Environment Agency

using science to
create a better place

Updated technical background to the CLEA model

Science Report: SC050021/SR3

SCHO0508BNQW-E-P

The Environment Agency is the leading public body protecting and improving the environment in England and Wales.

It's our job to make sure that air, land and water are looked after by everyone in today's society, so that tomorrow's generations inherit a cleaner, healthier world.

Our work includes tackling flooding and pollution incidents, reducing industry's impacts on the environment, cleaning up rivers, coastal waters and contaminated land, and improving wildlife habitats.

This report is the result of work undertaken by the Environment Agency's Science Programme.

Published by:
Environment Agency, Rio House, Waterside Drive,
Aztec West, Almondsbury, Bristol, BS32 4UD
Tel: 01454 624400 Fax: 01454 624409
www.environment-agency.gov.uk

ISBN: 978-1-84432-856-7

Author(s):
Jeffries, J. & Martin, I.

Dissemination Status:
Publicly available / released to all regions

Keywords:
Contaminated land, CLEA report, exposure assessment, guideline values, human health, land contamination, risk assessment, soil pollution

Environment Agency's Project Manager:
Jo Jeffries
Science Department

Science Project Number:
SC050021/SR3

Product Code:
SCHO0508BNQW-E-P

This report is printed on Cyclus Print, a 100% recycled stock, which is 100% post consumer waste and is totally chlorine free. Water used is treated and in most cases returned to source in better condition than removed.

Further copies of this report are available from:
The Environment Agency's National Customer Contact Centre by emailing:
enquiries@environment-agency.gov.uk
or by telephoning 08708 506506.

Legal Status and Disclaimer

The CLEA Guidance incorporates the following

1) *Science Report SC050021/SR2: Human health toxicological assessment of contaminants in soil.*
2) *Science Report SC050021/SR3: Updated technical background to the CLEA model.*
3) *Science Report SC050021/SR4: CLEA Software (Version) Handbook.*
4) *CLEA Software version 1.04 (2009)*

The CLEA Guidance can help suitably qualified assessors to estimate the risk that a child or adult may be exposed to a soil concentration on a given site over a long period of exposure that may be a cause for concern to human health. The CLEA Guidance does not cover other types of risk to humans, such as fire, suffocation or explosion, or short-term and acute exposures. Nor does it cover risks to the environment or the pollution of water.

The CLEA Guidance is non-statutory. It does not purport to interpret the policies or procedures of the Environment Agency and shall not operate as a statutory licence, waiver, consent or approval from the Environment Agency. Nothing in the CLEA Guidance shall prejudice, conflict with or affect the exercise by the Environment Agency of its statutory functions, powers, rights, duties, responsibilities, obligations or discretions arising or imposed under the Environment Act 1995 or any other legislative provision enactment, bye-law or regulation.

The CLEA guidance describes the soil concentrations above which, in the opinion of the Environment Agency, there may be concern that warrants further investigation and risk evaluation for both threshold and non-threshold substances. These levels are a guide to help assessors estimate risk. It does not provide a definitive test for telling when risks are significant.

Regulators are under no obligation to use the CLEA Guidance.

Science at the Environment Agency

Science underpins the work of the Environment Agency. It provides an up-to-date understanding of the world about us and helps us to develop monitoring tools and techniques to manage our environment as efficiently and effectively as possible.

The work of the Environment Agency's Science Department is a key ingredient in the partnership between research, policy and operations that enables the Environment Agency to protect and restore our environment.

The science programme focuses on five main areas of activity:

- **Setting the agenda**, by identifying where strategic science can inform our evidence-based policies, advisory and regulatory roles;
- **Funding science**, by supporting programmes, projects and people in response to long-term strategic needs, medium-term policy priorities and shorter-term operational requirements;
- **Managing science**, by ensuring that our programmes and projects are fit for purpose and executed according to international scientific standards;
- **Carrying out science**, by undertaking research – either by contracting it out to research organisations and consultancies or by doing it ourselves;
- **Delivering information, advice, tools and techniques**, by making appropriate products available to our policy and operations staff.

Steve Killeen

Steve Killeen

Head of Science

Acknowledgements

The Environment Agency would like to thank the Food Standards Agency and CIRIA for the use of information in this report. We would also like to thank those individuals and organisations too numerous to mention that responded with feedback on the draft circulated in October 2007 and the report published in August 2008.

Contents

List of Tables

Table of Figures

1 Introduction

1.1 Update to R&D Publication CLR10

In December 2006, the Department for Environment, Food and Rural Affairs (Defra) issued a discussion paper entitled *Soil Guideline Values: The Way Forward*. The paper sought views from key organisations and groups on various ideas for how non-statutory technical guidance might be amended to make it more useful to assessors carrying out risk assessments, and to make clearer when land qualifies as contaminated land under Part 2A of the Environmental Protection Act 1990 in England and Wales. This exercise culminated in the publication by Defra of *Improvements to contaminated land guidance. Outcome of the "Way Forward" exercise* (Defra, 2008a).

This report updates the technical basis of the Contaminated Land Exposure Assessment (CLEA) model and reconsiders the rationale for the generic land use scenarios used to derive **Soil Guideline Values** (SGVs). It is based on the outcome of the review undertaken by the Environment Agency as part of the discussions with Defra and other organisations to improve the guidance and takes into account:

- Consolidation of technical guidance on the CLEA model into a single report, focussed on the derivation of SGVs with improved readability and accessibility.
- Update of the data sets and model **algorithms** used in the CLEA model based on recent scientific literature.
- Reconsideration of the generic land use scenarios and default assumptions used in the CLEA model to derive SGVs including improvements in clarity, internal consistency, and practical usability of the approach.

This report updates and replaces R&D Publication CLR10, published in 2002, and CLEA Briefing Notes 1 to 4, published in 2004 and 2005 (Defra and Environment Agency, 2002c; Environment Agency 2004a, 2004b, 2005b and 2005c). It incorporates many of the changes to exposure assessments that were introduced in *Soil Guideline Values: The Way Forward*, but includes other changes as well.

1.2 Background

This report describes the technical principles of the CLEA model developed by the Environment Agency to derive SGVs. The CLEA model uses generic assumptions about the fate and transport of chemicals in the environment, and a generic conceptual model for site conditions and human behaviour to estimate child and adult exposures to soil contaminants for those living, working, and/or playing on contaminated sites over long time periods. SGV are derived using the CLEA model by comparing the estimated exposure with **Health Criteria Values** (HCVs) that represent a tolerable or minimal risk to health from chronic exposure. The derivation of HCVs is described in detail within the TOX guidance report (Environment Agency, 2009a).

SGVs are scientifically based **generic assessment criteria** that may be used to simplify the assessment of risk to human health from chronic exposure to contaminants in soil. SGVs are a screening tool for the **generic quantitative risk assessment** of land contamination (Defra and Environment Agency, 2004). They represent "trigger values", indicators to a risk assessor that above this level soil concentrations may pose a *possibility of significant harm* to human health (Defra, 2008b), although further investigation and evaluation of risk will usually be required.

SGVs do not of themselves represent the threshold at which there is a *significant possibility of significant harm* nor do they automatically represent an *unacceptable intake* in the context of Part 2A of the Environmental Protection Act 1990 (Part 2A), but they can be a useful starting point for such an assessment (Defra, 2008b). Science alone cannot answer the question of whether or not a given *possibility of significant harm* is *significant*, since what is either *significant* or *unacceptable* is a matter of socio-political judgement, and the law entrusts decisions on this to the enforcing authorities (Defra, 2008b).

Land contamination is a material consideration within the planning regime. A planning authority has to consider the potential implications of contamination both when it is developing structure or local plans (or unitary development plans) and when it is considering applications for planning permission. Planning Policy Statement 23 (England), in the granting of planning permission for new development including permission to carry out remediation, states that remediation must remove unacceptable risk and make the site suitable for its intended use (ODPM, 2004a and 2004b). As a minimum, after development and commencement of its use, the land should not be capable of being deemed contaminated land under Part 2A.

1.3 Advice on using this report

This report explains the CLEA model and the assumptions used to define generic land use scenarios to derive SGVs. Used in conjunction with the TOX guidance report (Environment Agency, 2009a), it sets out the technical approach that underpins the derivation of SGVs. This report has been prepared with the support of Defra, the Welsh Assembly Government, the Food Standards Agency and the Health Protection Agency. It is published by the Environment Agency as non-statutory technical advice in the context of Part 2A and the consideration of land affected by contamination under the planning regime (Defra, 2008a and 2008b).

In the context of Part 2A, a risk assessor using an SGV can conclude the following (Defra, 2008b):

- At a representative average soil concentration close to or below an SGV, there is unlikely to be *a significant possibility of significant harm*.
- At a representative average soil concentration above an SGV, there might be a *significant possibility of significant harm* with the significance linked to the margin of exceedance, the duration and frequency of exposure, and other site-specific factors that the enforcing authority may wish to take into account.

The information in this report will assist users of SGVs in judging whether it is appropriate to apply such guideline values in assessing the risks posed by a contaminated site. Critical to this judgement is whether the conceptual model used to describe exposure within a generic land use scenario is appropriate to the site in question. If not, then a more **detailed quantitative risk assessment** will usually be required (Defra and Environment Agency, 2004).

This technical document has been written for professionals who are familiar with assessing risks to human health from land contamination, but who are not experts in exposure modelling. Assessors evaluating the use of SGVs will find Chapters 2 and 3 particularly useful, as they set out the key assumptions behind the generic land use scenarios central to the assessment. Important assumptions are highlighted in these chapters with the help of grey-shaded text boxes. Chapters 4 through 9 provide a more detailed discussion of the scientific and technical principles behind predictions of the environmental fate and transport of chemicals, and estimations of human exposure.

Assumptions in the CLEA model apply to the derivation of SGVs, but offer a useful starting point for assessors developing their own **site-specific assessment criteria**. Thus, the Environment Agency has published a software version of the model for use with Microsoft Excel (Environment Agency, 2009b). The software and its accompanying handbook contain further information on using the CLEA model outside the scope of this report (Environment Agency, 2009b).

The remainder of this publication has been divided into the following Chapters:

- Chapter 2 provides an overview of the CLEA model and explains how it is used to derive SGVs.
- Chapter 3 describes the conceptual models for the standard land uses.
- Chapter 4 describes the collation of data sets for use in the CLEA model including human characteristics, soil types, and physical-chemical data.
- Chapter 5 covers prediction of the fate and transport of chemicals in soils for use in the CLEA model.
- Chapters 6, 7, 8, 9 and 10 describe predictive modelling of the ingestion, skin contact and inhalation pathways.
- Chapter 11 offers a list of references, abbreviations and a glossary of terms.

Other risks from land contamination

This report describes the CLEA model, a tool used by the Environment Agency to develop SGV. SGV are used for the generic assessment of human health risks arising from long-term and on-site exposure to chemical contamination in soil. There are other potential health risks from land contamination that are not covered by this guidance but which nevertheless may be critical on a site-specific basis such as:

- Short term exposure resulting in human health risk such as poisoning or by direct bodily contact
- Explosion or suffocation risk associated with the build-up of gases such as methane and carbon dioxide
- Contamination through the food chain, other than from the consumption of homegrown fruit and vegetables
- Sources of contamination other than surface soils including groundwater, surface waters such as ponds and lakes, and drinking water
- Off-site migration and potential impacts on health

In addition, land contamination may pose a risk to the wider environment including groundwater, surface waters, buildings, pets and livestock, soil quality and protected habitats. These risks should also be assessed where necessary. See the *Model Procedures for the Management of Contaminated Land* (Defra and Environment Agency, 2004) for further information and guidance on carrying out a comprehensive and systematic assessment of all possible risks.

2 Estimating human exposure to soil contaminants

This chapter introduces the technical principles for modelling human exposure to soil contaminants. It provides an overview of the CLEA model and its role in the derivation of SGVs. It also discusses the interface between exposure and health effects, and considers the methods available for managing uncertainty in exposure estimates.

2.1 Principles of human exposure assessment

Exposure assessment is "*the process of estimating or measuring the magnitude, frequency, and duration of exposure to an agent, along with the number and characteristics of the population exposed. Ideally, it describes the sources, pathways, routes, and the uncertainties in the risk assessment*" (IPCS, 2004).

The CLEA model is a spreadsheet-based application used to estimate exposure to chemicals from soil sources by adults and children living, working and/or playing on land affected by contamination, over long periods of time. By comparing predicted exposure with HCVs, the model outputs are used to derive SGVs which are examples of generic assessment criteria (Defra and Environment Agency, 2004). Such criteria may be used to simplify the assessment of a site, provided the assessor is satisfied that the assumptions underlying the derivation of SGVs are reasonably representative of the site (see Section 2.2.2).

2.1.1 Defining exposure

The CLEA model predicts human exposure to a chemical in soil by direct contact (such as soil ingestion) or following transport from the soil into another medium (such as homegrown produce or indoor air).

Exposure is defined as contact between a chemical and the external surfaces of the human body (IPCS, 2005).

There are three main routes of entry for chemicals into the body:

- by ingestion through the mouth;
- by inhalation through the nose and mouth;
- by absorption through the skin.

Intake is the amount of a substance ingested or inhaled by an individual. It is a function of chemical characteristics and the nature and behaviour patterns of the target population. Intake is expressed in terms of a mass of chemical per kilogram body weight per day (for example, mg kg^{-1} bw day^{-1}). The intake dose is the most commonly used metric for exposure in toxicity studies in laboratory animals. Therefore, although the internal (uptake) dose causes the majority of **adverse effects** on health, it is the intake dose which is the exposure metric that is often of most use to risk assessors.

Uptake is the amount of a substance that enters the body following absorption by the gastrointestinal and/or pulmonary systems, or through the skin. The proportion of an ingested chemical that is absorbed from the gut into the body and reaches **systemic circulation** unchanged is referred to as the bioavailable fraction. This fraction is known as the **systemic dose** (Environment Agency, 2009a). The term uptake dose is used to refer to the total amount of a chemical that enters the body, including for example for oral exposure that which acts on or is metabolised by the liver before entering the systemic circulation.

In reality, it is very difficult to measure uptake by the body directly. This is a significant limitation on the use of uptake data in risk assessments and in the evaluation of **dose-response relationships** in experimental or **epidemiological studies** of chemical toxicity. Indirect estimates of uptake can be obtained from biological markers, **pharmacokinetic models**, and studies of **bioavailability** and **bioaccessibility** (Environment Agency, 2009a; IPCS, 2000). However, the use of these methods is extremely limited and it is seldom taken into account in chemical risk assessment.

2.1.2 Quantifying exposure

The aim of the CLEA model is to estimate human exposures to chemicals in soil in terms comparable with relevant HCVs including the **Tolerable Daily Intake** (TDI) and the **Index Dose** (ID) (see Section 2.3). Most HCVs are expressed as an intake based on the administered dose from animal studies or an estimate of exposure from occupational or epidemiological studies (Environment Agency, 2009a). Most HCVs are reported in units of the amount of chemical per kilogram body weight per day (for example, mg kg^{-1} bw day^{-1}) but there are exceptions to this including asbestos.

Skin contact is more difficult to characterise because there is often little or no information on chemical toxicity via this route, and it is usual to compare dermal exposures with data on toxicity from oral studies (see Section 2.3.1). Compared with such oral exposures, the skin represents a highly efficient barrier between chemicals in the environment and the human body (IGHRC, 2006). It is therefore more meaningful to use estimates of skin absorption (uptake) in comparisons with HCV based on intake.

The CLEA model estimates the **Average Daily Exposure** (ADE) to a contaminant in soil via the following routes:

- ingestion of contaminated soil, dust, and homegrown produce via the mouth (as intake);
- inhalation of contaminated dust[1] and vapour via the nose and mouth (as intake);
- absorption of the contaminant through the skin (as uptake).

ADE is defined as the average daily amount of a contaminant per kilogram bodyweight, which a **critical receptor** might take in over the duration of exposure. **Equation 2.1** expresses the calculation of ADE on a mathematical basis. This equation is widely adopted internationally for chemical risk assessment (ASTM, 2000; USEPA, 1996, 2002a; Lijzen *et al.,* 2001).

Chemical intake/uptake rate (IR) is a function of two parameters: the concentration of a contaminant in the relevant medium (soil/water/food/air) and the daily human exposure rate to that medium. For example:

- The intake rate for cadmium by soil ingestion would depend on the cadmium soil concentration and the amount of soil ingested daily by the critical receptor.
- The intake rate for the inhalation of benzene vapour would depend on its air concentration and the amount of air inhaled daily by the critical receptor.

---

[1] Inhaled dust can also be ingested and swallowed as part of mucus/spittle after inhalation.

The CLEA model estimates daily exposure from up to ten different pathways based on the concentration of chemical in soil (see Figure 2.1), with the selection of pathways dependent on the conceptual model for the generic land use scenario (see Chapter 3). Although a single daily rate is used for ease of calculations, it is unlikely that many such exposures would occur during a single exposure event. For example, direct soil ingestion results from a number of discrete instances of hand-to-mouth contact, usually lasting only a few minutes duration over an extended period of time.

Equation 2.1

$$\text{ADE} = \frac{\left(IR_{ing} \times EF_{ing} \times ED_{ing}\right)}{BW \times AT} + \frac{\left(IR_{inh} \times EF_{inh} \times ED_{inh}\right)}{BW \times AT} + \frac{\left(IR_{derm} \times EF_{derm} \times ED_{derm}\right)}{BW \times AT}$$

Where

ADE is the average daily human exposure to a chemical from soil, mg kg^{-1} bw day^{-1}

IR is the chemical intake/uptake rate, mg day^{-1}

EF is the exposure frequency, days $year^{-1}$

ED is the exposure duration, year

BW is the human body weight, kg

AT is the averaging time, days

The subscripts *ing*, *inh*, and *derm* apply to the inhalation, ingestion and dermal contact routes respectively. IR_{ing} and IR_{inh} are normally estimated as intakes. IR_{derm} is normally estimated as an uptake.

Exposure frequency (EF) is related closely to the chemical intake/uptake rate. It represents the number of days per year in which a daily exposure event is considered to occur. For example, the conceptual model for a residential property might assume that the exposure frequency for inhalation of household dust is 365 days per year (that is, the occupants breathe the air inside their homes every day).

In the conceptual model, a frequency is assigned to each **exposure pathway**. Most of the exposure frequencies used in the CLEA model are derived directly for each generic land use scenario (see Chapter 3) but some frequencies must also take into account the methods used to derive the chemical intake/uptake rate. **Equation 2.1** shows that the exposure frequency multiplied by the exposure duration gives the total exposure period in days for each pathway. See text box for further examples.

Exposure frequency

Exposure frequencies are an important parameter in estimating ADE. They should be assigned on a pathway-by-pathway basis taking into account the site conceptual model and other factors relating to the derivation of the chemical intake/uptake rate.

For example, consider the generic land use scenario for an allotment site in Chapter 3. It may be assumed that for most exposure pathways, the number of site visits by the adult or child to the allotment would be the basis for setting the exposure frequency. In effect, exposure is considered likely only when the receptor comes into contact with the contaminated soil. However, this is not true for all pathways. Consumption of produce grown on the allotment may be consumed more or less frequently than the number of site visits might suggest. In extreme circumstances, a child that never accompanies a parent to the allotment may be exposed to soil contamination through consumption of produce at home.

In some cases, the exposure frequency will be dictated by factors other than the site conceptual model. For example, the chemical intake/uptake rate from homegrown fruit and vegetables is calculated from an annual average from national survey data (see Section 4.4 and 7.2.3) and therefore the exposure frequency is taken to be 365 days per year. In reality, it is unlikely that consumers would eat such small amounts of individual fruit and vegetables every day but would have a larger portion maybe once or twice per week.

Fixed soil concentration

An important generic assumption in deriving SGVs is that soil concentration is fixed over the duration of exposure. Although natural degradation and dispersion processes will gradually reduce the concentration of contaminants in surface and near-surface soils, the rate at which this occurs is highly site-specific.

SGVs are generic assessment criteria and therefore are intended to be applicable across a wide range of different sites where the rate of loss of any substance in soil is highly variable. The precautionary position must therefore be to assume no degradation without the results of a detailed and site-specific assessment.

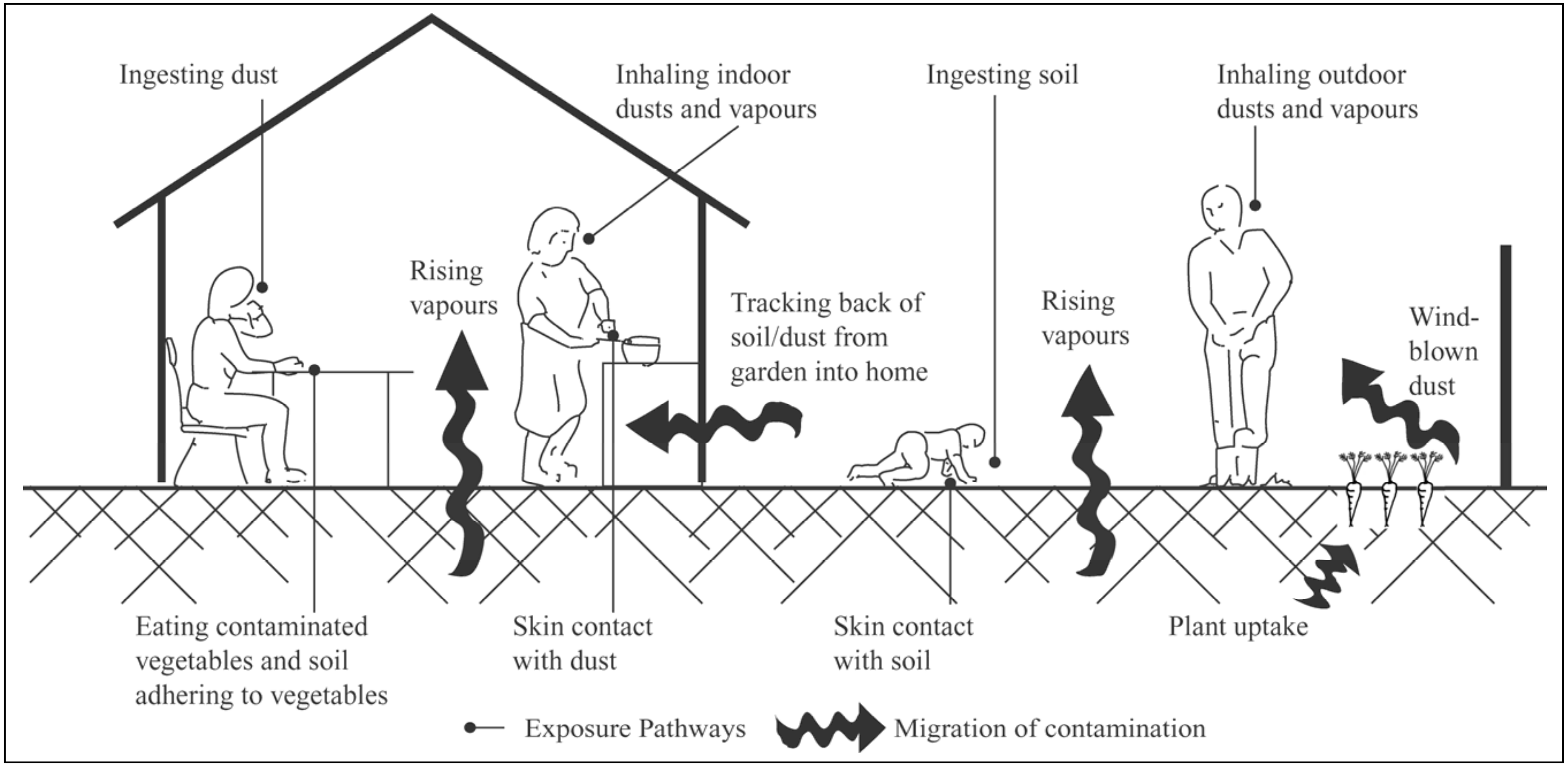


Figure 2.1: Illustration of the potential exposure pathways in the CLEA model

Average daily exposure is estimated from chemical intake/uptake rates over a specified time period, the **exposure duration** (ED). The CLEA model considers chronic exposure scenarios (that is, long-term low levels of exposure). It is not designed to consider exposures for periods shorter than one year and where acute exposures are likely to drive the risk assessment.

