOSURE APPROACH – ADVANTAGES AND LIMITATIONS

Appendix 3

*Excerpt taken from the '***EFSA/WHO INTERNATIONAL CONFERENCE WITH SUPPORT OF ILSI EUROPE ON RISK ASSESSMENT OF COMPOUNDS THAT ARE BOTH GENOTOXIC AND CARCINOGENIC' 16-18 November 2005. ISSN 1725-9843.**

Advantages of the MOE approach compared with other approaches

Since the three documents from ILSI Europe, EFSA and JECFA proposed, or in the case of ILSI Europe and JECFA used, the MOE as the preferred approach for risk assessment advice for substances that are both genotoxic and carcinogenic, the conference discussion was framed in terms of the advantages and limitations of the MOE approach in comparison with other approaches.

The conference considered that the MOE approach offers the following advantages:

• It is a pragmatic approach and has the potential to be explained and understood in a transparent way.

• It lends itself to a narrative presentation of the underlying scientific assumptions.

• It takes account of both carcinogenic potency and exposure, which the ALARA approach does not.

• It makes good use of all the available data.

• It does not extrapolate the curve orders of magnitude outside the observable dose-effect range.

• It only has to consider uncertainties in the toxicity data and in the exposure data; it does not have to contend with the uncertainties associated with selection and use of a mathematical model for low dose extrapolation.

• When appropriate human epidemiological data are available, they can be used to calculate MOEs that can be considered instead of, or alongside, those derived from experimental animal data.

• Where uncertainties are identified by the MOE approach, these can indicate what further steps or data may be needed to refine the risk assessment.

• MOEs can be calculated for subsets of the population with different exposures.

• It provides an additional piece of information in a 'weight of evidence' risk assessment.

• At the risk assessment stage, the question of acceptability of risk (a risk management task) can be avoided.

• It can be used to compare and rank substances.

• It can provide guidance on setting priorities for risk management actions.

• It can provide useful guidance for choosing between different risk management options for a substance.

• It can be used to set targets for risk reduction strategies.

• It can assist the risk manager in decision-making when regulatory limits for a substance are exceeded.

• It can be used by risk managers to distinguish between situations of larger, intermediate and lesser concern and may point to situations of minimal concern.

• It can be used to set priorities for testing and for further research.

• In contrast to linear extrapolation, the MOE approach does not give a risk estimate which may be (mis)interpreted as precise, or as the level of actual risk in the exposed population.

• It can be used to compare the relative risks of exposure to a substance via different routes.

• It can be used to aid decision-making in application of an ALARA/ALARP policy by risk managers.

Limitations of the MOE approach compared with other approaches

The conference considered the limitations of the MOE approach:

• It provides a numerical value (a ratio) but, in contrast to linear extrapolation, does not provide a quantitative estimate of risk.

• The abstract nature of a ratio may result in problems of understanding.

• Although it does not define the possible magnitude of the risk, it may be misinterpreted as giving a measure of the risk.

• Good intake/exposure data are critical; the confidence that can be placed in any particular MOE is dependent on the reliability of the exposure/intake assessment.

• Provision of a single value for the MOE could result in over-interpretation of the reliability and applicability of the value.

• As, with all other approaches, it requires a clearly and carefully expressed narrative to provide perspective and context and to explain it to risk managers and consumers.

• Interpretation of the significance of a particular value of an MOE lies on the borders between risk assessment and risk management.

• It does not provide a tool for performing risk/benefit or risk/cost assessments.