Using the CLEA model, it is possible to vary the exposure duration from a single year in childhood up to a lifetime of 75 years. Many physical characteristics (such as bodyweight) and those exposure parameters influenced by behaviour vary with age. For example, the soil ingestion rates for young children are likely to be significantly different from those of an adult (see Chapter 6).

The CLEA model divides a lifetime into eighteen age intervals (or **age classes**) to account for variations in **exposure characteristics** with age (see Figure 2.2). The first sixteen age classes correspond to the first sixteen years of life, the seventeenth interval is typical of an adult working life (age 16 to 65), and the eighteenth represents retirement (age 65 to 75). The age classes have been chosen to represent those stages in life where the most significant differences in exposure characteristics are likely to occur. Childhood is considered in more detail, bearing in mind the rapid changes in children's use of a site and their physical development compared to adults.

ED is a critical parameter in exposure assessment and depends on the underlying conceptual model. In particular, the length of time and the choice of time interval depend on the critical receptor (see Section 2.2.1).

The CLEA model estimates the *average* daily exposure over the period of exposure. **Averaging time** (AT) is assumed to be equal to the exposure duration. For example, a period of exposure covering the first six years of a child's life has an averaging time of 2190 days (six years at 365 days per year).[2]

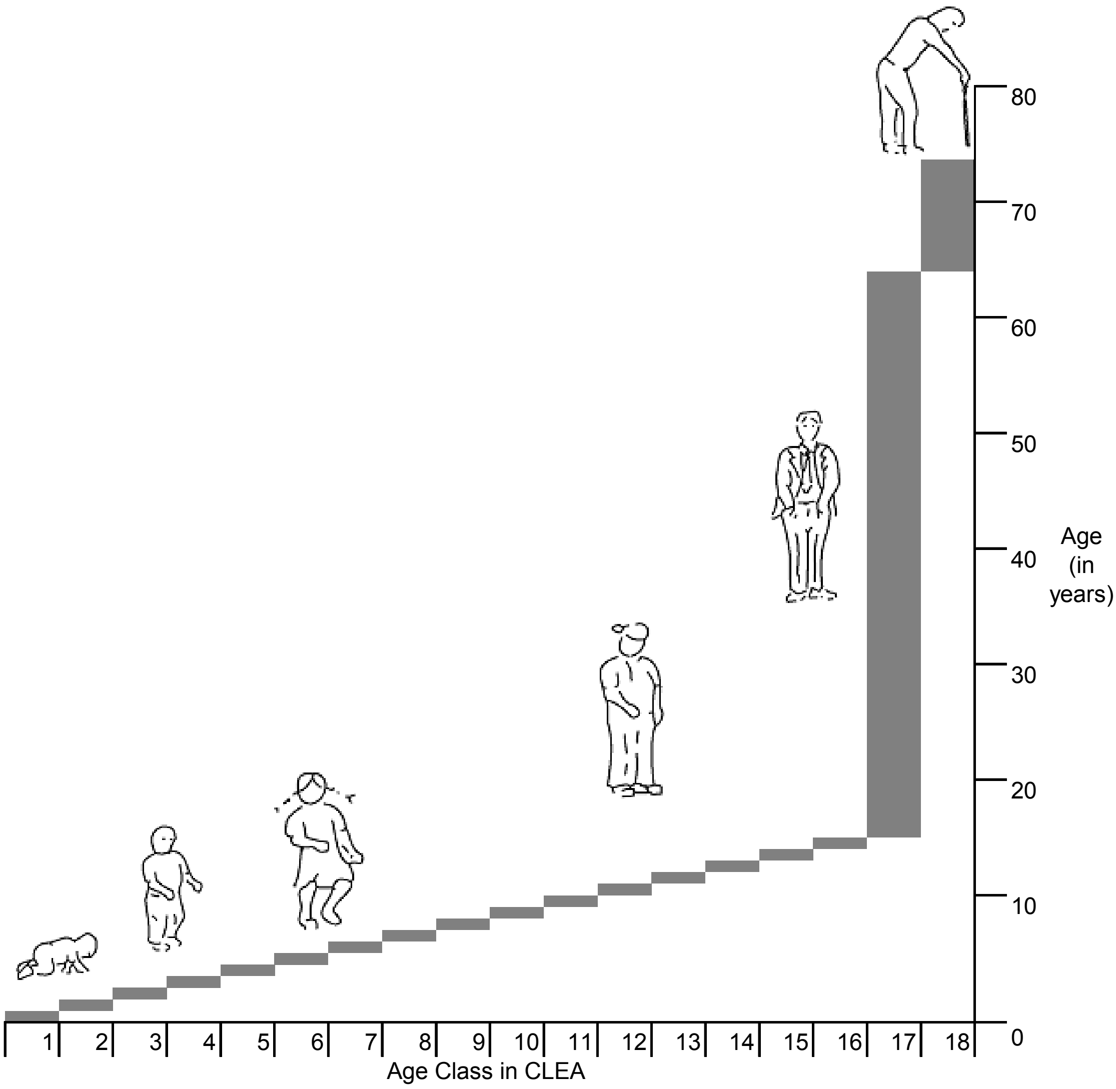
Most exposure assessment models are based on the principle that exposures are aggregated over the duration of exposure, and hence assume that peaks and troughs in exposure are not significant compared with the final outcome. As exposure duration increases, the effect of aggregating exposure becomes more pronounced, as illustrated in Figure 2.3.

Actual daily exposures to soil contamination will vary considerably, especially where daily exposure is an amalgamation of individual events such as hand-to-mouth contacts, skin contact with soil, and consumption of contaminated produce.

Aggregating such exposures over a year will generate a smoother curve because much of the daily variation is subsumed within average chemical intake rates. The peak that is observed in Figure 2.3 reflects the higher average exposures to soil contaminants observed for children compared with adults. It is generally recognised that young children, predominantly because of exposure pathways such as soil ingestion, are likely to have higher average daily exposures to soil contaminants than are seen in adults. Combining these higher exposure rates with their lower body weight means that a child's exposure to soil contaminants over the first six years is likely to be considerably higher than for a corresponding adult over the same duration. Aggregating exposure over a lifetime assumes a linear relationship and therefore neglects the higher exposures that children might receive.

---

[2] International approaches to the risk from non-threshold chemicals such as genotoxic carcinogens typically adopt a lifetime averaging time, which may differ from the exposure duration (Lijzen *et al.*, 2001; USEPA, 2002).



Age class	Age (years)
1	0 – 1
2	1 – 2
3	2 – 3
4	3 – 4
5	4 – 5
6	5 – 6
7	6 – 7
8	7 – 8
9	8 - 9

Age class	Age (years)
10	9 - 10
11	10 - 11
12	11 - 12
13	12 - 13
14	13 - 14
15	14 - 15
16	15 - 16
17	16 - 65
18	65 - 75

Figure 2.2: Subdividing the human lifetime into age classes

For wholly practical reasons, aggregation of exposure over some specified period is required. Ideally, this exposure period would be short enough to ensure that there are few, if any, exceedances of a HCV on a daily basis. However, such is the uncertainty and variability in modelling environmental exposure that this is in reality impossible to achieve, and would have little or no applicability beyond a particular site or individual. In risk assessment, a compromise position is usually adopted, with childhood exposures rather than lifetime exposures considered where the child is the default critical receptor (USEPA, 1996 and 2002a). Thus, short-term exceedances of a HCV, in the order of a few days or weeks, may still occur at soil concentrations equal to or less than the SGV. Whether such exceedances are important in protecting human health is discussed more fully in the relevant substance-specific SGV and TOX reports.

Much of the discussion above considers the sensitivity of the receptor in the context of exposure only. For certain contaminants, the exposure duration may be longer or shorter because of considerations of toxicology. In considering the toxicology of lead, the developing foetus and child have generally been accepted as being most at risk because of sources and pathways of exposure and because of their greater susceptibility to its toxic effects (Defra and Environment Agency, 2002a).

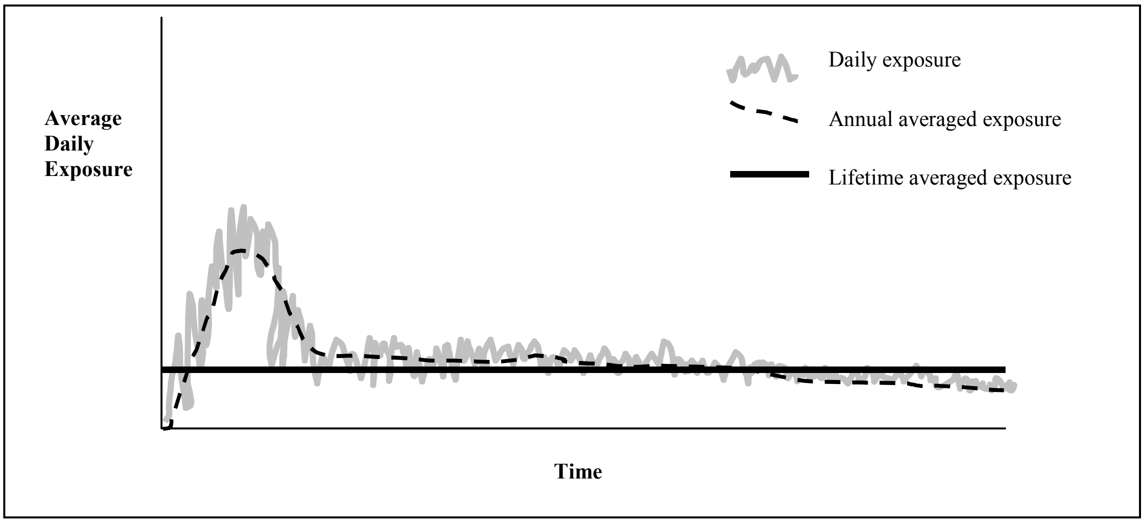


Figure 2.3: Effect of aggregating soil exposures over longer timescales

Exposure duration and averaging time

Generic assumptions for the conceptual models described in Chapter 3 are summarised in the table below.

Standard land use	Sensitive receptor	Exposure duration	Averaging time
Residential	Young child	6 years	2,190 days
Allotments [1]	Young child	6 years	2,190 days
Commercial	Working adult	49 years	17,885 days

Notes: [1] It is assumed that children spend time with parents and/or grandparents at the allotment, and that they consume allotment produce with the family at home.

2.2 Conceptual models for exposure assessment

The CLEA model is an **exposure assessment** tool used to estimate the magnitude of exposure to soil contaminants, taking into account the number and characteristics of the exposed population (IPCS, 2005). It is an integral component of risk assessment.

Exposure assessment is based on defined **exposure scenarios,** a specific conceptual model that sets out a discrete set of circumstances where exposure may occur including the source, pathways, exposed population, and timeframe of exposure (IPCS, 2004). In the context of land contamination, the **conceptual model** represents the characteristics of the site in diagrammatic or written form that shows the possible relationships between contaminants, pathways and receptors (Defra and Environment Agency, 2004).[3] The conceptual models used in the derivation of SGVs are called generic land use scenarios and are described in Chapter 3.

2.2.1 Defining the exposure scenario

The CLEA model estimates chronic exposure to contaminants for people living and/or working on a contaminated site. Central to defining the exposure scenario is the land use, since this helps to identify the types of people that use a site, the types of activity they undertake, and the extent to which such **activity patterns** involve direct or indirect contact with soil. This is also consistent with UK policy on land contamination where the risks to health are assessed against the use of the land (Defra, 2006).

In reviewing land use, the assessor seeks to identify the types of people using the site, and in particular the **critical receptor**, that is, the individuals or subgroup of the population most likely to be exposed and/or susceptible to the presence of soil contamination. There are three factors to consider when identifying the critical receptor:

- susceptibility of the receptor to the presence of soil contamination;
- likelihood that a receptor is present based on the category of land use;
- likely degree of contact with soil or indirect contact with other contaminated media such as homegrown produce or indoor air.

In many cases, a young child is considered the critical receptor because of the combination of higher childhood exposure for key pathways such as soil ingestion and lower bodyweight, which results in a higher estimated ADE (see **Equation 2.1**). In addition, there is evidence that children are more sensitive to the toxicity of some chemicals.

Land use provides boundaries to formal and informal activities and helps to describe how people potentially behave. Factors considered include the frequency and duration of visits to the site (and specific areas within a site), the likely activities that could bring about contact with soil contamination (for example, growing fruit and vegetables), and other physical site factors (such as garden area and the amount of hard standing). Combining the choice of critical receptor with the pattern of likely exposure will define the choice of exposure duration and averaging time (see discussion of exposure duration in Section 2.1.2).

By default, the CLEA model includes up to ten different exposure pathways that may be applied to a range of common land uses including residential, public open space,

---

[3] The individual relationships that exist between a contaminant, a receptor, and a pathway are described in contaminated land risk assessment as a **pollutant linkage** (Defra and Environment Agency, 2004).

and commercial sites (see Figure 2.1). These pathways have been consistently identified internationally as those being the most important for assessing human exposure from soil contamination (Lijzen *et al*., 2001; USEPA, 1996 and 2002a). However, a risk assessor should always consider whether additional exposure pathways might be present (such as the use of water from a private supply borehole) in considering the suitability of using an SGV at a particular site.

Contamination depth

Many of the exposure pathways considered by the CLEA model assume that the adult or child is in contact with the contaminated ground or that such contamination is easily mobilised from the surface (as is the case for dust and tracked back soil). Therefore, it is assumed that the pollution is at the surface or close to it. However, plant uptake of chemicals and the release of soil vapours may occur to much greater depths.

Plant uptake for many chemicals is a passive process through the root zone (see Chapter 7 for further details). Thorne et al. (2005) noted that for many crop plants, root depths are between one and two metres although the highest density of roots occurs in the top 80 cm, with the notable exception of trees. Vapours can potentially migrate to the surface over distances of tens of metres, although the amount of transport greatly reduces with depth.

Whether or not soil contamination at greater depth or beneath hard standing poses a risk to health depends on the importance of the contact pathways (primarily ingestion and dermal contact) and the likelihood that such soils may be brought to the surface through activities such as gardening or building works.

Consideration of the fate and transport of contaminants also helps us to understand the likely pathways of exposure and the relative contribution of any one pathway to overall human exposure. Fate and transport are strongly influenced by the physical, chemical and biological properties of individual contaminants and their interaction with the environment. For example, most metal contaminants, with the notable exception of elemental mercury, are not sufficiently volatile at ambient temperatures to pose an appreciable risk to human health by vapour inhalation. Therefore, exposure to metal contamination will typically occur by direct contact with contaminated soil and the likelihood for human exposure will be greatly reduced if it is not present at the soil surface or lies beneath hard standing (see text box for further discussion).

Where the influence of specific activities or fate and transport behaviour on likely exposure is uncertain, the use of an exposure model such as the CLEA model can be used to evaluate impacts across a range of different pathways.

2.2.2 Generic versus site-specific exposure assessment

Figure 2.4 illustrates the steps within the CLEA model to estimate human exposure based on a defined conceptual site model. The term “site-specific risk assessment” is commonly used by contaminated land practitioners (Defra and Environment Agency, 2004). However, in reality all risk assessments are site-specific, differing only in the detail of their approach.

In common with other mathematical applications, the CLEA model can be used in **forward** and **backward mode** (see Figure 2.4). Operating in forward mode[4], the model takes a prescribed soil concentration and estimates human exposure from knowledge of the chemical properties of the contaminant and parameters of the exposure scenario. The output is the ADE, which can be compared with relevant HCVs. **Assessment criteria** are calculated by running the model in backward mode, starting with a prescribed level of exposure (usually equal to the HCV) and calculating the soil concentration that might give rise to that level of exposure.

The primary purpose of the CLEA model is to assist environmental risk assessments for land contamination through the derivation of SGVs. The UK framework for environmental risk assessment and management sets out a tiered approach where the level of effort put into assessing each risk is proportionate to its priority (in relation to other risks) and its complexity (DETR *et al*., 2000). Defra and Environment Agency (2004) incorporated these principles into the management of land contamination and identified three tiers in risk assessment:

- preliminary risk assessment;
- generic quantitative risk assessment;
- detailed quantitative risk assessment.

The CLEA model uses generic land use scenarios (see Chapter 3) as conceptual models to estimate exposure as part of a generic quantitative risk assessment. It also uses screening level predictions of the fate and transport of chemicals in the soil environment as a surrogate for site measurements. However, the overall structure of the model and many of its components are suitable for both generic and detailed quantitative risk assessment. Conceptually, Figure 2.4 applies to both tiers of risk assessment.

Generic assessment criteria, including SGVs, are derived using largely generic assumptions about the characteristics and behaviour of contaminants, pathways and receptors. These assumptions will usually be conservative within a defined range of conditions (Defra and Environment Agency, 2004). By broadening the conceptual models for land use and through simplifying the site data requirements, generic assessment criteria apply to a range of different sites. Generic assumptions used within the CLEA model are protective of health across a wide range of circumstances and reasonable range of possible activities. Key generic assumptions used in the CLEA model are summarised in Table 2.1 and identified throughout this report using grey-shaded text boxes.

Site-specific assessment criteria are derived using detailed site-specific information on the characteristics and behaviour of contaminants, pathways and receptors (Defra and Environment Agency, 2004). Usually, such criteria are calculated by replacing generic assumptions within the model with data collected from the contaminated site (such as soil properties, plant or air concentrations, and the outcomes of time use surveys). More rarely, more detailed pathway-specific modelling may be involved, for example, in estimating dust and vapour air concentrations using complex air-dispersion models. Site-specific assessment criteria are used in detailed quantitative risk assessments (Defra and Environment Agency, 2004). Table 2.1 illustrates where detailed assessment may be used to replace generic assumptions used to derive SGVs.

---

[4] Also known as "ratio mode" or the "hazard index" since in risk assessment, it is usual to compare the exposed dose with the relevant HCVs.

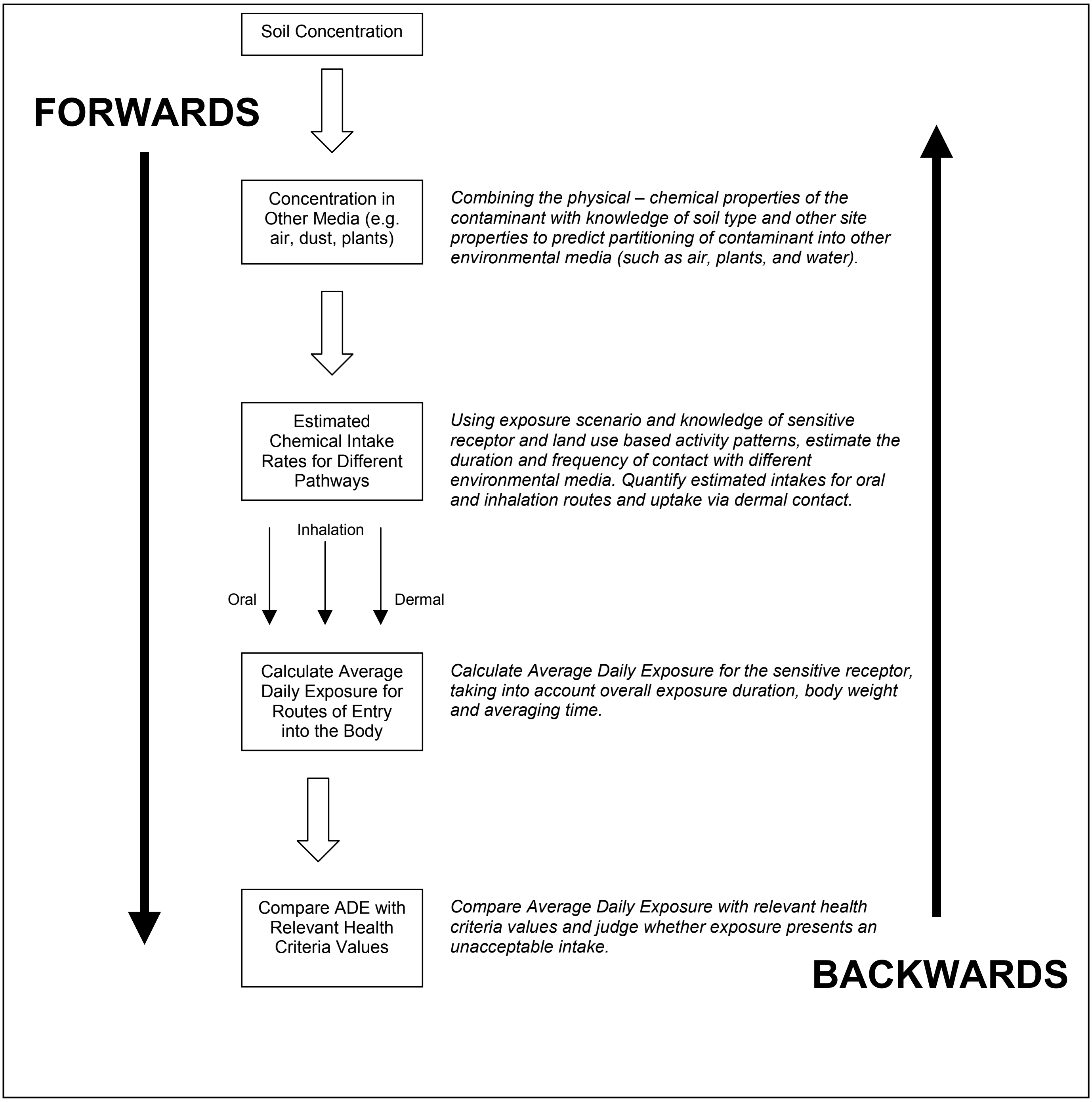


Figure 2.4: Steps to estimating human exposure using the CLEA model

Table 2.1: Generic assumptions in exposure assessment and options to refine these with further study

Stages [1]	Generic assumptions	Detailed assessment
Soil concentration	Chemical concentration is uniformly distributed from the soil surface to a depth consistent with the root zone of edible plants. Chemical form is often assumed to be the realistic worst case (for example, chromium VI). Chemical concentration is fixed over the duration of exposure.	Site investigations provide detail on the type of contaminant present and its likely distribution across the site (both horizontal and vertical). Loss mechanisms including physical transport, dilution, and degradation can be investigated and taken into account.
Media concentrations	Estimated using pseudo steady-state partitioning models and reasonable worst-case assumptions about the source of contamination and migration pathways. Soil is assumed to be relatively dry and porous (see Section 4.3).	Site investigations can measure chemical concentrations in various media including soil gas, plants and ambient and indoor air. Fate and transport pathways can be further investigated and key parameters determined (for example, soil type and moisture content).
Estimated intakes	Likely exposure pathways based on reasonable worst-case conceptual models (see Section 2.2.1). Exposure characteristics based on reasonable worst-case behaviours including fruit and vegetable consumption, soil ingestion and dermal contact. Tracking back of contamination into the home is assumed to be significant.	Site investigation may conclude that some exposure pathways are unlikely to be present because of management practices or physical barriers such as hard standing. Alternatively, it may be concluded that additional pathways exist or that generic assumptions may not be protective of health (for example, the more self-sufficient family may grow a significant proportion of their own fruit and vegetables). Exposure characteristics may be reviewed including exposure frequency and the degree of direct soil contact based on time-use surveys. Indoor dust investigations may better characterise the impact of off-site materials being tracked back.
Average daily exposure	Critical receptor, based on the standard land use, is assumed to be present.	Site investigation may better define site users, frequency and duration of exposure.

[1] Based on the steps outlined in Figure 2.4.

2.3 Exposure and Health Criteria Values

In deriving SGVs, the CLEA model compares an estimate of exposure to soil contamination with HCVs representing exposures associated with minimal health risk.

2.3.1 Health Criteria Values

All chemicals have the potential to cause harm to human health depending on the duration and level of intake (Environment Agency, 2009a). In the setting of Soil Guideline Values (SGVs), Health Criteria Value (HCV) is the collective term used to describe a level of exposure to a chemical derived from toxicity data for the purposes of safeguarding human heath. The Environment Agency (2009a) describes the process and terminology used to set HCVs and provides advice on their interpretation. The key principles are summarised in the following paragraphs.

In characterising the hazard posed by chemicals to human health, toxicologists distinguish between those chemicals for which there is a threshold dose below which there is no adverse effect on health and those chemicals for which no threshold can be detected or assumed. The Environment Agency (2009a) uses different approaches to deriving and using HCVs based on threshold and non-threshold chemical effects.

For threshold effects, a **Tolerable Daily Intake** or TDI is derived. Daily exposure equal to or less than the TDI is considered to be without appreciable health risk even if it is experienced over a whole lifetime (Environment Agency, 2009a). Where an assessment indicates that a TDI might be exceeded, this is undesirable but does not necessarily mean that adverse health effects will result. The likelihood and possible severity of adverse health impacts if a TDI is exceeded needs to be considered on a case-by-case basis and requires expert judgement.

When using a TDI to derive SGV, exposure of the population to the same chemical from sources other than soil (such as ambient air, drinking water and diet) needs to be taken into account (Environment Agency, 2009a). The **Tolerable Daily Soil Intake** or TDSI is derived from the HCV taking into account the **mean daily intake** (MDI) for non-soil background exposure (see text box).

The TDSI is calculated by the CLEA model using **Equation 2.2** and **Equation 2.3** for each route of exposure for which a TDI and an MDI is available. As noted by the Environment Agency (2009a), the background intake is expressed as the adult mean daily intake or MDI. The CLEA model makes corrections for younger age groups to account for differences in dietary consumption and inhalation rate. The chemical intake rates for oral and inhalation background exposures are calculated separately.[5] Since the intake rate for non-soil background sources must also be corrected for bodyweight, the TDSI will vary between different age classes.

For some threshold contaminants, the non-soil background exposure may already occupy a high proportion of the TDI or may even exceed it. It would therefore be impracticable to propose SGV on this basis without reserving a minimum proportion of the TDI for exposure from land (Environment Agency, 2009a; Defra, 2008b). In the derivation of SGV, this minimum proportion is 50 per cent and therefore at representative average soil concentrations greater than the SGV the contribution from the land will be greater than half the TDI.

---

[5] There is very little data on background dermal uptakes of common soil contaminants.

This minimum proportion from soil sources applies to comparisons with individual and multiple routes of exposure (see Section 2.3.2 for further discussion).

Contribution of non-soil sources of exposure

The mean daily intake (MDI) is the average "background intake" to which the UK population may be exposed. In the derivation of SGV, MDI is given separately for oral and inhalation routes. Typically, the MDI is estimated from published information on ambient air concentrations and average concentrations measured in water and food products. Where relevant to the specific chemical, other sources are also considered (for example, the exposure of the general population to mercury vapour from dental amalgam). If no data or information on background exposure is available, it should normally be assumed to be negligible and the MDI set to zero for all age groups. If only qualitative information is available, judgement will be required on how this is quantitatively accounted for (see Environment Agency, 2009a).

For threshold contaminants only, the MDI is taken into account in the derivation of SGV (see text for further discussion).

Equation 2.2

$$IR_{MDI} = MDI \times CF_{MDI}$$

Where

IR_{MDI} is the chemical intake rate from non-soil sources, mg day^{-1}

MDI is the adult mean daily intake from oral or inhalation pathway, mg day^{-1}

CF_{MDI} is the correction factor for the adult MDI to account for younger exposed groups from either the oral or inhalation pathway, unitless [6]

Separate IR_{MDI} are estimated for oral and inhalation exposure

Equation 2.3

$$TDSI = TDI - \frac{(IR_{MDI} \times EF \times ED)}{BW \times AT}$$

Where

TDSI is the tolerable daily soil intake, mg kg^{-1} bw day^{-1}

TDI is the tolerable daily intake, mg kg^{-1} bw day^{-1}

IR_{MDI} is the chemical intake from non-soil sources, mg day^{-1}

EF is the exposure frequency, days year^{-1} = [365]

ED is the exposure duration, year

BW is the human body weight, kg

AT is the averaging time, day

Separate TDSI are calculated for oral and inhalation exposure if TDI and background data is available (see Section 2.3.2 for further discussion of combined exposure). As noted in the text, in the derivation of SGVs the TDSI may not be less than half the value of the TDI.

---

[6] See Table 3.4 in Environment Agency (2009a) for correction factors according to age class.

In characterising non-threshold effects, the HCV used is the **Index Dose** or ID. The most well known group of non-threshold chemicals are the non-threshold genotoxic chemical carcinogens which include benzene and benzo[*a*]pyrene. Exposure at the ID level is therefore considered to carry some, albeit minimal and often unquantifiable, level of risk (Environment Agency, 2009a). Where an ID is exceeded, there will be an increased risk to health, the significance of which requires expert judgement although often it will also not be quantifiable (Environment Agency, 2009a). In managing the risk to health from non-threshold chemicals, the **ALARP (as low as reasonably practicable) principle** will automatically apply in the UK.

It is accepted that any exposure to non-threshold contaminants from other, non-soil, sources will increase the overall risk of cancer of an individual but such additional sources are not taken into account in the setting of SGV (Environment Agency, 2009a). This is consistent with current standard practice; for example, WHO does not consider other sources of exposure when setting drinking-water guidelines for non-threshold carcinogens.

2.3.2 Comparing exposure with HCV

The basic principle used by the Environment Agency to establish SGV is that they are set at the soil concentration where the ADE from soil sources by a particular exposure route, as predicted by the CLEA model, equals the HCV for that route (that is, the TDSI or the ID).

Environment Agency (2009a) describes the methods and procedures for deriving HCVs that characterise the risk for each route of exposure. For some chemicals, intake and/or uptake via different routes (via the nose, mouth, or through the skin) may lead to different local effects or may affect different organs. Adults and children using a contaminated site may be concomitantly exposed to the same chemical via all three routes of exposure. If the contaminant produces systemic critical toxicity, therefore, each route of exposure may contribute to an aggregate **systemic effect** even when exposure via each separate route would be less than its corresponding HCV (Environment Agency, 2009a). Even if a contaminant has an oral, dermal and inhalation HCV, each derived based on local toxic effects, it is still possible that exposures within these limits could contribute to a total systemic load that results in adverse systemic effects if the systemic effects are seen at intakes not much exceeding those causing the local effects (Environment Agency, 2009a).

Unless the toxicity data indicates otherwise, derivation of the SGV takes this possible effect into account using **Equation 2.4** (Lijzen *et al.,* 2001). Using this equation, the SGV is set at a soil concentration where the total risk from soil exposure via all routes of entry into the body is mathematically no greater than the risk due to exposure by any single route of entry compared to relevant pathway-specific HCVs. **Equation 2.4** is based on the following assumptions:

(a) Total risk is the sum of risks from exposure by all routes.

(b) The reciprocal of the HCVs is a useful indicator of the relative toxicological potencies by each route of exposure.

(c) Exposures are proportional to the soil concentration.

Where there are oral, dermal and inhalation HCVs, the SGV is set at a soil concentration *C* such that Equation 2.4 holds.

Equation 2.4

$$\frac{C\,R_{oral}}{HCV_{oral}} + \frac{C\,R_{dermal}}{HCV_{dermal}} + \frac{C\,R_{inhalation}}{HCV_{inhalation}} = 1$$

Where: *C* is the representative concentration of the chemical in soil, mg kg^{-1} dw
R_x is the ratio of ADE from soil sources over the soil concentration for a particular exposure route *x*, mg kg^{-1} bw day^{-1} over mg kg^{-1} dw soil
HCV_x denotes the relevant HCV for a particular exposure route *x* (for example, a TDSI or ID), mg kg^{-1} bw day^{-1}

Assessing the hazard to health from exposure to chemicals is based on an incomplete data set from experimental and epidemiological studies (Environment Agency, 2009a; IGHRC, 2006). Ideally, toxicological information should always be available for the same routes of exposure as arise in practice, but this is not practical for a number of reasons (IGHRC, 2006). A common problem with many environmentally important chemicals is the lack of dermal toxicity data (Environment Agency, 2009a). Extrapolation of toxicity data from the oral route of administration to the dermal route of exposure is the most straightforward **route-to-route extrapolation**, as it offers less potential for underestimating the toxicity of a chemical (IGHRC, 2006). In the derivation of SGVs, the default assumption is to compare dermal uptake with the HCV for the oral exposure pathway (and to add this directly to the oral intake in the calculation of ADE from soil sources). [7] This is a precautionary position for most chemicals and is in line with advice from UK expert committees (IGHRC, 2006). Where the dermal toxicity of a chemical is greater than its oral toxicity, a chemical-specific approach to the derivation of the SGV will be required (Environment Agency, 2009a).

There is only limited evidence for a few chemicals on which to quantify risk and produce an HCV directly or by route-to-route extrapolation. In such cases where HCV are not available for other routes of entry, it is still precautionary to include all exposure routes in estimating the background in calculating the TDSI (that is, the combined chemical intake within **Equation 2.3**) and the ADE (within **Equation 2.5**), unless there is toxicological evidence to the contrary, such as a clear absence or barrier to systemic toxicity via one or more routes.

Where there is only a single HCV, the SGV is therefore set at a soil concentration *C* such that Equation 2.5 holds.

Equation 2.5

$$\frac{C\,R_x}{HCV_x} = 1$$

Where: *C* is the representative concentration of the chemical in soil, mg kg^{-1} dw
R_x is the ratio of ADE from soil sources for a particular exposure route *x* over the soil concentration, mg kg^{-1} bw day^{-1} over mg kg^{-1} dw soil.
HCV_x denotes the relevant HCV for a particular exposure route *x* (for example, TDSI or ID), mg kg^{-1} bw day^{-1}

Exposure route x *is normally oral or inhalation (Environment Agency, 2009a)*

---

[7] Although dermal uptake is evaluated on a chemical-by-chemical basis, the default assumption in the CLEA model is that dermal absorption is ten percent of chemical exposure from skin contact for organic chemicals (see Chapter 8).

In setting SGVs using **Equation 2.4**, an additional problem to consider is the impact on the contribution of non-soil sources to total exposure when combining pathways. This problem arises from the fact that background exposure is independent of soil concentration and the SGV calculated using **Equation 2.4** will be lower (with a reduction in total and soil exposure) than a corresponding guideline derived for each individual pathway. The CLEA model automatically corrects for this effect when setting SGV by limiting the non-soil background exposure when calculating the oral or inhalation TDSI to be no greater than that from soil, ensuring that soil always contributes a minimum of half of the total exposure when combining pathways using **Equation 2.4**.

Another consideration in applying **Equation 2.4** to the setting of SGVs is the situation where one of the HCVs is an ID and the other a TDSI. As noted previously in Section 2.3.1, non-soil background exposure is not subtracted from the ID. It would be inconsistent therefore to account for such exposure when considering a wider systemic effect using **Equation 2.4**, even when the **critical adverse effect** by the other exposure route has a threshold. For example, where a chemical has an oral TDSI and inhalation ID, non-soil inhalation background exposure will not be subtracted from the oral TDI in the setting of the SGV. However, in managing the risk to health from the combined effect, the ALARP principle will apply.

The CLEA model solves **Equation 2.4** by simultaneous calculation to find the soil concentration *C*, which is the basis for the overall SGV. This assumes that human exposure to a chemical in soil will increase and decrease in proportion to soil concentration. This is normally the case in the derivation of SGV, but there are circumstances where this assumption of proportionality breaks down.

Many exposure models, including the CLEA model, partition contaminants in soil between the solid (adsorbed to soil surfaces), dissolved and gas phases. This partitioning is modelled using theoretical coefficients and is limited by the maximum **aqueous solubility** and the saturated vapour concentration of the pure chemical (see Chapter 5). Exposure pathways that depend on the dissolved or gas phase concentration (including indoor and outdoor vapour inhalation), and plant uptake[8], may not in reality continue to increase with soil concentration above these physical limits (see Section 5.3). Above these limits, the relationship between human exposure and soil concentration will change depending on the overall contribution of these pathways to total exposure. In these circumstances **Equation 2.4** will no longer be applicable. The risk assessor should review the physical limits for each chemical, taking into account their robustness when considering whether they represent a real limit to exposure under modelled conditions.

2.3.3 Considering chemical mixtures

Knowledge about the toxicology of a chemical comes, in the main, from studies in which relatively large doses of that single substance have been administered to experimental animals (Environment Agency, 2009a). In contrast, adults and children are exposed to vast numbers of chemicals every day, including many priority soil contaminants. The possibility exists, therefore, that the mixture of chemicals to which humans are exposed will have a greater cumulative effect on health than that predicted by toxicological risk assessment of the individual chemicals. Many of the more

---

[8] Note this applies only to estimates of plant uptake using the Briggs *et al.* (1982, 1983) equations, as other empirical numerical factors are based on the total soil concentration only.

complex interactions between chemicals are unlikely at exposures below the HCVs (Environment Agency, 2009a). As a general point, assessing the effect of chemical interactions where SGVs are exceeded requires expert judgement.

If multiple chemicals are present that act via the same threshold toxicological **mode of action**, dose addition may give rise to a health effect even when the exposure to each individual chemical is below its respective TDI.

In deriving a TDI for a chemical, consideration is given to whether the contaminant belongs to a chemical group with a shared or common mode of action. In such cases, the framework in Environment Agency (2009a) may propose a group TDI, which may additionally adopt the use of potency factors to adjust for within-group variability in toxic potency (for example, Toxic Equivalence Factors, or TEFs, for dioxin-like compounds). For such chemicals, it will be necessary to publish SGVs with supporting guidance on how to adjust for site-specific variations in group composition such as the relative weight fraction (Environment Agency, 2005d).

Where a group TDI is not available, provision for potential dose addition may be achieved by calculating the Hazard Quotient (HQ), the ratio of the ADE over the relevant pathway-specific HCV, and summing these to give the Hazard Index (HI). See **Equation 2.6** and **Equation 2.7**. As a starting point, however, it may be useful to obtain an indication of the potential for dose addition by dividing the representative average soil concentration for each contaminant by its corresponding SGV and summing the results (Environment Agency, 2009a).

For non-threshold carcinogens, there is a theoretical risk of cancer at any level of exposure. Therefore, combination effects may increase the risk of cancer irrespective of the mode of action (Environment Agency, 2009a). Unless there is evidence for a common mode of action, this potential increase in cancer risk does not affect ID derivation (though site-specific assessment may account for this using an approach similar to using HI for threshold substances). Where several non-threshold carcinogens share a common mode of genotoxic action, a group ID may be proposed.

In addition to considerations of toxicity, the fate and transport of chemicals may be strongly influenced by the presence of other contaminants. Examples include the potential for co-solvent mobilisation of organics in water, competition effects during plant uptake, and relative vapour pressures within the **soil gas** (Kabata-Pendias, 2001; TPHCWG, 1999; USEPA 2003). For the most part, SGVs are established at low levels in soil where competition or saturation effects are unlikely to be significant.

Equation 2.6

$$HQ_i = \frac{ADE_i}{TDSI_i}$$

Where: HQ_i is the Hazard Quotient for chemical i in soil, dimensionless
ADE_i is the average daily human exposure to a chemical i from soil for a particular exposure route, mg kg^{-1} bw day^{-1}
$TDSI_i$ denotes the relevant TDSI for chemical i for a specific exposure route, mg kg^{-1} bw day^{-1}

Equation 2.7

$$HI = \sum_{i=1}^{n} HQ_i$$

Where: HI is the Hazard Index for all chemicals i with a common mode of action, dimensionless
HQ_i is the Hazard Quotient for chemical i in soil, dimensionless
n is the number of chemicals present sharing a common mode of toxic action, unitless

2.4 Taking account of uncertainty

Although it is possible to observe and measure human exposure to soil contamination, most human health risk assessments rely on predictions from an exposure assessment model (Defra and Environment Agency, 2004). This relies on an understanding of how risks might arise from characterising the sources of contamination, the fate and transport of chemicals in the environment, and the scientific and social aspects of human behaviour leading to exposure. All of these introduce **uncertainty**, as understanding of the risks may be incomplete and modelling results in an imperfect representation of the real world. Quantifying risk and exposure gives rise to several different areas of uncertainty and variability whose impact on any assessment should be evaluated (DETR *et al*., 2000; IPCS, 2005).

2.4.1 Types of uncertainty

Uncertainty is a lack of knowledge about specific factors in a risk or exposure assessment including parameter uncertainty, model uncertainty and scenario uncertainty (Defra and Environment Agency, 2004).

There are different types of uncertainty (IPCS, 2004; USEPA, 1997a):

- *Parameter uncertainty* relates to the value of any individual parameter in an assessment and includes sampling, analysis and systematic errors. For example, there is uncertainty associated with measurement of the concentration of a contaminant in soil or the wind speed across a site.
- *Model uncertainty* relates to limitations in the way that a model represents the real world. A model is in essence a simplification of reality in order to aid our understanding of and/or predict the outcomes of the real system. There are many situations in exposure assessment where our scientific understanding is restricted to simplistic observed relationships between parameters.
- *Scenario uncertainty* relates to limitations in the conceptual model for the exposure assessment. For example, simple assumptions may be included to make a specific assessment approximate to a broad range of conditions and to take account of wider practical, social and economic considerations.

Variability gives rise to uncertainty in risk assessment but refers to observed differences attributable to true heterogeneity or diversity in a population (USEPA, 1997a). Unlike the types of uncertainty described above, variability cannot be reduced by further study, only better described and understood. For example, by taking a larger sample of the UK population it is possible to determine in more detail the variation in body weights associated with gender and age.

Uncertainty gives rise to two kinds of built-in error within exposure models (IPCS, 2005). Selecting algorithms and their parameterisation causes practical problems to the model developer and user. Many of the algorithms used in the CLEA model are semi-empirical in nature and draw on the limited results of laboratory and field trials (see Chapters 6 to 10). Although more complex and mechanistic approaches to modelling soil systems are always being proposed, there is often a paucity of data to parameterise such approaches (Environment Agency, 2006b). Inevitably, many semi-empirical approaches are based on observations from a small number of real world situations and consider very few combinations of environmental conditions and other variables. In principle, such errors can be corrected for by greater understanding of how systems work and with improved input data, but in reality, scientific progress in these areas may take several years (IPCS, 2005).

The second type of model error is more fundamental (IPCS, 2005). Full validation of quantitative exposure models in natural systems is impossible because real world situations are never closed systems and results are always unique.[9] Scenario uncertainty is a big factor in exposure modelling and is an inevitable consequence of designing exposure scenarios that are intended to be appropriate for screening purposes. Conceptual models used for *generic* risk assessment are intended to be protective of health across a wide range of circumstances and incorporate a precautionary element to account for a *reasonable* range of possible activities (see Section 2.2). In such circumstances, validation is limited to confirming the existence of causal relationships, that is, to confirm that assumptions, choices and hypothetical relationships are reasonable (CSTEE, 2001; IPCS, 2005). In the case of the CLEA model, will contact with soil contamination along identified exposure pathways result in possible health effects?

2.4.2 Managing the uncertainty

One of the most important factors in evaluating uncertainty and variability in an exposure model is to set in context the purpose and scale of the exposure model (IPCS, 2005). As noted previously, the CLEA model estimates exposure by children and/or adults living, working, and playing on land affected by contamination. Several qualifying statements define the scale and boundaries (the domain) to the conceptual models proposed in Chapter 3 and the algorithms/parameters described in Chapters 6 to 10. These are the receptor domain, the location domain, and the time domain (IPCS 2005).

The CLEA model uses land use-based exposure scenarios for a hypothetical individual, whose aggregated exposure from all pathways is likely to be well above average. This will be health protective of the vast majority of the UK population, taking into account a wide range of different situations and site conditions. However for each exposure pathway, parameter choices are not automatically based on either a maximally exposed individual or a worst-case exposure situation.[10] The CLEA model estimates exposure for a hypothetical individual site and the results should not be extrapolated to a regional or national geographical scale. The CLEA model estimates average exposure over an extended time period of several years. It is not a dynamic model and cannot estimate the rate of change in exposure with time in any detail or to predict short periods of acute exposure.

---

[9] The only truism in modelling terms is that a model is always wrong.

[10] For example, the consumption of homegrown produce for the residential land-use scenario is based on the typical UK population and not the subgroup that grows a high proportion of the fruit and vegetables consumed by the household.

The CLEA model is **deterministic**, meaning that in any calculation a single value is assigned to each variable. Many of these values are assigned on the basis of average or conservative (the most health protective) measurements and by expert judgement.

Historically, in dealing with parameter uncertainty and variability in a deterministic model, it has been good practice to select values representative of a worst-case exposure scenario (IPCS, 2005). This has the assumed comfort of being more protective against an unforeseen situation or risks to sensitive individuals. However, the problem with this approach can be that such choices, however defensible individually, tend to be implausible collectively. If a deterministic model consists of the product of only three exposure parameters chosen at the 90th percentile, then the outcome would represent a 99.9th percentile assessment.

As an illustration of this point, Keenan *et al*. (1993) in their review of a dioxin exposure assessment for a child living close to a hypothetical municipal incinerator observed that: "*at first review, the analysis seemed reasonable until one noted that the child ate about a teaspoon of dirt each day, that his house was downwind of the stack, that he ate fish from a pond near the incinerator, his fish consumption was at the 95th percentile level, he drank contaminated water from the pond, he ate food grown primarily from the family garden, and he drank milk from a cow that had grazed on forage from the farm*."

Over recent years there has been an increasing desire on the part of authoritative bodies to move away from modelling a worst case or maximally exposed individual to more realistic or reasonable exposure scenarios (Rikken *et al*., 2001). This is the approach adopted in the CLEA model and takes into account not only the degree of conservatism from individual choices, but also the collective effect of these choices. This can be simplified to (examples provided in Table 2.2):

- Identify common activities or pathways likely to result in exposure and use reasonable worst-case estimates (that is, a high-end weighted value from the available technical literature).
- Identify an unusual (but not unlikely) worst-case activity and use typical case assumptions (that is, a central tendency weighted value from available studies).

An alternative to a deterministic approach is the **stochastic** model, which replaces single-value parameters in the exposure assessment with a family of values selected from a defined probability distribution. The original CLEA model pioneered such approaches for risk assessment in the UK but practical difficulties were encountered with using it directly in generic risk assessment. The current deterministic approach is consistent with international practice.

Stochastic techniques are useful in analysing and characterising uncertainty within complex multimedia models (IPCS, 2005; USEPA, 1997a; Saltelli *et al.,* 2004). These have been used along with other techniques to produce a comprehensive **sensitivity analysis** of the CLEA model (Environment Agency, in prep.). This analysis identifies the key parameters influencing estimates of exposure using the CLEA model and the critical areas of uncertainty driving risk considerations.

Table 2.2: Building reasonable worst-case exposures

Activity	Type	Example exposure parameters
Playing in the garden	Common	Above median soil ingestion rates combined with high-end exposure frequencies
Growing fruit and vegetables	Unusual	Mean homegrown fractions based on general population
Living in the home	Common	Breathing rate based on average body weight, combined with high-end exposure frequencies and indoor air concentrations of dust and vapour

3 Generic land use scenarios

Exposure assessment is based on defined exposure scenarios, a specific conceptual model that sets out a discrete set of circumstances where exposure may occur including the source, the pathways, and the exposed population (see Section 2.2). In assessing exposure from contaminated sites, the CLEA model uses land use as a central and unifying theme.

In this chapter, three generic land use scenarios are described. The CLEA model uses these conceptual models to derive the SGVs. Each land use is introduced in a general way, painting a picture of the envisaged use. This is followed by a more detailed discussion of the critical receptor, relevant pathways and frequency of exposure, based on a review of information on activity patterns.

3.1 Introduction

Generic land use scenarios have been used to derive SGVs and are considered appropriate for generic quantitative risk assessments for contaminated land. They are based on the grouping of a range of typical activities according to land use, and taken as a whole these scenarios represent a reasonable worst case that will be protective of human health for the majority of sites. However, it is extremely unlikely that every detail of the conceptual models presented here will accurately reflect the conditions found at any one specific site and the judgement on whether such differences are important must be made by the risk assessor. Such a decision should take into account:

- Whether the differences between actual site circumstances and assumptions within the generic land use scenario would mean that the estimated exposure or outcome decision would be vastly different.
- Whether site circumstances are based on robust observations and take into account reasonable foresight, given physical and other constraints on land use.

Minor differences between these conceptual models and the actual site circumstances, such as adjustments of a few days to exposure frequency, are unlikely to result in major differences to the resulting exposure estimate. If actual representative average soil concentrations across the site already exceed the SGV by a factor of three or more, further minor adjustment is unlikely to affect the outcome of the generic quantitative risk assessment. More important factors including consideration of actual plant uptake (see Chapter 7) or vapour intrusion (see Chapter 10), the presence or absence of the critical receptor, and/or the identification of additional exposure pathways, such as a private drinking water supply, would probably result in considerably different estimates of exposure and therefore are more likely to affect the outcome of the risk assessment.

Additional guidance is available on factors that are likely to vary significantly between sites and how to collect essential data as part of a detailed quantitative risk assessment (CIRIA, in press; Environment Agency, 2009b and in prep.). In such cases, the generic land use scenarios presented here can offer a starting point.

3.2 Residential land use

3.2.1 Summary

This generic scenario assumes a typical residential property consisting of a two-storey house built on a ground-bearing slab with a private garden consisting of lawn, flowerbeds, and a small fruit and vegetable patch. The occupants are assumed to be parents with young children, who make regular use of the garden area.

The key assumptions for the residential land use model are summarised in Box 3.1.

Box 3.1: Key generic assumptions for residential land use

The key features of the residential land use conceptual model are:

- Critical receptor is a young female child (aged zero to six years old).
- Exposure duration is six years.
- Exposure pathways include direct soil and indoor dust ingestion, consumption of homegrown produce, consumption of soil adhering to homegrown produce, skin contact with soils and indoor dust, and inhalation of indoor and outdoor dust and vapours.
- Building type is a two-storey small terraced house.

Figure 3.1: Residential land use

3.2.2 Overview

Government undertakes two surveys in England relevant to developing a residential exposure scenario. The Survey of English Housing (SEH) is an annual household survey which collects information by interview from approximately 20,000 households about their housing. DCLG (2006a) summarises the latest data from the 2004/05 survey. The English House Condition Survey (EHCS) includes a physical inspection of property by professional surveyors. The information obtained through the EHCS provides an accurate prediction of the type and condition of housing in England. DCLG (2006b) and DCLG (2006c) provide a detailed account of the condition of homes in 2003 and a mid-point survey position for 2004 respectively.[11]

In 2004, there were around 22 million homes in England (DCLG, 2006c). Of the 17 million households living in private sector homes in 2004, three million were classified as vulnerable (in receipt of at least one of the principal means-tested or disability-related benefits). More than one million of these vulnerable households included either infants (less than five years old) or elderly people (75 years or older) who tend to be more at risk in terms of health outcomes of poor housing (DCLG, 2006c).

In 2005, although a couple without dependent children was the most common type (36 per cent) of all households, 29 per cent did have dependent children living at home (DCLG, 2006a). The average household size in 2005 was 2.4 persons (DCLG, 2006a). In 2004/05, 82 per cent of households lived in a house or bungalow and 17 per cent in a flat or maisonette. About 74 per cent of households lived in two-storey buildings and 84 per cent had the use of a garden (DCLG, 2006a). Ninety-five per cent of those who lived in a house or bungalow had a garden.

In the 2005 survey, length of residence in current accommodation varied considerably between types of tenure. Owner-occupiers had lived in their current homes for a median 11.5 years, social renters for a median 7.4 years and private renters for 1.5 years (DCLG, 2006a).

3.2.3 Critical receptor

There is little doubt that adults and children are found together in a residential setting with up to 29 per cent of households with dependent children (DCLG, 2006a). As noted in Section 2.2.1, where young children and adults are likely to be present together, it is usual to consider the child as the critical receptor. The CLEA model estimates exposure for a young child over a period of six years from age zero to six years old. This is consistent with international practice.

3.2.4 Exposure pathways

The young child may be exposed to chemicals from soil in a number of ways through playing in the home and the garden, eating homegrown produce, and simply breathing indoor and outdoor air. The CLEA model predicts human exposure by up to ten different pathways and all are assumed to be applicable in the residential setting. The exposure pathways considered by this scenario are direct soil and dust ingestion, consumption of homegrown produce, consumption of soil adhering to homegrown

---

[11] Similar surveys were carried out in Scotland in 2003 and Wales in 1998. An interim survey was carried out in Northern Ireland in 2004.

produce, dermal contact with soil and indoor dust, and inhalation of indoor and outdoor dust and vapours.

An important judgement for the risk assessor is whether the household is able to grow its own fruit and vegetables in the garden and what sized garden is required to grow the default amounts used by the CLEA model. This scenario assumes that only a small proportion of produce is grown in the garden and therefore the average generic homegrown fraction is used (see Table 4.19 and Section 4.4.5 for further details). Applying the consumption rates in Table 4.17 to a household of two adults and two children, the required garden area could be as little as 20 m^2 (see Box 3.2 for a summary of this calculation and Section 3.2.6 for further information).

It is assumed that the property receives its water through public supply pipes only (not from a private well or spring which may be contaminated). If a private water supply is found on the site, the risk assessor should take into account additional exposure pathways such as consumption of drinking water and activities such as showering.

3.2.5 Activity patterns

Exposure frequencies are based on time-use studies and are set out for each pathway in Table 3.1 for age classes one to six. Although the assumption that the young child spends a portion of time at home for every day of the year appears conservative, the available data suggests that this may be typical of a significant proportion of the population. For example, data from the UK Tourism Survey in 1998 reported that 41 per cent of UK residents did not take a holiday of four nights or more in the calendar year, a proportion that has remained consistent over the past 30 years (Office of National Statistics, 2002c).

Although exposure frequencies are established on the basis of reviewing activity pattern data (such as the work of Gershuny *et al*. ,1986, and Gershuny, 2000) they must also take into account limitations in the underlying estimates of chemical intake. For example, with the exception of age class one, soil and dust ingestion is assumed to be 365 days per year although it is unlikely that a child will spend a substantial amount of time in the garden every day of the year. It is set at this frequency because the empirical studies that underpin estimates of soil and dust ingestion do not account for either the length of time outdoors or indoors and do not always distinguish between soil from outside and house dust that contains a soil-derived component (see Section 6.1.3). Similarly, the consumption rates for homegrown produce are based on annualised data and therefore a hypothetical exposure frequency of 365 days per year should always be assumed (see Section 4.4.4).

Data on indoor and outdoor **site occupancy** in hours per day are presented in Table 3.2 for each age class from one to six. This data is important for estimating child exposures via inhalation of dusts and vapours (see Chapters 9 and 10).

According to data from the UK Time Use Survey 2000, women spend on average 18 hours per day at home with children under the age of two, which progressively decreases to 15 hours per day for teenage children (Office of National Statistics, 2006a). In the same survey, analysis of children's activities (aged 15 years or under) by type and location suggests that on average they spend very little time outdoors, although they spend 16 hours per day in and around the home.[12]

---

[12] Children under the age of 15 years spend on average only twenty minutes per day outdoors doing physical exercise, gardening and pet care, resting, and pursuing a social life in and around the home (Office of National Statistics, 2006a).

Box 3.2: Calculation of required growing area for homegrown garden produce

Assume a household consisting of two adults (70 kg bw) and two children (15 kg bw) consume homegrown garden produce at the daily rate shown in Table 4.17 for a year (adjusted for the homegrown fraction in Table 4.19). [1]

Category	Annual household consumption (kg fw)
Green vegetables	16.8
Root vegetables	5.7
Tuber vegetables	3.0
Herbaceous fruit	8.2
Shrub fruit	1.5
Tree fruit	7.8

Data from Pollock (2002) and Mobbs (2003) was used to provide estimated yields per square metre for a broad range of fruits and vegetables. Comparing these with the calculated consumption rates above gives an estimated garden area for crop production.

Category	Typical yields (kg fw m^{-2}) [2]	Area required (m^2)
Green vegetables	2.8	7.7
Root vegetables	4.7	1.7
Tuber vegetables	4.4	0.7
Herbaceous fruit	5.1	4.0
Shrub fruit	0.8	1.9
Tree fruit	1.8	3.9
	Total Area	19.9

[1] Consumption rates and homegrown fractions are based on data for individual fruit and vegetables as defined in Table 4.19 and 4.21 and not on produce group averages

[2] Indicative average values for each category based on individual species data (and have not been used directly in the area calculation)

The occupancy periods used in the residential land use exposure scenario have been based on the following assumptions:

- Children up to school age (that is, age classes one to four) spend all their time in or close to the home.
- In the case of school-age children in age classes five and six, the assumption is that they spend about seven hours per day at school during the term, resulting in a weighted average of time spent at home of 20 hours per day across the year.
- Outdoor activity has been limited to one hour per day, with the assumption that most indoor activity includes sleep and watching TV.

Table 3.1: Default exposure frequencies for each pathway for age classes one to six

	Standard residential land use exposure frequencies (day $year^{-1}$)					
Age class	Soil and dust ingestion	Homegrown produce	Dermal		Inhalation	
			Indoor	Outdoor	Indoor	Outdoor
1	180 [1]	180 [2]	180 [1]	180 [1]	365	365
2	365	365	365	365	365	365
3	365	365	365	365	365	365
4	365	365	365	365	365	365
5	365	365	365	365	365	365
6	365	365	365	365	365	365

[1] It is assumed that an infant has limited contact with garden soils or household dust for the first six months.

[2] Department of Health (2006) recommends that infants are introduced to solid food from about six months starting with pureed fruit and vegetables such as pear, carrot, and potato as suitable first foods.

Table 3.2: Default site occupancy periods for age classes one to six

	Standard residential land use occupancy periods (hour day^{-1})	
Age class	Garden	Indoors
1	1	23
2	1	23
3	1	23
4	1	23
5 [1]	1	19
6 [1]	1	19

[1] It is assumed that the child is at school for seven hours per day (from 9am to 4pm) for 180 days per year and at home for 24 hours per day on non-school days.

3.2.6 Other assumptions

The Environment Agency (2005) reviewed available literature on the UK housing stock to identify default values for several building parameters that could be used in screening models for soil vapour intrusion into buildings. Many of the figures used by this report were taken from the English House Condition Survey 2001. Given that most households live in a two-storey property, a two-storey small terraced house has been adopted as the default for this exposure scenario, since this is the most health protective selection of the two-storey building types in Table 4.21.[13] The building parameters used in the CLEA model are discussed further in Section 4.5 and for this land use are summarised in Table 3.3.

MAFF (1999) estimated that 85 per cent of residential gardens occupied an area greater than 100 m^2 and that 34 per cent were greater than 450 m^2. The default garden area used in this exposure scenario is 100 m^2 (allowing for 20 per cent of the area to be given over to the growing of fruit and vegetables). Accounting for the lawn and hard standing such as a patio, it is assumed that about 75 per cent of the garden area is covered for the purposes of calculating ambient dust concentrations

Parameters for estimating the chemical intake for this type of land use are discussed in Chapters 6 to 10. This conceptual model assumes that a certain proportion of contaminated soil may reasonably be tracked back from the garden into the home and that this contributes to exposure to contamination from the soil-derived fraction of indoor dust (see Section 4.3.2 for further details).

The soil contamination is uniformly distributed across the site at the surface in garden soils (to a depth of at least one metre) and from 0.5 m beneath the building foundations (that is, 0.65 m from the soil surface). The depth to source beneath the building is a compromise between consistency with the overall conceptual model and technical limitations of the Johnson and Ettinger (1991) model to predict indoor air levels at very shallow depths (see Chapter 10). As noted previously, the soil concentration does not decrease with time either as a result of transport and dispersion or by chemical/ biological degradation (see Section 2.1.2).

Table 3.3: Default building parameters for the standard residential land use (after Environment Agency 2005)

Parameter	Value	Notes
Footprint area (m^2) [1]	28	Simple square footprint
Living space height (m)	4.8	Two-storey living area
Air exchange rate ($hour^{-1}$)	0.5	
Pressure difference between soil and indoor air (Pa)	3.1	
Foundation thickness (m)	0.15	Ground bearing slab design
Floor crack area (m^2)	0.04	

[1] Two-storey small terraced residential house with an assumed square footprint. Table 4.21 provides default values for other residential building types.

---

[13] The screening models described in Chapter 10 may predict higher indoor air concentrations of volatile compounds for different building configurations, most notably bungalows and other single storey properties. Care should therefore be taken in applying SGVs for volatile compounds, where a two-storey property is not present.

3.3 Allotment land use

3.3.1 Summary

This generic scenario assumes a plot of open space (about 250 m^2), commonly made available by the local authority to tenants to grow fruit and vegetables for their own consumption. There are usually several plots to a site and the overall site area may cover more than a hectare. The tenants are assumed to be parents or grandparents and that young children make occasional accompanied visits to the plot.

Key assumptions for the allotment land use model are summarised in Box 3.3.

Box 3.3: Key generic assumptions for the allotment land use

The key features of the allotment land use conceptual model are:

- Critical receptor is a young female child (aged zero to six years old).
- Exposure duration is six years.
- Exposure pathways include direct soil ingestion, consumption of homegrown produce, consumption of soil adhering to homegrown produce, skin contact with soils, and outdoor inhalation of dust and vapours.
- There is no building.

Figure 3.2: Allotment land use

3.3.2 Overview

Allotments, community gardens and city farms are valuable green spaces that can help improve people's quality of life by promoting healthy food, exercise and community interaction (DCLG, 2006d). An allotment is a plot of land where individuals can grow fruit and vegetables for consumption by themselves and their family. Allotments are managed by 'allotment authorities', which can include district authorities, unitary authorities and local councils (DCLG, 2006d). Crouch (1997) identified nearly 300,000 allotments in England, occupying a total area of more than 10,000 hectares. Allotments are enjoyed by more than a quarter of a million people and their families (Crouch, 1997).

Allotments derive from the enclosure legislation of the eighteenth and nineteenth centuries and the word "allotment" originates from land being allotted to an individual under an enclosure award (SCETRA, 1998). Local authorities have a statutory duty under Section 8 of the Small Holdings and Allotments Act 1908 to provide a sufficient number of allotments when they consider that there is a demand (DCLG, 2006d). Within the relevant legislation, there are various restrictions placed on the use of allotment sites. In particular, the plot must be "*mainly cultivated by the occupier for the production of vegetables and fruit crops for consumption by himself or his family*" (House of Commons, 1922). The implication of this is that only a limited proportion of a plot may be used for growing flowers and no commercial use may be made of produce (SCETRA, 1998). Subsequent legislation has restricted livestock to certain types of animal such as hens and rabbits (House of Commons, 1950).

3.3.3 Critical receptor

According to the national survey of allotments in 1993, more than 60 per cent of allotment gardeners are aged fifty and over (Saunders, 1993). Although 25 per cent of those surveyed had dependent children (less than eighteen years old) living at home, there is little or no formal survey data on children accompanying their parents or grandparents in the evening or at weekends, or on activities such as trespassing.

There is evidence that in recent years, the number of younger allotment gardeners has increased; for example, the GLA (2006) quotes the London Allotments Network as stating that half of the applicants for allotment plots are women with young children (citing awareness of food miles and requirements for organic produce as possible reasons for this change). In addition Birmingham City Council, the largest provider of allotments of any local authority in the UK, has stated that there is a growth in new tenants, particularly women and those aged 20 to 35 years (Birmingham City Council, 2007). This trend is consistent with best practice guidance on allotment management which encourages allotment sites to be made child friendly by converting unused plots into a play area for allotment holders' children (SCERTA, 1998).

During informal discussions with stakeholders as part of the Defra Way Forward exercise, several local authorities have indicated anecdotally that children were "*likely to be present*" on allotments on a regular but infrequent basis (Defra, 2006). As noted in Section 2.2.1, where young children and adults are likely to be present together, it is usual to consider the child as the critical receptor. The CLEA model estimates exposure for a young child for a period of six years from age zero to six years old. This is consistent with international practice.

Children and allotments

An important assumption in this generic land use scenario is the presence of children at the allotment site on a regular but infrequent basis. The risk assessor using a SGV based on this conceptual model should consider whether children are actually or likely to be present, for example, by talking with allotment holders or carrying out a site survey. An alternative scenario is to consider only the adult gardener; however, care should be taken where exposure is primarily via the consumption of homegrown produce, since the gardener's family would likely have similar intakes and child exposure may be high even if they rarely visit the site itself.

3.3.4 Exposure pathways

The young child may be exposed to chemicals from soil in a number of ways, through visiting the allotment to eating allotment produce. The CLEA model predicts human exposure by up to ten different pathways, but only the outdoor pathways and the consumption of allotment produce are considered relevant to this land use. Although Saunders (1993) reported that nearly 50 per cent of allotment plots had a shed or outhouse, high indoor exposure is unlikely because many sheds are small, used only for storage, and typically well ventilated. The pathways considered by this exposure scenario are direct soil ingestion, consumption of allotment produce (including consumption of soil adhering to allotment produce), dermal contact with soil, and outdoor inhalation of dust and vapours.

Although some allotment holders may choose to keep animals, including goats, rabbits and poultry, potential exposure to contaminated meat and eggs is not considered within the CLEA model. In evaluating the applicability of an SGV to assessing an allotment site, the assessor should consider the relative importance of other produce not otherwise considered by this exposure scenario.

In this scenario, allotment holders and their families are assumed to consume a higher proportion of homegrown fruit and vegetables from the allotment than the average family and therefore the high-end generic homegrown fraction is used (see Table 4.19 and Section 4.4.5 for further details). This is a reasonable worst-case assumption.[14] Applying the consumption rates in Table 4.17 to a household of two adults and two children, the required growing area is about 130 m^2 (see Box 3.4 for a summary of this calculation). This is about one-third of the available area of a typical allotment of 300 m^2 (Crouch, 1997).

---

[14] No national study has specifically targeted the habits of allotment holders and community gardeners, who might reasonably be expected to grow a significant proportion of their fruit and vegetable intake. The higher proportion used in this exposure scenario has been estimated by adjusting the average non-purchased fraction calculated from the Expenditure and Food Survey 2004/05 by the fraction of the survey population that reported any non-purchased items for specified vegetables in the earlier National Food Survey 1999. See Section 4.4.5 for further details.

Box 3.4: Calculation of required growing area for homegrown allotment produce

Assume a household consisting of two adults (70 kg bw) and two children (15 kg bw) consume homegrown allotment produce at the daily rate shown in Table 4.17 for a year (adjusted for the homegrown fraction in Table 4.19). [1]

Category	Annual household consumption (kg fw)
Green vegetables	111.8
Root vegetables	38.3
Tuber vegetables	20.2
Herbaceous fruit	54.5
Shrub fruit	10.3
Tree fruit	52.2

Data from Pollock (2002) and Mobbs (2003) was used to provide estimated yields per square metre for a broad range of fruits and vegetables. Comparing these with the calculated consumption rates above gives an estimated allotment area for crop production.

Category	Typical yields (kg fw m^{-2}) [2]	Area required (m^2)
Green vegetables	2.8	51.5
Root vegetables	4.7	11.3
Tuber vegetables	4.4	4.6
Herbaceous fruit	5.1	26.9
Shrub fruit	0.8	12.9
Tree fruit	1.8	25.7
	Total Area	132.9

[1] Consumption rates and homegrown fractions are based on data for individual fruit and vegetables as defined in Table 4.19 and 4.21 and not on produce group averages

[2] Indicative average values for each category based on individual species data (and have not been used directly in the area calculation)

3.3.5 Activity patterns

Activity patterns for allotment use, including the frequency and duration of visits, have been surveyed for England and Wales by Saunders (1993), a study which updated the earlier comprehensive survey known as the Thorpe Report (Ministry of Housing and Local Government, 1969). The survey results are summarised in Table 3.4.

Saunders (1993) reported a large seasonal variation with fewer visits, and of a shorter duration, during the winter months. During the summer, more than 80 per cent of those questioned visited their allotment several times per week and 36 per cent virtually every day. More than 90 per cent spent at least an hour or two per visit. In winter, about 30 per cent visited the allotment several times a week or more, with more than 50 per cent spending at least one or two hours per visit. Assuming that the allotment gardener visits the plot every day in the summer and three times per week in the winter (based on a reasonable worst case), the annual average exposure frequency would be 258 days per year.

None of the allotment surveys have differentiated between age and gender for the purposes of reporting the frequency and duration of visits. In the case of Saunders (1993), approximately two-thirds of the survey sample was aged over 50 and therefore the reported data is likely to be more representative of the older age group. It has therefore been necessary to make assumptions about the frequency with which children will accompany parents and grandparents to the allotment (see Table 3.5).[15]

Exposure frequencies are set out for each pathway in Table 3.6 for age classes one to six, and for the most part are based on the number of site visits from the allotment survey. The consumption rates for homegrown allotment produce are based on annualised data and therefore a hypothetical exposure frequency of 365 days per year should always be assumed (see Section 4.4.4).

Table 3.4: Frequency and duration of visits to allotments (Saunders, 1993)

	Summer		**Winter**	
	No. of respondents	**%**	**No. of respondents**	**%**
Frequency				
Virtually every day	300	36	58	7
Several times a week	421	51	197	23
Once a week or so	95	11	348	41
Two or three times a month	14	2	165	20
Once a month or less	4	1	73	9
Duration				
Only a few minutes	2	-	30	4
Less than 30 minutes	4	1	109	13
Less than one hour	22	3	253	30
One to two hours	431	52	367	44
Three hours or more	373	45	75	9

Table 3.5: Children accompanying a parent/grandparent during allotment visits

Age Group	**Visits accompanying parents (%)**	**Visit frequency (days per year)** [1]
Infants (0-1 years)	10	25
Toddlers (1-4 years)	50	130
Young person (4-11 years)	25	65
Young person (12-16 years)	10	25

[1] As a proportion of the adult frequency of 258 days per year

Averaged over the year, most allotment holders typically spent between one and two hours at the allotment per visit (Saunders, 1993). However, in the summer months nearly half of those surveyed spent more than three hours per visit and a value of three hours has been chosen as a reasonable upper bound for the time a child stays on site. Data on the site occupancy periods (hours per day) for outdoor exposure are presented in Table 3.7 for each age class from one to six. This data is important for estimating child exposures via inhalation of dusts and vapours (see Chapters 9 and 10).

---

[15] The Environment Agency is undertaking a review of these assumptions with the National Society of Allotment and Leisure Gardeners and this will be used to update the assumptions for this generic land use scenario.

3.3.6 Other assumptions

According to Crouch (1997), about half of individual allotment plots are about 10 rod or about 300 m^2 in size. There were 7,796 sites identified in the English survey, covering more than 10,200 hectares, with an average of 1.3 hectares per site (Crouch, 1997).

Parameters for estimating the chemical intake for this type of land use are discussed in Chapters 6 to 10. Since airborne dust and vapours from one plot may be easily mixed with dust and vapours from other plots, the area of generation and dispersion is assumed to be about 5,000 m^2, which is much larger than a standard plot but often less than a complete site. It is assumed that only 50 per cent of the source area is covered by plants and limited hard standing such as paths and sheds for the purposes of calculating ambient dust concentrations.

This conceptual model does not assume that a certain proportion of contaminated soil is tracked back into the home (see Section 4.3.2 for further details). Although Saunders (1993) observed that more than two-thirds of allotments were less than a mile from the home, the much lower frequency of visits to the allotment compared with a residential garden and the use of reasonable standards of hygiene (such as leaving boots outside or in the car) means this exposure route is less likely to be significant. In evaluating the applicability of an SGV to an allotment, the assessor should consider whether tracked back contamination is more likely to occur because of factors such as the proximity of the site to home and the location where tools, plants, and outdoor clothes are stored.

The soil contamination is uniformly distributed across the site from the surface to a depth of at least one metre. Soil concentration does not decrease with time as a result of transport and dispersion or by chemical/ biological degradation (see Section 2.1.2).

Table 3.6: Default exposure frequencies per pathway for age classes one to six

	Standard allotment land use exposure frequencies (day year^{-1})					
Age class	Soil ingestion	Homegrown produce	Dermal		Inhalation	
			Indoor	Outdoor	Indoor	Outdoor
1	25	180 [1]	0	25	0	25
2	130	365	0	130	0	130
3	130	365	0	130	0	130
4	130	365	0	130	0	130
5	65	365	0	65	0	65
6	65	365	0	65	0	65

[1] Department of Health (2006) recommends that infants are introduced to solid food from about six months starting with pureed fruit and vegetables such as pear, carrot, and potato.

Table 3.7: Default on-site occupancy periods for age classes one to six

Age Class	Standard allotment land use occupancy periods (hour day^{-1})
1	3
2	3
3	3
4	3
5	3
6	3

3.4 Commercial land use

3.4.1 Summary

There are many different kinds of workplace and work-related activities. This generic scenario assumes a typical commercial or light industrial property consisting of a three-storey building at which employees spend most time indoors and are involved in office-based or relatively light physical work.

The key assumptions for the commercial land use model are summarised in Box 3.5.

Box 3.5: Key generic assumptions for the commercial land use scenario

The key features of the commercial land use are:

- Critical receptor is a working female adult (aged 16 to 65 years old).
- Exposure duration is a working lifetime of 49 years.
- Exposure pathways include direct soil and indoor dust ingestion, skin contact with soils and dusts, and inhalation of dust and vapours.
- Building type is a three-storey office (pre-1970).

Figure 3.3: Commercial land use

This conceptual model is not designed to consider those sites that involve 100 per cent hard cover (such as car parks), where direct contact with contaminated soils is extremely limited. However, direct contact is not the main pathway for volatile chemicals and risk assessors should consider whether an SGV is still applicable where vapour pathways are driving the risk.

Many commercial premises actively welcome children on site, such as sports and shopping centres, and therefore the risk assessor should carefully consider whether the exposure scenario presented here is protective of such situations. This exposure scenario is not suitable for any part of a site occupied by a workplace nursery.

3.4.2 Overview

A modern economy has a diverse range of commercial enterprises including agriculture and fishing, manufacturing and distribution, construction, and service industries. There were 2.5 million business sites registered in 2004 (Office of National Statistics, 2006b).

Over one-quarter of the business sites across regions of the UK were in wholesale and retail sales, maintenance and repair of vehicles and household goods, and the hotels and catering sector, with the North East having the highest proportion at almost one-third (Office of National Statistics, 2006b).

According to the Annual Business Inquiry, the largest sector by number of enterprises with 33 per cent of all businesses is real estate management, rental companies, legal services, management consultancy, advertising and recruitment services, and other professional activities such as architects and design (Office of National Statistics, 2006c). Together with retail sales and repair services, these two sectors account for more than half of all businesses (Office of National Statistics, 2006c; Small Business Service, 2006a).

Small and medium-sized businesses (defined as those with less than 250 employees) accounted for over 99 per cent of all UK enterprises at the start of 2002 and 56 per cent of employment (Small Business Service, 2006a). However, 73 per cent of businesses are sole traders – that is, self-employed people operating without any employees (Small Business Service, 2006b). Many small businesses operate out of houses or properties that have been converted into offices or shops.

Urban areas have seen a growth in total employment in the 1990s (DETR, 2001). However, in many cities and towns there has been a shift away from employment in manufacturing and construction to finance and retail services (DETR, 2000). Over the period 1992 to 1996, commercial land use accounted for only 17 per cent of all new urban uses, although it had the highest rate of recycling previously developed land than any other land use (DCLG, 2001). This trend continued into the new millennium with some 68 per cent of new commercial development provided by previously developed land over the period 2001 to 2004 (DCLG, 2006e).

During the 1980s and early 1990s, many new retail and industrial parks were built on the edge of towns and cities (Urban Task Force, 1999; Office for National Statistics, 2000b). This peaked in 1989 when in one year 79 out-of-town shopping developments (of more than 50,000 square feet) were built (Office for National Statistics, 2000b). However, from 1998 this trend started to reverse, with predicted town-centre developments in 2000 outstripping those on the edge of towns by about ten to one in terms of floor space area (Urban Task Force, 1999).

3.4.3 Critical receptor

There are many different kinds of workplace and work-related activities that could be covered by this exposure scenario; however, for it to be effective, certain bounding assumptions must be used to limit the possibilities. This conceptual model assumes a small to medium-sized commercial or light industrial property at which the employees spend most time indoors and are involved in office-based or light physical work.

As noted in Section 2.2.1, where young children and adults are likely to be present together, it is usual to consider the child as the critical receptor. However, in many workplaces children are not permitted and where they are regular visitors such as in shops or leisure facilities, both duration and frequency of exposure are likely to be much lower compared to a full-time employee. An adult of working age is more likely to be the critical receptor in most cases. The CLEA model estimates exposure for a working adult over a period of forty-nine years from age 16 to 65 years old. The use of a working adult is consistent with international practice.

3.4.4 Exposure pathways

The working adult may be exposed to chemicals from soil in a number of ways at the workplace. The critical assumption in this exposure scenario is that the worker spends most time indoors, with limited opportunity for direct contact with soil. Contamination may be tracked back into the building from nearby ground such as a grassed/ landscaped areas or an undeveloped part of the site. The pathways considered by this exposure scenario are direct soil and dust ingestion, dermal contact with soil directly and from indoor dust, and inhalation of dust and vapours. The primary exposure routes are therefore vapour intrusion into the building and contact with indoor dust containing soil contamination tracked back from outside.

Children and commercial land use

As a rule-of-thumb, the exposure scenario presented here is not suitable to circumstances where a young child regularly spends more than seven hours per day at the site (that is, a significant proportion of a typical working day). For example, there has been a rapid increase in pre-school childcare provision since the late 1990s and a significant minority are located at the workplace (Daycare Trust, 2005; National Audit Office, 2004). The exposure scenario presented here would not be suitable for assessing risks from this type of commercial use.

The risk assessor should also carefully consider informal land use, especially where the commercial premises are vacant or site security is poorly managed. Children may trespass on derelict land on a regular and frequent basis; often, such unsupervised activity leads them directly into contact with ground contamination.

3.4.5 Activity patterns

The activity pattern for this generic scenario depends on work habits including the job tenure, the length of working hours, and the frequency and length of breaks.

Where the working adult is the receptor, a working lifetime of 49 years is used. Since estimated exposure from year to year does not vary[16], the critical factor is the assumed length of service with the same employer. Table 3.8 from the Labour Force Survey gives the length of service data for UK employees from 1986 to 2002 (Office of National Statistics, 2002b, 2003). The average length of service of employees has remained stable since 1975, with one in ten employees of working age having been in their job for less than six months and a similar proportion having been with the same employer for over 20 years. The average length of service for women with children has risen due to the increased provision and use of maternity leave (Office of National Statistics, 2003). A recent commercial survey found that 76 per cent of respondents had left their last organisation within three years and the length of service for women had increased (Reed Consulting, 2005). Burgess and Rees (1996) observed a similar pattern for younger workers in their study of labour market data over the period 1975 to 1992. However, they also observed a second group, estimated to be around 24 per cent of the working population that had worked for one employer for at least thirty years (Burgess and Rees, 1996). This figure is much higher than the observed trend to 2000.

The exposure frequencies for outdoor and indoor exposure pathways are 170 and 230 days per year respectively (see Table 3.9). It is assumed that employees work a five-day week and have up to six weeks leave (including statutory holidays such as Easter and Christmas) per year. This results in an indoor exposure frequency of 230 days per year. The outdoor exposure frequency assumes that the employee spends part of the day outside, typically their lunch break, for about three-quarters of the year, staying totally indoors only during the coldest and wettest periods. The outdoor exposure frequency is 170 days per year.

Table 3.8: Employee length of service (Office of National Statistics 2002b, 2003)

	Percentages of UK workforce				
Length of service	**1986**	**1991**	**1996**	**2000**	**2002**
Less than three months	5	5	5	5	5
Three months but less than six months	4	4	5	5	5
Six months but less than one year	9	10	9	10	10
One year but less than two years	11	13	12	13	13
Two years but less than five years	20	24	19	21	22
Five years but less than ten years	21	16	21	15	15
Ten years but less than twenty years	20	19	19	20	19
Twenty years or more	9	9	11	11	10

In a review of working time patterns, Bishop (2004) noted that the UK has a higher proportion of employees working more than 45 hours per week than many other European countries including France, Denmark and Sweden. However, the number of people working long hours in the UK has declined over the past decade. Part-time work continues to be a characteristic of working time patterns, with 24 per cent of employees working part-time in the UK (Bishop, 2004). The UK is distinguished from other European countries by the relative long hours worked by full-time employees, estimated to be 44 hours per week on average. In certain industrial sectors such as agriculture, manufacturing, and services, significant minorities of employees (between 15 and 40 per cent) work in excess of 50 hours per week (Bishop, 2004). Although not specified in the approach used by Bishop (2004), it is assumed that the reported working hours exclude the main meal break.

---

[16] This is because the averaging time is assumed to be equal to the exposure duration (see Section 2.1.1 for further information) and the exposure characteristics, such as body weights, are defined for the working age class as a whole.

Table 3.9: Default exposure frequencies for each pathway for age class 17

	Standard commercial land use exposure frequency (days per year)
Soil and dust ingestion	230
Dermal contact with indoor dust	230
Dermal contact with soil	170
Inhalation of dust and vapours from indoor air	230
Inhalation of dust and vapours from ambient air	170

For many workers in the UK, the lunch break is no longer synonymous with “the lunch hour”. A market survey by analysts Datamonitor (2000) suggested that the “*majority of UK workers take between 25 and 30 minutes for their lunch break*”. However, in many businesses including manufacturing, distribution and retail it is still common practice for employers to allow their employees one or two additional short breaks during the day, especially where the work is monotonous and intensive, requiring a high level of concentration.

In this exposure scenario, the average working week is assumed to be 45 hours, including a one-hour break each day. For a five-day week, this corresponds to an average time on site of nine hours per day. Site occupancy periods (hours per day) for indoor and outdoor exposure are also weighted according to the frequency of time spent indoors and outdoors and are 8.3 hours per day and 0.7 hours per day respectively. See Box 3.6 for further explanation.

Data on the site occupancy periods (hours per day) is important for estimating adult exposures via inhalation of dusts and vapours (see Chapters 9 and 10). Throughout their time on site, the worker is assumed to undertake no energetic activity since few current occupations are regarded as being very active (Department of Health, 1991).

3.4.6 Other assumptions

The Environment Agency (2005) reviewed available literature on the UK non-domestic building stock to identify default values for several building parameters that could be used in screening models for soil vapour intrusion into buildings. Most commercial buildings are relatively old, with around 50 per cent of buildings dating from before the Second World War. The non-domestic building stock is much more diverse than the housing stock in terms of size, shape and construction materials (Environment Agency, 2005), which reflects the diversity of end uses from office and retail premises to schools and hospitals. The building parameters used for this scenario are based on a pre-1970s office with a three-storey living space and are listed in Table 3.10 and discussed further in Section 4.5. This selection is consistent with the age of many commercial buildings and is the most protective of health (based on estimates of vapour intrusion) of the different building types discussed in Section 4.5.

Box 3.6: Calculations for the weighted average site occupancy periods

The commercial land use exposure scenario assumes that the worker spends 230 days per year on site. The worker is assumed to go outside the office or warehouse building on only 170 days per year for no more than one hour per day. However, for 60 days per year, the worker spends no time outside and therefore it is necessary to calculate the weighted average value.

	Days inside hours day^{-1}	Days inside/outside hours day^{-1}	Weighted average hours day^{-1}
Inside hours	9.0	8.0	8.3
Outside hours	0.0	1.0	0.7

It is assumed that all respiration periods are engaged in passive activities.

The area of land occupied by commercial properties is highly variable. Environment Agency (2005) reported that the plan area of offices and warehouses from a survey of four English towns varied from only 4 m^2 to over 20,000 m^2. Assuming a plan area of 424 m^2 for an average-sized office (see Table 3.10), the whole site then occupies a land area in the range of one to two hectares, with about 80 per cent hard standing.

Parameters for estimating the chemical intake for this type of land use are discussed in Chapters 6 to 10. This conceptual model assumes that a certain proportion of contaminated soil may reasonably be tracked back from outside into the office area and that this contributes to exposure to contamination from the soil-derived fraction of indoor dust (see Section 4.3.2 for further details).

The soil contamination is uniformly distributed across the site at the surface in landscaped soils (to a depth of at least one metre) and from 0.5 m beneath the building foundations (that is, 0.65 m from the soil surface). The depth to source beneath the building is a compromise between consistency with the overall conceptual model and the technical limitations of the Johnson and Ettinger (1991) model to predict indoor air concentrations at very shallow depths (see Chapter 10). As noted previously, the soil concentration does not decrease with time either as a result of transport and dispersion or by chemical/biological degradation (see Section 2.1.2).

Table 3.10: Default building parameters for the standard commercial land use (after Environment Agency, 2005)

Parameter	Value	Notes
Footprint area (m^2) [1]	424	Simple square footprint
Living space height (m)	9.6	Three-storey office area
Air exchange rate (hour^{-1})	1.0	
Pressure difference between soil and indoor air (Pa)	4.4	
Foundation thickness (m)	0.15	Ground-bearing slab design
Floor crack area (m^2)	0.165	

[1] Three-storey office (pre-1970) with an assumed square footprint (Table 4.21 provides default values for other commercial building types).

4 Chemicals, soils, receptors and buildings

Chapter 2 introduced the key factors in estimating human exposure to chemicals from soil including the chemical intake/uptake rate (IR). This parameter represents the predicted daily amount of contaminant inhaled, ingested, or absorbed through skin contact, by adults and children who are living, working and/or playing on contaminated sites. This chapter discusses the data needed to quantify exposure using the CLEA model and serves as an introduction to the pathway modelling in subsequent chapters.

4.1 Introduction

Chemical intake/uptake rate is the predicted daily amount of chemical taken in by the human body based on the exposure scenario and our understanding of the fate and transport of chemicals in the environment. It can be simply described in quantitative terms as the product of the chemical concentration in an environmental media (for example, soil or ambient air) and the degree of human exposure to that media. For example, the chemical intake/uptake rate from direct soil ingestion is the product of soil concentration and daily soil ingestion rate (see also Chapter 6).

4.1.1 Fate and transport models

Fate and transport of a chemical is a collective term to describe a number of complex and highly variable processes including:

- persistence of a chemical in soil, water, and air;
- partitioning of a chemical between different environmental media (for example, a chemical may be absorbed to soil organic matter, dissolved in the pore water solution, or reside in the soil gas phase);
- transport of a chemical from one place to another (for example, the leaching of a chemical from soil to groundwater).

The fate and transport of chemicals in the soil environment depends on many different physical, chemical and biological processes. Ideally, monitoring data would be available to assess many of these processes for a wide range of chemicals (ECB, 2003). However, this is not usually the case and chemical concentrations must be modelled.

Although more than a century of research has established the principles of how chemicals behave in the environment, predictive models are still in the early stages of development and appraisal. Many of these models are useful under the conditions for which they have been validated, although outside these boundaries their utility is limited and their reliability questionable (ECB, 2003).

In general, there are two types of fate and transport model: (a) empirical/knowledge-based, and (b) mathematical/mechanistic (ECB, 2003). **Empirical models** are based on experimental observation and often establish plausible relationships between system parameters based on expert opinion. **Mechanistic models** establish plausible relationships based on scientific opinion, but they are often more systematic and will try to follow processes within the system being investigated from theoretical principles.

Empirical and mechanistic models range in complexity and the required number of input parameters (Environment Agency, 2006b; IPCS 2005). In undertaking both generic and detailed risk assessments, the choice of suitable model is based on its applicability to the specific situation, extent of validation and critical review, and the availability of good quality data to populate the model for a range of circumstances.

The CLEA model uses several empirical and mechanistic models to provide a simplified understanding of fate and transport processes. The approach adopted is considered suitable for generic quantitative risk assessment and balances low complexity/data requirements with robust suitability for a wide range of chemicals and site conditions. This is consistent with international practice.

In many cases the output from these models will result in reasonable worst-case predictions of likely concentrations and subsequent chemical intake rates, but this will depend on the correct characterisation of soil and site conditions. Fate and transport estimates depend on several parameter data sets including the physical-chemical properties of the soil contaminant and site conditions including soil type, wind conditions, and the physical dimensions of any buildings.

4.1.2 Quantifying chemical intake

Estimating the chemical intake/uptake rate depends also on the amount of exposure, which varies according to the pathway (see Chapters 6 to 10). However, many of these approaches are based on a common understanding of receptor characteristics such as body weight, height, inhalation rate, and exposed skin area.

The common data sets used in the CLEA model to estimate human exposures via different pathways are described in Sections 4.2 to 4.5. Table 4.1 provides an overview of the exposure pathways available in the CLEA model along with the main environmental media, fate and transport processes, and the key chemical, site, and receptor characteristics for estimating the chemical intake rate.

Fate and transport processes – key assumptions

Chemical concentration is not reduced over time by destruction, transformation, and fixation processes including chemical and biological degradation.

Chemical partitioning between environmental media and different phases including air, water, soil, and lipids is assumed to reach dynamic chemical equilibrium. It is assumed to be a proportional relationship and depends on known chemical properties such as the octanol-water partition coefficient. Partitioning does not take into account the presence of free phase contaminants.

Chemical transport processes are primarily driven by diffusion in combination with simplified advection along a single direction (for example, diffusion of a chemical through soil and the drawing of soil air into a building along a pressure gradient).

Table 4.1: Overview of exposure pathways in the CLEA model

Pathway	Environmental media	Chemical characteristics	Site characteristics	Receptor characteristics
Soil and dust ingestion	Soil and indoor dust	Persistence	Soil chemical concentration Fraction of soil in indoor dust	Ingestion rate Body weight
Consumption of homegrown fruit and vegetables	Produce	Persistence **Soil-to-plant concentration factors** Partitioning from soil to water Partitioning from water to lipids	Soil chemical concentration Soil type Organic matter content Plant type	Consumption rate Fraction of produce consumed that is homegrown Body weight
Skin contact (indoors)	Indoor dust	Persistence Dermal absorption fraction	Soil chemical concentration Fraction of soil in indoor dust Soil type	Contact rate Body weight Exposed skin area
Skin contact (outdoors)	Soil	Persistence Dermal absorption fraction Skin permeability rates	Soil chemical concentration Soil type	Contact rate Body weight Exposed skin area
Inhalation of dust (indoors)	Air	Enrichment potential in finer soil fractions	Soil chemical concentration Soil type Fraction of soil in indoor dust	Body weight Inhalation rate Time spent indoors
Inhalation of dust (outdoors)	Air	Enrichment potential in finer soil fractions	Soil chemical concentration Wind erosion potential Air dispersion factors Fraction of site with hard or vegetative cover	Body height and weight Inhalation rate Time spent outdoors
Inhalation of vapours (indoors)	Air	Persistence Partitioning from soil to air Diffusion through soil pores	Soil chemical concentration Soil type Building type	Body height and weight Inhalation rate Time spent indoors
Inhalation of vapours (outdoors)	Air	Persistence Partitioning from soil to air Diffusion through soil pores	Soil chemical concentration Soil type Air dispersion factors	Body height and weight Inhalation rate Time spent outdoors

4.2 Chemicals

Table 4.2 summarises the chemical data required by the modelling approaches outlined in Chapters 6 to 10. Not all the input data is required for both inorganic and organic compounds for two reasons:

- Significant differences in the chemistry of inorganic and organic chemicals result in different fate and transport properties and processes.
- Similarities in the composition and structure of organic chemicals mean that there are often empirical relationships that describe the behaviour of organic chemicals as a group.

The CLEA model uses data reported in the International System of Units (SI). Values from the scientific literature are corrected to SI units using conversion factors presented in the *Guide for the Use of the International System of Units* (NIST, 1995).

Many chemical processes are sensitive to temperature and pressure (Boethling and Mackay, 2000). Chemical properties are often measured or calculated at room temperature (typically 20°C to 25°C). As noted in Section 4.3, the average annual soil temperature in the UK is 10°C and therefore many of the reference properties of a chemical should be adjusted to this lower temperature. Methods for the most common adjustments are presented in *Compilation of Data for Priority Organic Pollutants for Derivation of Soil Guideline Values* (Environment Agency, 2008c). Certain chemicals will have insufficient data in the scientific literature to adjust their measured properties according to ambient temperature and pressure. In most cases, using values at higher reference temperatures (in the range 20°C to 30°C) will likely over-predict fate and transport behaviour and are useful only as a conservative screen.

Chemical data is available from a wide range of sources including handbooks, scientific papers and journals, toxicological reports, and internet databases. Care should be exercised in selecting data for modelling, since parameter uncertainty and variability may have a significant effect on the predicted exposure (Environment Agency, in prep.). The Environment Agency (2008c) offers further guidance on the selection of parameters for use in the derivation of SGVs for a number of different organic chemicals including petroleum hydrocarbons, chlorinated solvents and pesticides.

In using chemical data, it is important to select values following a review of the scientific and technical literature. The most common sources of information include:

- values routinely used by scientists within the field and peer-reviewed databases[17];
- values used by the EU consistent with Technical Guidance Document (ECB, 2003);
- values used by the IPCS such as reported in the Environmental Health Criteria series of monographs;
- values reported by national agencies such as USEPA (1996, 2002a, and 2003);
- values estimated using a recognised property estimation or QSAR method (Boethling and Mackay, 2000; ECB, 2003; Lyman *et al*., 1990)

---

[17] These may include research data for groups of related chemicals, such as the information on dioxins, furans, and dioxin-like PCBs maintained by the University of Lancaster (Centre for Chemicals Management, 2007) or for specific properties such as chemical solubility held by IUPAC-NIST (IUPAC-NIST, 2006). It may also include information from respected desk references such as Lide (2008), MERCK (2006), Mackay *et al*. (2006), and Montgomery (2007).

Any review of chemical data should take into account the guidelines in the box below.

Selecting chemical data from the literature

Any review should clearly state the reference sources examined, the range of variability, and the approach used to identify the recommended value within individual references and for the review as a whole. For example, Otte et al. (2001) proposed to use the geometric mean of data selected from twelve databases in the re-evaluation of the Dutch Intervention Values.

It is also important to understand whether the value was measured experimentally or predicted using a property estimation method. In comparing values from different sources the review should account for:

- *differences in reported units;*
- *differences in temperature and pressure conditions;*
- *interdependent relationships between values (for example, between the octanol-water coefficient and the organic carbon-water coefficient)*
- *confidence levels associated with any individual recommended value (for example, the IUPA-NIST (2006) provides a qualitative indication of a recommended value from doubtful to recommended).*

The availability of data will vary significantly between common industrial chemicals such as benzene and less studied compounds such as 2,3,4,6-tetrachlorophenol. In many cases, chemical properties may be predicted using an appropriate property estimation method or QSAR method (Boethling and Mackay, 2000; ECB, 2003; Lyman et al., 1990). The availability of data and range of variation observed will also depend on the chemical property examined. For example, there is often a strong consensus and limited variation in the molecular weight of a compound, while the Henry's Law constant may be found to vary by several orders of magnitude (Environment Agency, 2008c). The range variation within and between references should be recorded by any review, including the decree of consensus and the age of any recommended value as well as that of the original study.

Table 4.2: Chemical data for inorganic and organic compounds

Parameter	SI Units	Description
Air-water partition coefficient (K_{aw}) [1]	$cm^3\ cm^{-3}$	This is the constant of proportionality between the concentration of a chemical in air and in water at low partial pressures, a specified temperature and pressure, and below the saturation limits in either air or water. It is calculated from Henry's Law constant, which is the constant of proportionality between water solubility and the partial pressure of the gas phase and is reported in units of Pa $m^3\ mol^{-1}$. The air-water partition coefficient is used by the CLEA model to predict the partitioning behaviour of an organic chemical between environmental compartments such as soil pore water and air.
Dermal absorption fraction (ABS_d)	-	An empirical measure of the proportion of chemical in soil that is absorbed through the skin by a typical soiling event. It is used in the CLEA model to estimate chemical uptake during skin contact with soil and indoor dust (see Chapter 8).
Diffusion coefficients in air (D_{air}) and water (D_{water}) [1]	$m^2\ s^{-1}$	Molecular **diffusion** is the net transport of a chemical in a liquid or gas medium and is a result of intermolecular collisions rather than turbulence or bulk transport. The **diffusion coefficient** or diffusivity of a chemical is the proportionality constant in **Fick's law** of diffusion. The rate of diffusion is the property of two substances (that is, it depends not only on the chemical being transported but also on the medium through which it moves). Diffusion coefficients are used by the CLEA model for how fast chemicals migrate through the environment from one media into another in the absence of advective or bulk transport flow.
Molecular weight (M) [1]	$g\ mol^{-1}$	Relative molecular mass of an organic chemical. It is used in the CLEA model to calculate the theoretical saturated vapour concentration for a chemical in soil (see Chapter 5).
Octanol-water partition coefficient (K_{ow})	-	This is the experimentally measured ratio of the concentration of an organic chemical in water to the concentration in octanol (an organic solvent). It has been used as a surrogate measure of **chemical lipophilicity** by many researchers and has been observed to predict the partitioning behaviour of a chemical between an organic and aqueous media. For example, it is used in the CLEA model in several empirical relationships to predict the uptake of an organic chemical by plant tissues from water (see Chapter 7).
Organic carbon-water partition coefficient (K_{oc})	$cm^3\ g^{-1}$	This is the experimentally measured or estimated ratio of the concentration of an organic chemical in water to the concentration sorbed to organic soil carbon. It is used in the CLEA model to predict the relative distribution of an organic chemical in soil between the organic matter and pore water (see Chapter 5).

Parameter	SI Units	Description
Soil-to-dust transport factor (TF)	-	An empirical measure of the tendency of a chemical to concentrate in indoor dust from soil. It is used in the CLEA model to estimate the indoor dust concentration of chemicals from the soil concentration (see Chapters 8 and 9).
Root-plant part factor (f_{int})	-	An empirical measure of the tendency of an inorganic compound to concentrate in the plant shoots or fruits or tubers compared to the roots. It is used in the CLEA model to estimate the transfer of chemicals from the roots to other plant parts for estimating chemical concentrations in the edible portions of fruit, leafy and tuber vegetables (see Chapter 7).
Soil-plant availability correction (δ)	-	A proportionality constant for the relationship between soil solution and plant concentration for inorganic compounds. It is used in the CLEA model to estimate the root concentration of inorganic compounds in fruit and vegetables (see Chapter 7).
Soil-to-plant concentration factor (CF)	mg kg^{-1} plant per mg kg^{-1} dw soil	Ratio of the chemical concentration in the edible fractions of fruit and vegetables to that found in the adjacent soil derived from empirical measurements or estimated by a generic model. It is used in the CLEA model to calculate the plant concentration of a chemical from a known soil concentration (see Chapter 7).
Soil-water partition coefficient (K_d)	cm^3 g^{-1}	A measure of the tendency of a chemical to adsorb to the mineral and organic phases in soil compared to water. It is used in the CLEA model to predict the partitioning behaviour of a chemical between environmental compartments including air, soil, and water and to estimate the plant uptake of inorganic compounds (see Chapters 5 and 7).
Vapour pressure (P) [1]	Pa	The vapour pressure of a substance is the pressure its vapour exerts in equilibrium with its solid or liquid phase. It increases rapidly with temperature and is an important controlling factor on the volatility of substance. It is used in the CLEA model to predict the partitioning behaviour of an organic chemical between environmental compartments including air, soil, and water and to determine the vapour-based saturation limit in soil (see Chapter 5).
Water solubility (S)	mg L^{-1}	The maximum concentration of a chemical in water at the specified temperature. It is used in the CLEA model to determine the solubility-based saturation limit in soil (see Chapter 5).

---

[1] Few inorganic compounds readily volatilise under ambient conditions. However, where this is the case this chemical property will be required to effectively describe the fate and transport processes involved.

4.3 Soil and dust

In this section, default properties are presented for different soil types according to particle size or textural classes. Soils have been differentiated on the basis of the system used by the Soil Survey Handbook (Hodgson, 1997). Figure 4.1 shows the soil types superimposed on a triangular diagram of the varying proportion of sand, silt and clay particles. Soil pH and the soil organic matter content (SOM) are set independently of soil type. The data used by the CLEA model is described in Section 4.3.1.

Indoor dust, containing a proportion of soil-derived particles, is also an important source of exposure in land use settings where local contamination may be tracked back from outdoors (Paustenbach, 2000). This is discussed further in Section 4.3.2.

4.3.1 Soil properties for fate and transport modelling

Table 4.3 summarises the soil data required by the modelling approaches outlined in Chapters 6 to 10. Table 4.4 tabulates the default values for nine of the eleven soil types shown in Figure 4.1. In the sources reviewed, there was insufficient information to derive class average values for the loamy sand and sandy clay soil types in data on UK topsoils. Although the *sand* soil type represents the most conservative choice for modelling diffusion and **advection** transport processes, it is not geographically widespread.[18] Most common UK sandy soils are in fact closer to a *sandy loam* and it is this default soil type that is used in the derivation of SGVs.

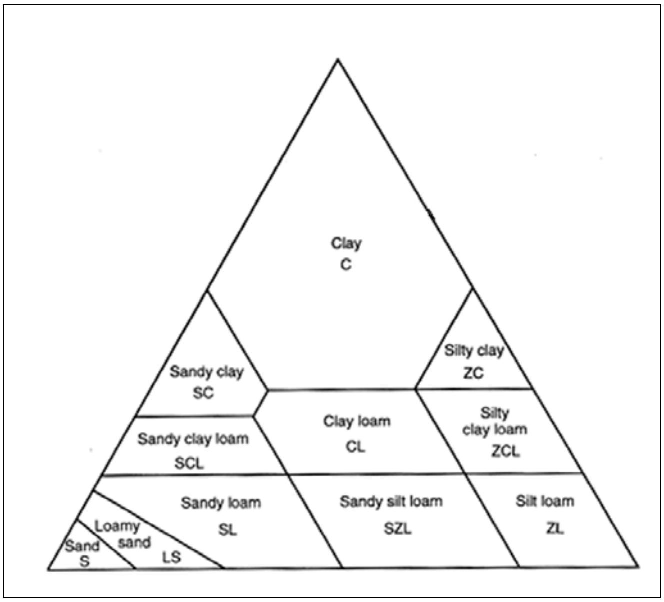


Figure 4.1: Soil classification scheme according to particle size distribution (Reproduced from National Soil Resources Institute [Hodgson, 1997]. © Cranfield University [1997]. No part of this publication may be reproduced without the express written permission of Cranfield University)

---

[18] Coarse-grained soils, like *sand,* typically have a higher air-filled porosity, greater saturated hydraulic conductivity, and poorer water retention capability than finer soils. However the fine-grained soils will contain a higher proportion of silt and clay particles, which are important in exposure via soil contact because such fractions adhere more strongly to surfaces including the skin, fruit and vegetables (Sheppard and Evenden, 1992 and 1994).

Table 4.3: Soil data

Parameter	SI Units	Description
Dry soil bulk density	g cm^{-3}	Apparent density of field soil calculated from the oven-dry mass divided by the volume occupied in the field. It is used by the CLEA model in the partitioning calculations for a chemical between soil, water and air phases.
Organic carbon fraction	g g^{-1}	Amount of organic carbon in soil expressed as a mass fraction. It is used in the CLEA model to estimate the partitioning of organic chemicals between soil, water and air phases. In many soils, chemical adsorption to soil depends strongly on the amount and type of organic matter present.
Organic matter content	% dry weight	Amount of organic material in soil including humus. The primary source of organic matter is plant material and is used by the CLEA model to estimate the organic carbon fraction.
pH	-	Measure of the acidity or alkalinity of a soil and the corresponding soil solution. pH conditions influence the **cation exchange capacity** of soils and the degree to which a chemical partitions between soil and water phases. It also influences the solution chemistry of pollutants, which affects their ionisation potential, reactivity, and their aqueous solubility.
Porosity	cm^3 cm^{-3}	Total soil **porosity** is the volume of the sample not occupied by solid material. Water-filled porosity is the amount of pore space occupied by water based on a suction head at 50 cm H_20. Air-filled porosity is the remainder of the pore space. Porosity is important for the mobility of a chemical through soil by diffusion or advection transport processes.
Residual soil-water content	cm^3 cm^{-3}	Soil moisture content under a suction head at 15,000 cm H_2O, which is used to estimate the effective soil-air permeability. It helps to describe the soil-water release curve under increasing suction.
Saturated hydraulic conductivity	cm s^{-1}	Quantitative measure of the ease with which the pore spaces of a saturated soil permit water movement. It helps to describe the potential for a chemical to move through soils either by diffusion or advection.
Temperature	K	Ambient soil temperature, which is used to adjust chemical properties including aqueous solubility and volatility.
van Genuchten shape parameters	cm^{-1}, -	Empirical parameter, which is used to estimate the effective soil-air permeability. It helps to describe the soil-water release curve under increasing suction. Parameter n is derived from the Landis dataset. m is calculated from n.

Soil porosities are highly variable (Brady and Weil, 1990) and depend largely on the arrangement of the solid particles, the particle size distribution and their shape. If the particles lie close together (that is, they are compacted) the total porosity will be low. If they are arranged in porous aggregates, as is often the case in medium- to fine-textured soils, the pore space per unit volume will be high. Sandy surface soils typically have a total porosity in the range 0.35 to 0.5 cm^3 cm^{-3}, whereas medium- to fine-textured soils vary from 0.4 to 0.6 cm^3 cm^{-3} (Brady and Weil, 1990).

Table 4.4 lists the default porosity data used in the CLEA model for the various soil types. Average values have been calculated according to soil type from analysis of the HORIZON Hydraulics library data held by the National Soil Resources Institute (NSRI) based at Cranfield University. The NSRI holds very detailed descriptions of the hydraulic properties of a large number of soils sampled across England and Wales. The average values are estimated from data taken only from the horizon A (that is, the top soil). Water-filled porosity has been estimated for an unsaturated soil at field capacity with an approximate suction head of 50 cm H_2O (Hall *et al*., 1977). Residual water content has been estimated for an unsaturated soil under extreme drought conditions with an approximate suction head of 15,000 cm H_2O (Hall *et al*., 1977). As soils become more porous, they also become less dense. The dry bulk soil density depends on the proportion of the total volume of soil occupied by air and on the density of the particles themselves (Rowell, 1994). Cultivated mineral soils with a medium to heavy texture have a dry bulk soil density in the range 0.8 to 1.4 g cm^{-3} and porosity in the range 0.46 to 0.69 cm^3 cm^{-3} (Rowell, 1994).

Table 4.4 presents the default dry bulk densities and saturated hydraulic conductivities used in the CLEA model according to soil type. These values are the average densities for each soil type according to analysis of the HORIZON Hydraulics library data.

The moisture retention properties of soil are critical parameters for understanding the transport behaviour of gases and liquids in the unsaturated zone (van Genuchten *et al*. 1991, and USEPA, 2003). As a soil dries out, it is increasingly more difficult to remove the remaining moisture (Hall *et al*., 1977). Water contained within large and well-connected interstitial pore spaces is more easily lost from a soil than water contained in small poorly connected pore spaces, or within mineral grains. A water retention curve describes the volume of water present in soil under an increasing negative pressure head or suction. Van Genuchten *et al*. (1991) presented several empirical methods for predicting the water retention curve from more easily measurable characteristics including **Equation 4.1**. These empirical parameters are used by USEPA (2003) to estimate the effective air permeability of a soil for calculating the rate of vapour ingress into a building (see also Chapter 10).

Equation 4.1

$$\theta = \theta_r + \frac{(\theta_s - \theta_r)}{\left[1 + (\alpha h)^n\right]^m}$$

Where: θ is the volumetric moisture content at a pressure head h cm H_2O, cm^3 cm^{-3}

θ_r is the residual water content, taken as the moisture content at 15,000 cm H_2O, cm^3 cm^{-3}

θ_s is the saturated moisture content, cm^3 cm^{-3}

α is equal to the reciprocal of pressure head at which the moisture content starts to fall below saturation - the bubbling pressure, cm^{-1}

H is the pressure head – although for unsaturated soils this is a suction (negative), in this derivation it is taken as positive, cm H_2O

n is the van Genuchten shape parameter

m is $(1-\frac{1}{n})$

Table 4.4: Default properties according to soil type

Soil type [1]	Bulk Density (g cm^{-3})	Porosity (cm^3 cm^{-3}) Air	Porosity (cm^3 cm^{-3}) Water	Porosity (cm^3 cm^{-3}) Total	Residual Water Content (cm^3 cm^{-3})	Saturated Hydraulic Conductivity (cm s^{-1})	van Genuchten α (cm^{-1})	van Genuchten m (dimensionless)
Clay	1.07	0.12	0.47	0.59	0.24	9.93E-04	0.0385	0.2972
Silty clay	0.94	0.12	0.51	0.63	0.26	1.17E-03	0.0541	0.3155
Silty clay loam	1.07	0.12	0.46	0.58	0.21	1.17E-03	0.0291	0.3072
Clay loam	1.14	0.14	0.42	0.56	0.19	1.51E-03	0.0437	0.3039
Sandy clay loam	1.20	0.16	0.37	0.53	0.15	2.37E-03	0.0560	0.3098
Silt loam	1.09	0.14	0.44	0.58	0.18	1.58E-03	0.0375	0.3078
Sandy silt loam	1.19	0.14	0.38	0.52	0.15	2.20E-03	0.0410	0.3174
Sandy loam [2]	1.21	0.20	0.33	0.53	0.12	3.56E-03	0.0689	0.3201
Sand	1.18	0.30	0.24	0.54	0.07	7.36E-03	0.1221	0.3509

[1] Most exposed areas of residential and commercial sites (such as gardens and landscaped areas) will be covered by a layer of top soil. However, many former industrial sites may have limited/no top soil and care should be taken in applying the data in this table to subsoil horizons, made ground, and drift geology.

[2] Also includes data from loamy sand soils since it has a very narrow particle size range.

Table 4.4 presents the default empirical van Genuchten values, α and *m* according to soil type. These values are estimated by curve fitting using average values of moisture retention at varying pressures from the HORIZON Hydraulics library data.[19]

Soil temperature depends directly or indirectly on three factors, namely the net amount of heat absorbed, the heat energy required to bring about a specified change in temperature in soil, and the energy lost through processes such as evaporation (Brady and Weil, 1990). Considerable seasonal and monthly variations in soil temperature can occur as a result of climatic changes in hours of sunshine, rainfall and wind speed and direction. The surface soil layers respond quickly to the ambient air temperature with increasing lag observed at depth in the subsoil. According to Met Office data, the annual average UK air temperature ranges between 7 - 11°C at low altitudes (Met Office, 2007). An annual average temperature of 10°C, or 283 K, has been selected as representative of UK surface soils.

The organic carbon content of soils is an important predictor of chemical partitioning between the soil and soil solution (Mackay, 2001). Many empirical relationships have been established between the lipophilicity of organic chemicals and organic carbon content of soils (ECB, 2003). The fraction of organic carbon can be estimated from the amount of soil organic matter measured in soil using **Equation 4.2** (Rowell, 1994).

Equation 4.2

$$f_{oc} = \frac{SOM}{100} \times 0.58$$

Where: f_{oc} is the fraction of soil organic carbon, g g^{-1}
SOM is the amount of soil organic matter, weight %

---

[19] Curve fitting was undertaken using a dynamic non-linear regression tool provided by Sigma Plot Version 10.

Made ground

"Made ground" consists of materials including brick, concrete rubble, ash slag, clinker, pulverised fly ash and other excavation debris that overlies the natural ground surface on many industrial sites. Risk assessors should be aware that very little is known about contaminant behaviour in made ground. Its heterogeneity, however, is well known and assessors should consider very carefully whether assessment criteria based on soil conditions could be used reliably in such situations. Where made ground comprises a mixture of rubble with a finer matrix of soil, it is the properties of the matrix that are more likely to be relevant to contaminant behaviour.

4.3.2 Indoor dust and tracking back of contamination

An important pathway for indirect human exposure to soil-borne contamination is through contact with indoor dust (Hunt *et al*., 2006; Oomen and Lijzen, 2004; Paustenbach *et al*., 1997; Rieuwerts *et al*., 2006). Soil may contribute to indoor dust through being tracked back on clothing, footwear, push chairs, toys and boxes of gathered produce, and in the fur of pets such as cats and dogs. Soil dust may also enter buildings and be deposited as wind-blown dust through open doors and windows (Paustenbach *et al*., 1997). At the Bunker Hill Superfund site in Idaho, Sheldrake and Stifelman (2003) noted that the interiors of homes that were completely cleaned of lead dust in 1990 were re-contaminated by outdoor sources within one year.

Several researchers have examined the tracking back of contamination from soil into buildings and mitigation of these routes for risk management. Thatcher and Layton (1995) showed that the dust mass in a house decreases with distance from the external doors and could be related to the household traffic pattern. Hunt *et al*. (2006) investigated the likely rates of dry and wet soil deposition on hard floors from soiled footwear, concluding that repeated tracking could lead to widespread surface contamination. Roberts *et al*. (1990) found that the amount of lead in a household carpet was reduced by 90 per cent when occupants removed shoes or used doormats.

The contribution that local soil makes to indoor dust, and the relationship between the concentration of contaminants in indoor dust and in the outdoor soil, is difficult to quantify with certainty (Paustenbach *et al*., 1997). Calabrese and Stanek (1992) performed a correlation analysis of trace elements in paired samples of soil and house dust and found that the soil component of house dust was about thirty-one per cent. Reviewing the evidence from five studies, Paustenbach *et al*. (1997) concluded that approximately half of house dust originates from local soil (with a reported range from twenty to eighty per cent). USEPA (1998) proposed a default mass fraction of soil in indoor dust of seventy per cent for modelling exposure to lead.

Several studies have reported a diluted dust concentration consistent with soil being a component of indoor dust. Although Rieuwerts *et al*. (2006) found no correlation between arsenic concentrations in house dust and in garden soil within a mining community, the overall mean dust concentration was about half the mean garden soil value. Cotter-Howells and Thornton (1991) studied environmental exposure to lead for children living in a Derbyshire mining village and found mean soil concentrations four and a half times greater than mean dust concentrations, suggesting a significant dilution effect. Chuang *et al*. (1995) found a correlation between PAH concentrations in entryway soil and in indoor dust suggestive of tracking back, with dust concentrations consistently lower than those measured in outdoor soil for the eight homes studied.

However, adopting a soil mass fraction approach to calculate the house dust contaminant concentration assumes that there are no processes of relative enrichment or dilution other than mass transfer (Oomen and Lijzen, 2004; Rasmussen, 2004). Many studies including those for lead, cadmium, nickel, herbicides and pesticides, and PCBs have shown that the concentration of contaminants appears to be greater in house dust relative to the outside soil by a factor of up to thirty (Paustenbach *et al.*, 1997; Rasmussen, 2004).[20] Oomen and Lijzen (2004) concluded, from a wide range of literature studies, that the lead concentration in house dust is on average three times higher than in the exterior soil, and that such enrichment should be included within soil-based risk assessments for lead.

Many studies have reported a direct association between garden soil and indoor dust concentrations, either supporting enrichment or demonstrating a significant soil component in indoor dust (Berny *et al.*, 1994; Culbard *et al.*, 1988; Davies *et al.*, 1990; Louekari *et al.*, 2004; von Lindern *et al.*, 2003). However, other studies have concluded that any observed enrichment has derived from non-soil sources inside the home and in many cases this is supported by a lack of correlation between soil and dust concentrations (Rasmussen, 2001; Rasmussen *et al.*, 2004). Sheldrake and Stifelman (2003) suggested that non-soil sources accounted for between 20 and 40 per cent of the lead found in house dust at the Bunker Hill Superfund site. Rasmussen (2004) observed a positive correlation between metal enrichment in indoor dust and organic carbon content, concluding that the higher carbon content in dust increases the potential for metal adsorption (from all sources) relative to soil.

Although it is clear from the literature that indoor dust is an important contributor to human exposure for many chemicals, the apparent contribution to this pathway from outdoor soil varies significantly from case to case. Several authors have recommended an enrichment factor for estimating indoor dust concentrations from outdoor soil data (Oomen and Lijzen, 2004; Paustenbach *et al.*, 1997). However, other studies have attributed enrichment to non-soil sources and it would not be appropriate to include such an effect in a model looking specifically at exposure from contaminated soil.

Qualitatively, dust enrichment may occur for some soil-derived chemicals where the house dust consists of finer soil particles (Paustenbach *et al.*, 1997). Metal contaminants are known to distribute preferentially to silts and clays because of their favourable sorption characteristics and higher relative surface (Alloway, 1995). This is not necessarily the case for organic chemicals that preferentially bind to organic matter in soil. USEPA (2000) recommends a cautious approach to including enrichment in risk assessment for lead, noting that although the finer soil fractions ($< 250\ \mu$m) may be enriched compared to the total soil, this would not be true for all types of contamination.

Sheppard and Evenden (1992 and 1994) studied the effect of enrichment within finer particle sizes compared to the bulk soil concentration in plant and skin adhesion studies. These enrichment factors were highest for coarse-grained soils because they begin with a smaller proportion of silt and clay particles, leading to the concentrating effect being more pronounced (Sheppard and Evenden, 1994). The authors observed typical enrichment factors between one and six for fine and sandy soils respectively.

In the generic CLEA model, it is assumed that the indoor dust concentration of a chemical from soil sources is related to the soil concentration by a transport factor, as defined in **Equation 4.3**. The dust concentration is used to determine the chemical uptake and intake from dermal and inhaled dust pathways only (see Chapter 8 and 9). As noted in Chapter 6, it is difficult to separate the components of soil ingestion attributed to outdoor soil and indoor dust and therefore the soil concentration only is used in the intake calculation.

---

[20] More typical range of this concentrating effect is between two and five times (Paustenbach *et al.*, 1997).

Equation 4.3

$$TF = \frac{C_{dust}}{C_s}$$

Where: TF is the soil to dust transport factor, g g^{-1} dw
C_{dust} is the chemical concentration in indoor dust, mg g^{-1} dw
C_s is the total soil concentration of the chemical, mg g^{-1} dw

It is also assumed that the minimum transport factor is proportional to the mass fraction of soil in indoor dust. The default value for the mass fraction is 50 per cent, which is in the middle of the range reported in the literature (Oomen and Lijzen, 2004; USEPA, 1998). Contaminant-specific transport factors will be based on a review of the literature and, where available, replace the default value. These will be provided in individual SGV reports.

Tracking back of soil particles into the home has been observed in several studies where the soil has been the dominant source of exposure. Although Rieuwerts *et al.* (2006) and von Lindern *et al.* (2003) have stressed the contribution of neighbourhood wide sources of soil contamination in influencing overall dust concentrations, recent studies have demonstrated that tracking back predominantly occurs over a short distance and is frequency dependent (Hunt *et al.*, 2006). In the generic CLEA model, tracking back into the building (and therefore the indoor exposure pathways) is only included where the building is located on the contaminated site.

4.4 Human characteristics

Table 4.5 summarises the default physical characteristics for the receptor included in the CLEA model. Some of these characteristics are dependent variables and are calculated from body weight using standard empirical relationships.

4.4.1 Weight and height

The body weight and height of adults and children according to age class has been established using analysis of data from the Health Survey for England 2003 (NCSR and UCL, 2003). This survey was designed to monitor trends in the nation's health through using a general population sample drawn from those living in private households (Jeffries, 2009). Up to three households per address were eligible for inclusion in the survey, which was conducted throughout the year to allow for seasonal differences. Table 4.6 presents the arithmetic mean body weight and height for males and females for each age class. In the generic CLEA model, the mean female body weights and heights are the default values.

Table 4.5: Human data

Parameter	SI Units	Description
Body weight	kg	Body mass is an important predictor of other human characteristics including total skin area and consumption rates. Mass is also an important factor in assessing the effect of chemical exposure on health.
Body height	m	Body height combined with weight is a predictor of total skin area. Height is also important for estimating exposure to soil contamination from the inhalation of dust and vapours.
Exposed skin area	cm^2	Exposed skin area is a fraction of the total skin area exposed to potential contact with contaminated soils and indoor dust. It takes into account the coverage of typical clothing and the effect of different activities in establishing likely soil contact rates.
Inhalation rate	m^3 $hour^{-1}$	Volume of air inhaled depends on a number of factors including age, sex, fitness level and also the type of activity undertaken, since physical exertion increases our requirement for air. Inhalation rate is important for estimating exposure to soil contamination from the inhalation of dust and vapours.
Consumption rate	g fw kg^{-1} bw day^{-1}	The amount of fruit and vegetables consumed per day is an important characteristic for estimating exposure to soil contamination from consumption of contaminated homegrown produce. Consumption depends on a number of different factors including age, deprivation status, and personal preferences.
Homegrown fraction	dimensionless	The proportion of fruit and vegetables consumed by the family that is assumed to be from the potentially contaminated garden or allotment. Not all fruit and vegetables consumed by the family are homegrown.

Table 4.6: Mean weight and height by sex and age class from the 2003 Health Survey for England (after Jeffries 2009)

Age class	Female		Male	
	Weight (kg)	Height (m)	Weight (kg)	Height (m)
1	5.6	0.7	6.9	0.7
2	9.8	0.8	10.5	0.8
3	12.7	0.9	13.2	0.9
4	15.1	0.9	15.8	0.9
5	16.9	1.0	17.6	1.0
6	19.7	1.1	19.6	1.1
7	22.1	1.2	22.8	1.2
8	25.3	1.2	25.4	1.2
9	27.5	1.3	28.0	1.3
10	31.4	1.3	33.2	1.3
11	35.7	1.4	35.6	1.4
12	41.3	1.4	40.2	1.4
13	47.2	1.5	43.7	1.5
14	51.2	1.6	49.8	1.6
15	56.7	1.6	58.8	1.6
16	59.0	1.6	61.2	1.7
17	70.0	1.6	83.2	1.8
18	70.9	1.6	82.7	1.7

4.4.2 Total skin area and exposed skin area

A number of studies have related total skin area to more easily measured body characteristics such as height and weight (ICRP, 1975; USEPA, 1985, 1997b). **Equation 4.4** shows the relationship used in the CLEA model to calculate total skin area. **Equation 4.4** is the approach proposed by Gehan and George (1970) to parameterise the earlier formula of Dubois and Dubois (1916) that related the body surface area to weight and height as independent variables. It is the approach recommended by USEPA (1997b, 2006) and is consistent with other studies such as the work of Haycock *et al*. (1978).

Equation 4.4

$$SA = 0.02350\, H^{0.42246}\, W^{0.51456}$$

Where: SA is the total body skin area, m^2
H is the body height, cm
W is the body weight, kg

However, it is reasonable to assume that not all parts of the body will come into contact with soil and indoor dust across a range of typical activities such as playing and gardening. It is therefore necessary to judge the amount of exposed skin during indoor and outdoor activity, where direct surface contact is possible.

Most studies assume that clothing blocks contact with contaminated surfaces and that the typical coverage of clothing can be used to establish the maximum exposed skin area for children and adults (Hawley, 1985; Keenan *et al*., 1989; McKone and Daniels, 1991; USEPA, 1997b, 2004a). These assumptions will vary according to land use and age class and will be based on a range of likely activities. Table 4.7 and Table 4.8

show the assumptions for the maximum exposed skin area used by the CLEA model for the commercial and allotment/residential land uses respectively. The maximum exposed skin fraction for age classes 1 to 16 have been calculated using estimates of the average combined male and female percentage of total surface area of body parts for children, for example, face and hands (USEPA, 2004a, 2006). For age class 17 and 18, they have been calculated using adult female body parts (USEPA, 1997, 2004a). For age class 17 and 18, the calculated maximum exposed skin fraction for the adult male is not significantly different to the adult female and therefore the female data is used within the CLEA model.

USEPA (2002a) showed that the proportions of total skin area for parts of the body change as children get older; for example, the leg area increases while the head area decreases as a proportion of total skin area. The maximum exposed skin fraction is used in **Equation 4.5** to calculate the exposed skin fraction for each age class.

Many activities are unlikely to result in the maximum exposed skin area coming into contact with soil and dust. It is therefore assumed that the typical exposed skin area is about one-third of the maximum value. This is an arbitrary, albeit reasonable, estimate of exposed area as there is little or no data that relates such behaviour to the degree of soiling. The calculation of exposed skin area is summarised in **Equation 4.5** and the results according to sex, age class, and land use are presented in Table 4.9.

Equation 4.5

$$SE = \frac{SA\,\phi_{\max}}{3}$$

Where: SE is the exposed skin area, m^2
SA is the total body skin area, m^2
Φ_{max} is the maximum exposed skin fraction, $m^2\ m^{-2}$

Table 4.7: Estimates of maximum exposed skin fraction during indoor and outdoor activities for the commercial land use

Age class	Outdoors		Indoors	
	Coverage	Φ_{max} ($m^2\ m^{-2}$)	Coverage	Φ_{max} ($m^2\ m^{-2}$)
17	Assumes face and hands exposed	0.08	Assumes face and hands exposed	0.08

Table 4.8: Estimates of maximum exposed skin fraction during indoor and outdoor activities for the residential and allotment land uses

Age class	Outdoors		Indoors	
	Coverage	Φ_{max} (m^2 m^{-2})	Coverage	Φ_{max} (m^2 m^{-2})
1	Assumes face, hands, forearms and lower legs exposed	0.26	Assumes face, hands, forearms, lower legs, and feet exposed	0.32
2		0.26		0.33
3		0.25		0.32
4		0.28		0.35
5		0.28		0.35
6		0.26		0.33
7	Assumes face, hands and forearms exposed	0.15	Assumes face, hands, forearms, and feet exposed	0.22
8		0.15		0.22
9		0.15		0.22
10		0.15		0.22
11		0.14		0.22
12		0.14		0.22
13		0.14		0.22
14		0.14		0.22
15		0.14		0.21
16		0.14		0.21
17	Assumes face, hands, forearms and lower legs exposed	0.27	Assumes face, hands, forearms, lower legs and feet exposed	0.33
18		0.27		0.33

Table 4.9: Calculated exposed skin values by age, sex, and land use

Age class	Exposed skin area (m^2)					
	Residential and allotment land use				Commercial land use	
	Female		Male		Female	Male
	Indoor	Outdoor	Indoor	Outdoor		
1	0.037	0.030	0.041	0.034		
2	0.053	0.042	0.056	0.044		
3	0.061	0.048	0.063	0.049		
4	0.076	0.061	0.077	0.062		
5	0.083	0.066	0.085	0.068		
6	0.087	0.068	0.087	0.068		
7	0.063	0.043	0.064	0.044		
8	0.069	0.047	0.070	0.048		
9	0.074	0.050	0.074	0.051		
10	0.080	0.055	0.083	0.057		
11	0.087	0.059	0.087	0.059		
12	0.096	0.065	0.094	0.064		
13	0.105	0.071	0.100	0.068		
14	0.110	0.075	0.109	0.074		
15	0.118	0.080	0.121	0.082		
16	0.120	0.082	0.125	0.086		
17	0.198	0.162	0.223	0.183	0.048	0.054
18	0.197	0.161	0.220	0.180		

4.4.3 Inhalation rate

In exposure assessment, the chemical intake is usually estimated as a function of the inhalation or ventilation rate, which is the product of the number of breathing cycles and the respired air volume for each cycle (USEPA, 1997b). The usual method of measuring the inhalation rate is the minute volume, which is reported in litres of air per minute. In chemical risk assessment, the inhalation rate is usually reported in units of cubic metres per hour.

Inhalation rate depends partly on physical characteristics (for example, age, sex, body size, and fitness level) and partly on the activity and work rate (Smith and Jones, 2003; USEPA, 1997b). It can be measured either directly using a spirometer and collection system or indirectly using heart rate measurements.

USEPA (1997b) reviewed the available literature including data from the International Commission on Radiological Protection (ICRP) and identified five key studies on which to base its recommended values. These values are summarised in Table 4.10 (allocated according to age class in the CLEA model) and depend critically on the work of Layton (1993). Layton (1993) estimated the inhalation rates from estimates of oxygen consumption associated with energy expenditure during physical activities of varying duration. Three different methods were used based on large survey data sets for energy expenditure and activity patterns, and estimates of metabolic rate and weighted average oxygen uptake. USEPA (1997b) concluded that Layton (1993) found similar results using three different approaches and explained differences between cohorts for age and sex, which were supported by observations in other studies.

Lordo *et al*. (2006) sought to improve upon the method used by Layton (1993) by calculating inhalation rates as a direct function of each person's oxygen consumption (derived from energy expenditure). Body weight, age, and gender data were also considered in the calculation and these data were obtained using statistical analysis of several data sets. Inhalation rates from Lordo *et al*. (2006) are listed in Table 4.10.

USEPA (2006) recommended age-specific inhalation rates for children from Lordo *et al*. (2006), which are also shown in Table 4.10 according to age class.[21] USEPA recommended these rates because they represented "*the most recent and geographically broad of the studies described*" and "*an improvement upon studies previously used*".

Smith and Jones (2003) summarised average inhalation rates for various ages from the ICRP working group report on modelling the respiratory tract (ICRP, 1994). These average rates were based on assumptions about the time and duration of different activities and were considered by the authors to be "*appropriate for most assessment purposes*". A comparison of these values with the recommendations of USEPA (1997b and 2006) and Lordo *et al*. (2006) is given in Table 4.11.

Inhalation rates vary as a function of activity; for example, breathing rates are lower when sleeping than when exercising. USEPA (1997b, 2006) recommend activity-based inhalation rates for children and adults based on short-term exposures. USEPA (1997b) recommended values are taken from various literature sources and are provided in Table 4.12. USEPA (2006) recommended values for children (aged nought to sixteen) were taken from Lordo *et al.* (2006) and are shown in Table 4.13. Values from Lordo *et al*. (2006) are provided for five activities, based on energy expenditure, rest (sleep or nap), sedentary (and passive), light, moderate and heavy.

For inhalation rates for long-term exposure studies, while there is good agreement between USEPA (1997b) and Smith and Jones (2003) for young children, the USEPA (2006) figures are considerably higher. USEPA (1997b) and USEPA (2006) are in

---

[21] Layton (1993) was considered as part of the USEPA (2006) review.

close agreement for activity-based rates, suggesting that the key differences between the two studies are the assumptions behind combined daily activities. In this respect, USEPA (2006) is based on actual survey information for the US population, whilst USEPA (1997b) is based on survey information from four communities in California. USEPA (1997b and 2006) and Lordo *et al*. (2006) values for older children and adults are much lower than those proposed using the ICRP model (Smith and Jones, 2003).

Table 4.14 sets out default values for the CLEA model for the residential and commercial land uses; values have been adjusted for body weight using the data in Table 4.6. Inhalation rates for children and adults are based on the work of Lordo *et al.* (2006) recommended by USEPA (2006) for children aged zero to sixteen years.

Table 4.15 sets out default values for the CLEA model for the generic allotment scenario. The default site occupancy period for allotment sites for age classes one to six is three hours per day. For this period, it is assumed that the young child (age class one to three) undertakes light activity for two-thirds of the time and moderate activity for the remainder. For the older child (age class four to six), it is assumed that the balance between light and moderate activity is half-and-half.

Actual air volumes respired depend also on site occupancy factors (see Chapter 3).

Table 4.10: Recommended inhalation rates for long-term exposure studies according to age and sex (from USEPA, 1997b, 2006; Lordo *et al.,* 2006)

Age class	Inhalation rate (m^3 day^{-1})					
	USEPA (1997b) [1]		USEPA (2006) [2]		Lordo *et al*. (2006)	
	Female	Male	Female	Male	Female	Male
1	4.5	4.5	8.5	8.8	8.5	8.8
2	6.8	6.8	13.3	13.5	13.3	13.5
3	8.3	8.3	12.7	13.2	12.7	13.2
4	8.3	8.3	12.2	12.7	12.2	12.7
5	8.3	8.3	12.2	12.7	12.2	12.7
6	10	10	12.2	12.7	12.2	12.7
7	10	10	12.4	13.4	12.4	13.4
8	10	10	12.4	13.4	12.4	13.4
9	13	14	12.4	13.4	12.4	13.4
10	13	14	12.4	13.4	12.4	13.4
11	13	14	12.4	13.4	12.4	13.4
12	12	15	13.4	15.3	13.4	15.3
13	12	15	13.4	15.3	13.4	15.3
14	12	15	13.4	15.3	13.4	15.3
15	12	17	13.4	15.3	13.4	15.3
16	12	17	13.4	15.3	13.4	15.3
17	11.3	15.2	-	-	14.8	19.4
18	11.3	15.2	-	-	12.0	16.4

[1] Inhalation rates are not differentiated according to sex from age classes one to eight.
[2] Based on Lordo *et al*. (2006). USEPA (2006) does not provide adult data.

Table 4.11: Summary of recommended values for radiological risk assessments (from Smith and Jones, 2003) compared with USEPA (1997b, 2006) and Lordo *et al.* (2006) values

Age group	**Inhalation rate (m^3 day^{-1})**			
	Smith and Jones (2003)	**USEPA (1997b)**	**USEPA (2006)**	**Lordo *et al.* (2006)**
One-year old	5.2	4.5	8.5 – 8.8	8.5 – 8.8
Five-year old	8.8	8.3	12.2 – 12.7	12.2 – 12.7
10-year old child	15.3	13 – 14	12.4 – 13.4	12.4 – 13.4
15-year old child	20.0	12 – 17	13.4 – 15.3	13.4 – 15.3
Adult	22.2	11 – 15	-	13.4 – 17.9

[1] Inhalation rates are differentiated according to sex in some age groups and a range is provided.

Table 4.12: Recommended inhalation rates for short-term exposure studies (from USEPA, 1997b)

Activity	**Inhalation rate (m^3 $hour^{-1}$)**	
	Children[1]	**Adults[2]**
Rest	0.3	0.4
Sedentary	0.4	0.5
Light	1.0	1.0
Moderate	1.2	1.6
Heavy	1.9	3.2

[1] Children aged zero to 16.
[2] Adults aged over 16.

Table 4.13: Inhalation rates for short-term exposure (based on Lordo *et al.,* 2006)

Activity	Age class	Mean inhalation rate[1] (m^3 $hour^{-1}$)	
		Female	Male
Sleep or nap	1	0.18	0.18
	2	0.28	0.27
	3	0.27	0.28
	4 to 6	0.25	0.26
	6 to 11	0.26	0.28
	12 to 16	0.29	0.32
	17	0.26	0.32
	18	0.27	0.36
Sedentary and passive	1	0.18	0.19
	2	0.28	0.28
	3	0.28	0.29
	4 to 6	0.26	0.27
	6 to 11	0.28	0.29
	12 to 16	0.31	0.34
	17	0.28	0.35
	18	0.30	0.40
Light intensity	1	0.44	0.48
	2	0.70	0.69
	3	0.72	0.70
	4 to 6	0.66	0.68
	6 to 11	0.66	0.70
	12 to 16	0.72	0.79
	17	0.68	0.83
	18	0.65	0.84
Moderate intensity	1	0.84	0.87
	2	1.26	1.28
	3	1.28	1.29
	4 to 6	1.20	1.26
	6 to 11	1.26	1.34
	12 to 16	1.41	1.58
	17	1.42	1.83
	18	1.28	1.77
High intensity	1	1.45	1.65
	2	2.19	2.42
	3	2.25	2.43
	4 to 6	2.07	2.34
	6 to 11	2.36	2.62
	12 to 16	2.79	3.05
	17	2.74	3.32
	18	2.42	3.20

[1] Original data reported in L min^{-1}. USEPA (2006) recommend Lordo (2006) for activity-based inhalation rates for children.

Table 4.14: CLEA default inhalation rates according to age and sex for residential and commercial land uses, based on long-term exposure

Age class	Inhalation rate (m^3 day^{-1})	
	Female	Male
1	8.5	8.8
2	13.3	13.5
3	12.7	13.2
4	12.2	12.7
5	12.2	12.7
6	12.2	12.7
7	12.4	13.4
8	12.4	13.4
9	12.4	13.4
10	12.4	13.4
11	12.4	13.4
12	13.4	15.3
13	13.4	15.3
14	13.4	15.3
15	13.4	15.3
16	13.4	15.3
17	14.8	19.4
18	12.0	16.4

Table 4.15: CLEA default inhalation rates according to age and sex for the allotment land use, based on short-term exposure

Age class	Inhalation rate[1] (m^3 day^{-1})	
	Female	Male
1	10.3	12.5
2	18.8	19.7
3	20.7	20.4
4	19.1	20.6
5	21.3	22.9
6	24.9	25.5

[1] Assuming an hourly rate for 24 hours

4.4.4 Consumption rates for fruit and vegetables

Both the generic residential and allotment land use scenarios described in Chapter 3 consider the consumption of homegrown fruit and vegetables. Produce has been divided into six groups in line with the Food Standard Agency's PRISM model (Thorne *et al.,* 2004). The produce included in each group is summarised in Table 4.16. Consumption rates for each fruit and vegetable category have been estimated by the Food Standards Agency using data from several different dietary surveys (Vazquez, *personal communication*, 2006). For ages one-and-a-half upwards, data from the most closely matching National Diet and Nutrition Survey (NDNS) was used: that is, the 1992 survey for children aged one-and-a-half to four-and-a-half years, the 1997 survey for young people aged four to 18 years, and the 2000 survey for adults (Gregory *et al*., 1995, 2000; Henderson *et al*., 2002). Children younger than one-and-a-half have not yet been considered in the survey and therefore an older 1986 dietary survey of 488 British infants aged six to 12 months was used (Mills and Tyler, 1992). Table 4.17 presents the consumption rates for each produce group according to age class.

Consumption data was estimated at the 90th percentile, in line with the Food Standard Agency's approach to generic risk assessment (Vazquez, *personal communication*, 2006). The data was reported per unit body weight, matching the body weights of individual respondents in the survey to their recorded consumption. The amounts of fruit and vegetables reported in the NDNS tends also to be "as consumed" using standard recipe information to translate meals into original ingredients. As a result, the data reported is not exactly fresh weight, as it does not account for some water loss during cooking (Vazquez, *personal communication*, 2006). Actual exposure also depends on the fraction of homegrown produce (see Section 4.4.5) since not all fruit and vegetables eaten at home are from the garden or allotment.

Table 4.16: Produce groups used in the CLEA model

Produce group		Included crops
Vegetables		
	Green	Beans (broad, French, green and runner beans), Brussels sprouts, cabbage (red, white, greens and kale), cauliflower, lettuce, spinach, peas (garden and mangetout), stem vegetables (broccoli, celery, asparagus), okra, globe artichokes, Chinese leaves, endives, chicory, chard, dandelion, watercress and fresh herbs (basil, coriander, tarragon, sage, parsley and mint).
	Root	Beetroot, carrot, casava, garlic, ginger, jerusalem artichoke, leeks, onions, parsnips, radish, rhubarb, salsify, swede, sweet potato, turnips and yam.
	Tuber	Potatoes.
Fruit		
	Herbaceous	Aubergine, courgettes, cucumber, marrow, pumpkin, strawberries, tomatoes.
	Shrub	Bilberries, blackberries, cranberries, gooseberries, loganberries, mulberries, physalis, raspberries, blackcurrants, redcurrants, and whitecurrants.
	Tree	Apples, apricots, cherries, peaches, pears and plums.

Table 4.17 Consumption rates for produce categories by age class

Age class	NDNS survey	Consumption rate (g fw kg^{-1} bw day^{-1})					
		Green	Root	Tuber	Herb.	Shrub	Tree
1	Infant 1986 [1]	7.12	10.69	16.03	1.83	2.23	3.82
2 – 4	Toddler 1992	6.85	3.30	5.46	3.96	0.54	11.96
5 – 16	Young person 1997	3.74	1.77	3.38	1.85	0.16	4.26
17 – 18	Adult 2000	2.94	1.40	1.79	1.61	0.22	2.97

[1] Not a NDNS survey

4.4.5 Proportion of homegrown produce

There is limited data for directly estimating the amount of garden and allotment produce consumed in the UK. Vazquez (*personal communication* 2006) noted that although a question on homegrown produce is now included in the National Diet and Nutrition Survey, there is insufficient evidence to provide a robust estimate for generic exposure assessment.

The Expenditure and Food Survey is a continuous survey of household expenditure, food consumption, and income (Defra, 2007). In 2004/05, 6,798 households were included in the sample taken from across the UK (Carr, *personal communication*, 2006). Fruit and vegetables brought into the home were categorised as purchased, takeaway, or free. The latter category included homegrown, "buy one get one free" offers, and other free meals such as fruit at school (Carr, *personal communication*, 2006; Defra, 2007). The survey information was filtered by Defra to remove quantities of processed food including tinned, frozen, and takeaway items. The remaining information was collated using the categories in Table 4.16 to ensure consistency with the food consumption data described in Section 4.4.4. Table 4.18 presents the average fraction of homegrown produce for each fruit and vegetable category, based on the proportion of non-purchased items to the total amounts brought into the home according to the Expenditure and Food Survey.

The majority of the UK population grows little or no homegrown produce and the mean data from the Expenditure and Food Survey 2004/05 reflects this. However, subgroups of the population like allotment holders would be expected to consume a much higher proportion of their own fruit and vegetables. In the National Food Survey 2000, approximately 85 per cent of the households sampled did not record any "non-purchased" items for a selection of vegetables including cabbages, leafy salads, carrots, onions and potatoes (Miller, *personal communication*, 2001; Rimmer, *personal communication*, 2001). This suggested that 15 per cent of the sample accounted for all the selected non-purchased items and that this subgroup may be more likely to represent the active home gardener or allotment holder. This opinion is consistent with estimates of garden use in surveys by MAFF over the period 1992 to 1996 (MAFF, 1999), where between 20 and 25 per cent of gardens surveyed were found to be growing fruit and/or vegetables.

Table 4.19 presents two sets of default values for the homegrown fraction, one based on the UK population average, and one transformed to account for subgroups of the population, assumed to be 15 per cent, that grow a considerable amount of their own produce. See Chapter 3 for consideration of growing space.

Table 4.18: Estimated proportion of homegrown fruit and vegetables from the Expenditure and Food Survey 2004/05

Produce type	Bought	Non-purchased	Total	Non-purchased fraction
	g person^{-1} week^{-1}	g person^{-1} week^{-1}	g person^{-1} week^{-1}	-
Vegetables				
Green	223.4	12.6	235.9	0.05
Root	271.4	16.6	288.0	0.06
Tuber	557.9	11.7	569.5	0.02
Fruit				
Herbaceous	211.8	14.5	226.3	0.06
Shrub	31.3	3.2	34.5	0.09
Tree	277.1	10.8	288.0	0.04

Table 4.19: Generic values for homegrown fraction for average and high-end scenarios (such as allotment holders)

Produce type	Homegrown Fraction	
	(average)	(high end) [1]
Vegetables		
Green	0.05	0.33
Root	0.06	0.40
Tuber	0.02	0.13
Fruit		
Herbaceous	0.06	0.40
Shrub	0.09	0.60
Tree	0.04	0.27

[1] Estimated from the average homegrown fraction by dividing by 0.15, therefore transforming the data to the 15 per cent of the population that recorded consumption of homegrown produce in the National Food Survey 2000 for the six vegetable types considered in the original CLR10 report (Rimmer, *personal communication*, 2001).

4.5 Buildings

The indoor environment is important to understanding human exposure to chemicals, because we spend so much of our time inside the home or workplace (Lioy *et al*., 2002; Office of National Statistics, 2006a; Paustenbach *et al*., 1997). Building data is required by the CLEA model to estimate vapour intrusion from contaminated soil into indoor air (see Chapter 10). Table 4.20 summarises the default building characteristics for use with the Johnson and Ettinger (1991) screening approach for predicting vapour intrusion from contaminated soil into buildings.

Table 4.21 summarises default characteristics for a number of residential and commercial building types (Environment Agency, 2005a). These values were selected from a review of the available literature including the English House Condition Survey (EHCS) (DCLG, 2001) and a sample survey of four UK towns carried out in the 1990s (Brown *et al*., 2000; Pout *et al*., 1998).

The residential footprint areas are the mean values for each building type and for all ages of building found in the EHCS (Environment Agency, 2005a). Residential building height is estimated from the number of habitable storeys and the average ceiling height of 2.4 metres (Environment Agency, 2005a). For non-residential buildings, the weighted-average plan area from the sample surveys is used to calculate the footprint and the building height is used to calculate the pressure difference resulting from the stack effect, with a distinction made between sample data from pre- and post-1970 construction (Environment Agency, 2005a). The number of occupied storeys in non-residential buildings is estimated by dividing the average building height from the survey data by the average storey height.

Environment Agency (2005a) suggested that a desirable level of ventilation in residential buildings is about 0.5 to 0.75 air changes per hour (ach). This range is sufficient to control moisture and other pollutants in the home while also minimising energy usage. There are few measurements of actual ventilation rates in residential properties because of the complexity of such investigations; however, a limited study found a yearly average of 0.52 ach in 35 homes (Environment Agency, 2005a). Although air change rate will vary by type and age of housing, a default value of 0.5 is used in the CLEA model for all residential buildings.

Table 4.20: Building Data

Parameter	SI Units	Description
Footprint	m^2	Building footprint in contact with contaminated soil. This parameter is often simplified to a square or rectangular shape with a known width and length in metres. It is used to determine the area of floor cracks in contact with the soil and also to determine the volume of living space.
Building height	m	Building height is important for determining the stack effect, which is the pressure difference between the warm air inside the building and the cold air outside. Building height does not necessarily equal living space volume, since the area under the roof is not always habitable.
Volume of living space	m^3	Volume of indoor air that may be contaminated by vapour intrusion. It is calculated from the building footprint, the number of habitable building storeys (which might include a habitable cellar or basement) and the height of each storey. Most screening models assume that the air volume is continuously well mixed.
Living space air exchange rate	$hour^{-1}$	This is the rate at which the indoor air mixes with outdoor air through gaps in windows, doors and walls. It is used to estimate the dilution effect of clean outdoor air entering the building and mixing with/displacing indoor air contaminated via vapour intrusion.
Pressure difference	Pa	This is the negative pressure difference between heated indoor air and colder outdoor air that drives advection of soil gas into buildings. As warm air rises, colder air is drawn in to replace it. The **stack effect** and the **dynamic effect** control pressure difference.
Foundation thickness	m	The thickness of the foundation slab, which sets the diffusion path length from soil into indoor air.
Floor crack area	cm^2	Advective contaminant transport through the floor is controlled by the number of openings within the floor, such as cracks or gaps between the floor and the wall.

Table 4.21: Default values for building data according to residential and commercial building type

Building Type	Building Footprint	LS Air Exchange Rate	Building Height	Storeys	Storey Height	LS Height	Pressure Difference	Foundation Thickness	Floor Crack Area
	m^2	hour^{-1}	m	-	m	m	Pa	m	cm^2
Residential									
Bungalow	78.0	0.5	2.4	1.0	2.4	2.4	2.6	0.15	706.5
Small terraced house	28.0	0.5	4.8	2.0	2.4	4.8	3.1	0.15	423.3
Medium/large terrace house	44.0	0.5	4.8	2.0	2.4	4.8	3.1	0.15	530.7
Semi-detached house	43.0	0.5	4.8	2.0	2.4	4.8	3.1	0.15	524.6
Detached house	68.0	0.5	4.8	2.0	2.4	4.8	3.1	0.15	659.7
Commercial									
Warehouse (pre-1970)	1089.0	1.0	5.2	1.0	4.6	4.6	3.2	0.15	2640.0
Warehouse (post-1970)	1914.0	1.0	5.9	1.0	5.1	5.1	3.4	0.15	3499.9
Office (pre-1970)	424.0	1.0	10.2	3.0	3.2	9.6	4.4	0.15	1647.3
Office (post-1970)	610.0	1.0	13.0	4.0	3.2	12.8	5.1	0.15	1975.9

[1] Living space (LS)

The Guidance to the Workplace (Health, Safety and Welfare) Regulations 1992 set minimum standards for the supply of fresh air to employees. BRE monitored six offices (five mechanically ventilated and one naturally ventilated) and found an average ventilation rate of 13 L s^{-1} per person (Environment Agency, 2005a). In a typical office, a person occupies 45 m^3 of space[22], which for a ventilation rate of 13 L s^{-1} corresponds to an air exchange rate of one per hour (Environment Agency, 2005a). This is the default value used for commercial buildings in the CLEA model.

The air pressure within a building is invariably slightly lower than that found outside because of stack, wind, and mechanical ventilation effects (Environment Agency, 2005a). The default values in Table 4.21 depend on the following assumptions:

- The air pressure difference, inside and outside the building, due to temperature difference is calculated using **Equation 4.6** with an assumed temperature difference between inside and outside of 12°C in winter and 0°C in summer (that is, an average annual difference of 6°C).
- An average wind effect of 2 Pa (USEPA, 2003).[23]
- No mechanical ventilation.

Equation 4.6

$$\Delta P = \frac{\rho_0 \, \Delta T \, g \, h}{T_i}$$

Where: ΔP is the air pressure difference due to temperature difference, Pa
ρ_0 is the external density, kg m^{-3} [1.2]
ΔT is the temperature difference between indoor and outdoor air, K [6]
g is the acceleration due to gravity, m s^{-2} [9.80665]
h is the height of building, m
T_i is the indoor air temperature, K [298]

Johnson and Ettinger (1991) make several assumptions about the building foundation (see also Chapter 10). Firstly, they assume that the foundation consists of a concrete ground-bearing slab rather than some form of suspended floor. Secondly, the cracks in the floor through which soil gas ingress occurs are assumed to be located at the perimeter between the floor and wall. Although such shrinkage joints can occur in aged slabs, further openings can be found across the slab either as planned expansion joints or more commonly as cracks and fractures (Environment Agency, 2005a).

In the EHC Survey (DCLG, 2001), solid foundations were found in about half of all residential properties irrespective of age and between 70 and 75 per cent houses built since the late 1960s (see Table 4.22). However, suspended floors are likely to be found in properties built prior to the Second World War and interpretation of the

---

[22] British Council of Offices (2000) gives typical occupancy rates of 15 m^2 of floor area per employee. The floor to ceiling height of an office building is in the order of three metres (Environment Agency, 2005a).

[23] Environment Agency (2005a) makes no specific recommendations for the pressure difference arising from the dynamic effect of wind pressure on the walls of the building. This is because the dynamic effect depends not only on wind speed, but also on the wind direction and the angle of incidence for each wall. Dynamic pressures on building surfaces can range from –20 to +20 Pa, but this does not represent the soil-building pressure difference that will drive soil gas entry (Environment Agency, 2005a). If, in a simple symmetrical example, air enters the building through the windward wall and then exits through the opposite wall (on the leeward side) then the dynamic pressure would be zero. USEPA (2003) suggests that an average value for the dynamic effect is 2 Pa.

Johnson and Ettinger (1991) should be applied more cautiously in these situations, since gas ingress rates could be considerably higher (Environment Agency, 2005a).[24]

Specifications for thickness of the ground-bearing slab vary considerably with age and between houses constructed to the same specification. Environment Agency (2005a) recommended a generic value of 150 mm for the thickness of the concrete layer, consistent with practice during the 1980s.

The density of cracks and other gaps in the floor will strongly influence the advective flow of soil gas into a building (see Chapter 10). USEPA (2003) estimate crack densities by assuming that the crack is present as a gap between floor and wall, either by design or as a result of the slab shrinking during construction. BRE experience with radon gas ingress into buildings suggests that there is an average gap of one to two millimetres between an in situ concrete slab and the wall in houses constructed since the 1960s (Environment Agency, 2005a). However in older houses, this gap can be larger (between two and three mm).

Table 4.21 lists floor crack areas for the different building types, assuming that the wall to floor crack width is two mm. The average floor crack area for all residential housing is 569 cm^2, much higher than the 300 cm^2 found by Eaton and Scott (1984) in a Canadian survey. Van Wijnen and Lijzen (2006) cited a range of residential values for the area of floor openings of between 0.5 and 50 cm^2 with an average of 5 cm^2, conclusions consistent with the findings of Waitz *et al*. (1996).

Table 4.22: Proportion of solid floors in different types of English housing (Environment Agency, 2005a)

Type	**Proportion of solid floors by age and type of property as a proportion of all properties built within time period (%)**				
	< 1919	**1919 - 1944**	**1945 - 1964**	**1965 - 1980**	**> 1980**
Small terraced house	11.0	2.2	6.0	8.2	13.9
Medium/large terraced house	9.2	3.2	10.8	15.3	7.1
Semi-detached house	6.1	9.8	29.8	19.2	14.4
Detached house	6.9	2.2	5.5	14.5	29.0
Bungalow	0.8	3.1	7.0	13.3	9.5
Proportion of all housing with solid floors	34.0	20.5	59.0	70.4	73.9

---

[24] See more detailed site-specific guidance in *The VOCs Handbook* (CIRIA, in press).

5 Chemical partitioning

The starting point for predicting the fate and transport of chemicals in the soil environment is the degree to which they partition between the main soil phases including mineral and organic particles, and the air/water in pore spaces. This chapter describes the simplified linear approach used by the CLEA model to predict these processes and the circumstances in which this approach breaks down.

Soil is a complex heterogeneous medium comprising mineral and organic solids, aqueous and gaseous components (Alloway, 1995). Chemical contaminants enter soil in a variety of forms and under vastly different circumstances, from natural mineralisation through long-term diffuse deposition to short-term high volume releases such as pipe leaks and tank spills. Chemicals entering soil systems can partition between several different solid, liquid and gas phases. For example, metals in soil can occur in at least five solid phases including a component of the mineral lattice, as a precipitate, as an exchangeable ion on mineral surfaces, as an organic chelate or within the bio-phase (Alloway, 1995). Chemicals may also dissolve in the water or volatilise into the air contained within the spaces between soil aggregates. The relationship between these different phases is often complex, depending on a range of different soil conditions and chemical properties (see Figure 5.1). Typically, only a few per cent of the total contaminant content in soil will be in aqueous solution or the gas phase; however, it is this proportion that strongly influences transport and exposure.

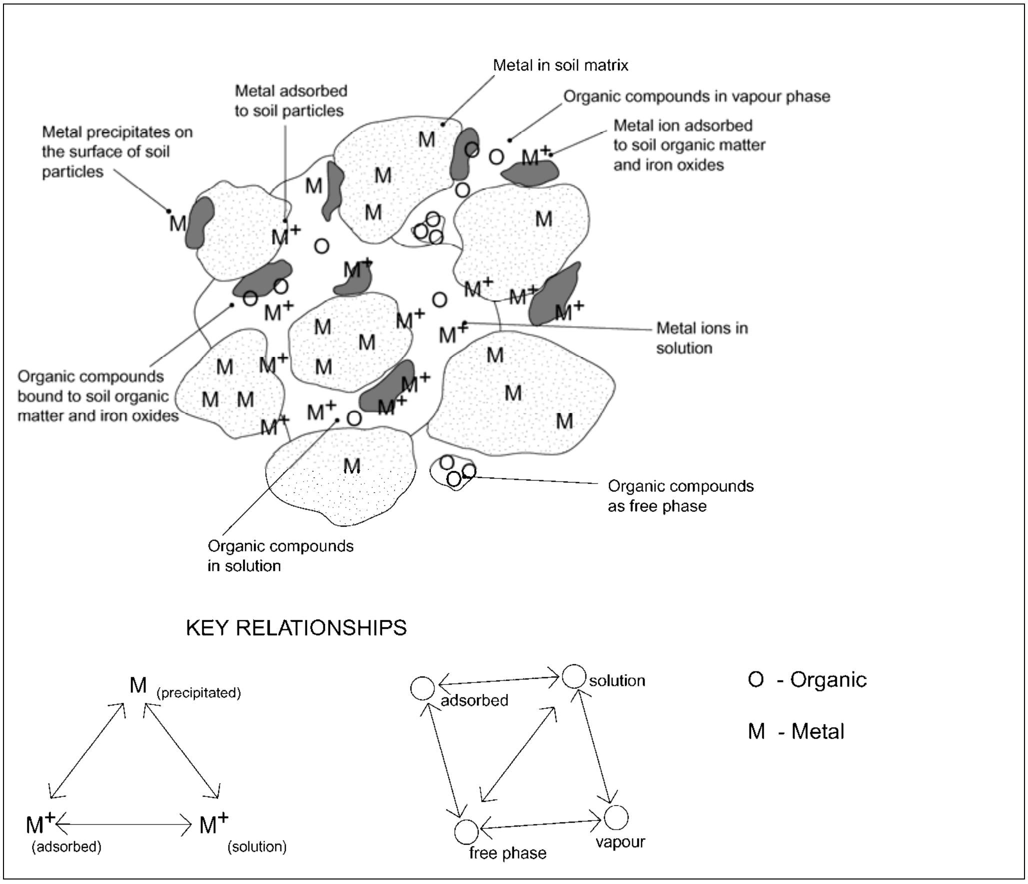


Figure 5.1: Illustration of the key processes in chemical partitioning in soil

Chemical partitioning in the soil will not always be relevant to exposure pathway calculations in the derivation of SGVs for one or more of the following reasons:

- partitioning is irrelevant to the mechanism of exposure (for example, chemical intake by direct soil ingestion);
- partitioning is empirically accounted for in the pathway calculations (for example, if the dermal absorbed fraction is estimated from experimental study and calculated in the CLEA model from the total soil concentration);
- partitioning is empirically accounted for by direct measurement of exposure (for example, several soil-to-plant concentration factors are based on the direct relationship between plant concentration and total soil concentration).

5.1 Predicting chemical behaviour in soil

Increasingly sophisticated computer models are becoming available to assess soil partitioning of substances, especially metals and their salts (Allison *et al.,* 1991; Bourg 1982). However, their applicability to generic modelling remains limited because of their data requirements to specify soil conditions. The alternative approach, and the one most commonly used in generic models, is to predict the equilibrium partitioning behaviour between two phases and to answer the question "*Given a concentration in one phase, what will be the concentration in another phase that has been in contact with it long enough to achieve equilibrium?*" (Mackay, 2001). There are two methods to describe this partitioning behaviour (Mackay, 2001):

- an experimental or empirical **partition coefficient** that relates to the ratio of the chemical concentration in each of the two phases;
- use of an intermediate quantity as a criterion of equilibrium, which can be related to the concentration in either phase (for example, chemical potential or **fugacity**).

The CLEA model adopts the partition coefficient approach to predicting chemical concentration in different soil phases (Environment Agency, 2002b). The soil system is divided into three phases (Environment Agency, 2002b; Jury *et al*., 1983):[25]

- **sorbed phase**, where the chemical is reversibly bound to the surface of mineral and organic matter particles;
- **aqueous phase**, where the chemical is dissolved in the interstitial pore water;
- gas phase, where the chemical is a gas within the interstitial pore air.

Table 5.1 summarises the key partitioning relationships within this three-phase system (Jury *et al*., 1983). The most important of these relationships is the one between the sorbed or bound chemical and its concentration in aqueous solution. This is described by the experimental or calculated soil-water partition coefficient (K_d), which is the ratio of observed soil concentrations to that measured in solution from experimental studies (see **Equation 5.1**). Linear and non-linear trends can be assumed for a variety of different soil properties[26] (Alloway, 1995; Jury *et al*., 1983; Waitz *et al*., 1996).

---

[25] The CLEA model does not consider a fourth phase, that is the chemical itself is not present in a pure form as either a solid or liquid, since it estimates exposure to very low concentrations of such chemicals in the environment.

[26] The higher the soil-water partition coefficient, the more strongly bound the contaminant is to the soil.

Equation 5.1

$$K_d = \frac{C_{sb}}{C_w}$$

Where: K_d is the soil-water partition coefficient, cm^3 g^{-1}
C_{sb} is the chemical concentration sorbed to soil, mg g^{-1}
C_w is the chemical concentration in aqueous solution, mg cm^{-3}

K_d values are reported widely in the literature for inorganic compounds and their elements in a wide range of different soil conditions. Care must be taken in the selection of default values, since they often obscure a wide range of real soil-to-soil solution characteristics. For example, a compendium of values for use in modelling radionuclide transport in the environment reported a K_d value for cadmium in a 'loam soil' of 40 cm^3 g^{-1}, which has been widely used as a default value (Sheppard and Thibault, 1990). This number was derived from the **geometric mean** of just eight values reported in the literature, with a possible range from 7 to 962 cm^3 g^{-1}. Clearly, this K_d value is subject to significant uncertainty. In the CLEA model, representative K_d values for inorganic substances are selected from the literature according to the guidelines in Section 4.2.

In some respects, the behaviour of organic compounds in soil is made simpler by the opportunity to consider families of chemically related compounds. For neutral organic compounds (those without a strongly ionic character) and in the absence of free phase, the soil-water partition coefficient has been found to correlate strongly to the amount of soil organic carbon (ASTM, 2000; Mackay, 2001; USEPA 2003). The K_d value can therefore be predicted for organic chemicals from their chemical affinity to organic carbon and the amount of organic matter in soil (see **Equation 5.2**).

Equation 5.2

$$K_d = K_{oc}\, f_{oc}$$

Where: K_d is the soil-water partition coefficient, cm^3 g^{-1}
K_{oc} is the organic carbon-water partition coefficient, cm^3 g^{-1}
f_{oc} is the fraction of organic carbon in soil, g g^{-1}

Experimental and calculated organic carbon-water partition coefficients (K_{oc}) are reported in the literature (Environment Agency, 2003; Mackay *et al.*, 2006). Several researchers have also derived semi-empirical relationships between K_oc and the **lipophilic tendency** of an organic compound, as predicted by the octanol-water partition coefficient, K_{ow}.

Table 5.1: Soil phases and chemical partition coefficients

Relationship	Partition coefficient
Sorbed and aqueous phase	Soil-water partition coefficient (K_d)
Sorbed and gas phase [1]	Soil-vapour partition coefficient
Aqueous and gas phase [2]	Air-water partition coefficient (K_aw)

[1] This is typically not a very important transport pathway in assessing the fate of chemicals in the soil environment under ambient conditions (Mackay, 2001)

[2] Measured directly or calculated from Henry's Law constant (Environment Agency, 2008c)

There are often considerable variations in the experimental values of K_{oc} for chemical compounds reported in the literature, even where the results have been normalised to standard organic carbon content (Environment Agency, 2008c). Using a calculated K_{oc} has the advantage of a consistent relationship between K_{oc} and K_{ow} for modelling purposes and is the approach recommended by the *Technical Guidance Document on Risk Assessment* (ECB, 2003). **Equation 5.3** describes the two general relationships used in the CLEA model to calculate K_{oc} and their range of applicability (ECB, 2003; Environment Agency, 2003). ECB (2003) also lists 17 other relationships that are applicable to specific chemical families including phenols, esters and organic acids.

Equation 5.3

$$(1)\quad \log K_{oc} = 0.81 \log K_{ow} + 0.10 \qquad \textit{(predominantly hydrophobic compounds)}$$

$$(2)\quad \log K_{oc} = 0.52 \log K_{ow} + 1.02 \qquad \textit{(non-hydrophobic compounds)}$$

Where: K_{oc} is the organic carbon-water partition coefficient, cm^3 g^{-1}
K_{ow} is the octanol-water partition coefficient, dimensionless

Equation (1) is applicable to most organic chemicals with log k_{ow} values in the range 1.0 to 7.5 and containing only carbon, hydrogen or halogen atoms.

Equation (2) is applicable to organic chemicals with log K_{ow} values in the range –2.0 to 8.0 and applies to hydrocarbons not covered by Equation (1) including those which contain oxygen and nitrogen such as phenols, esters, and amines.

Volatile compounds including benzene and elemental mercury may partition from aqueous solution into air and be transported through the soil into ambient air and inside buildings (Boethling and Mackay, 2000; Environment Agency, 2008c; Johnson and Ettinger, 1991; Mackay, 2001). The tendency for a pure chemical to volatilise to air is controlled by its vapour pressure and from aqueous solution by the air-water partition coefficient (K_{aw}), which is measured directly or calculated from Henry's Law constant (see also Section 4.2).

The reported values of Henry's Law constant may vary over many orders of magnitude for the same chemical (Environment Agency, 2008c). There is a common misconception that substances with a low volatility, such as DDT, will also have a low Henry's Law constant but this is not necessarily the case, because such substances may also have very low aqueous solubilities (Mackay, 2001). ITRC (2007) noted that several regulatory agencies have defined volatile chemicals as those with a Henry's Law constant greater than 1 x 10^{-5} atm m^3 mol^{-1} (that is, greater than 1 Pa m^3 mol^{-1}).

Where a chemical has an appreciable volatility, the partitioning tendency from solution to air, must also be taken into account when assessing the equilibrium concentration between soil and water (ASTM, 2000). **Equation 5.4** describes the total soil concentration to pore water concentration ratio (K_{sw}) used in the CLEA model for organic substances and inorganic substances with an appreciable volatility (ASTM, 2000).

Equation 5.4

$$K_{sw} = \frac{\theta_w + (K_d \rho_s) + (K_{aw} \theta_a)}{\rho_s}$$

Where: K_{sw} is the total soil- water partition coefficient, $cm^3\ g^{-1}$
K_d is the sorbed soil-water partition coefficient, $cm^3\ g^{-1}$
θ_w is the water-filled soil porosity, $cm^3\ cm^{-3}$
θ_a is the air-filled soil porosity, $cm^3\ cm^{-3}$
ρ_s is the dry soil bulk density, $g\ cm^{-3}$
K_{aw} is the air-water partition coefficient at ambient temperature, $cm^3\ cm^{-3}$

5.2 Calculated soil phase concentrations

The CLEA model calculates the various soil phase concentrations using chemical partition coefficients from a total soil concentration value inputted by the user.

5.2.1 Soil gas phase

Soil gas concentration is calculated using **Equation 5.5**, which is derived from the calculation of the gas concentration at source in USEPA (2003) substituting the partition coefficient K_{sw} for K_d. The soil gas concentration may exceed the theoretical saturated vapour concentration (see Section 5.3).

What is the effect of using K_{sw} instead of K_d?

K_{sw} will be appreciably larger than K_d for volatile substances in soils with a low organic carbon content. This means that using K_d directly will over-predict the concentration in aqueous solution. For semi-volatile compounds and soils with an organic matter content greater than five per cent by weight, the differences between partitioning behaviour will be less significant. This is illustrated by the calculations for benzene (log K_{ow} 2.13, K_{aw} 1.16 x 10^{-1}) and benzo[a]pyrene (log K_{ow} 6.18, K_{aw} 1.76 x 10^{-6}) for a sandy loam soil at varying organic matter contents.

Chemical	**K_d ($cm^3\ g^{-1}$)**	**K_{sw} ($cm^3\ g^{-1}$)**	**Difference (%)**
Benzene			
1.0 per cent SOM	7.82E-01	1.07E+00	27.2
2.5 per cent SOM	1.96E+00	2.25E+00	13.0
5.0 per cent SOM	3.91E+00	4.20E+00	6.9
Benzo[a]pyrene			
1.0 per cent SOM	8.78E+03	8.78E+03	0.0
2.5 per cent SOM	2.19E+04	2.19E+04	0.0
5.0 per cent SOM	4.39E+04	4.39E+04	0.0

Equation 5.5

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

Where: C_{vap} is the soil gas concentration, mg cm^{-3}
C_s is the total soil concentration, mg g^{-1}
K_{aw} is the air-water partition coefficient at ambient temperature, cm^3 cm^{-3}
K_{sw} is the total soil-water partition coefficient, cm^3 g^{-1}

5.2.2 Soil aqueous solution phase

Soil solution concentration is calculated using **Equation 5.6** for inorganic substances with no appreciable volatility and **Equation 5.7** for organic substances and volatile inorganic substances. The soil solution concentration may exceed the theoretical maximum aqueous solubility (see Section 5.3).

Equation 5.6

$$C_w = \frac{C_s}{K_d}$$

Where: C_w is the soil solution concentration, mg cm^{-3}
C_s is the total soil concentration, mg g^{-1}
K_d is the sorbed soil-water partition coefficient, cm^3 g^{-1}

Equation 5.7

$$C_w = \frac{C_s}{K_{sw}}$$

Where: C_w is the soil solution concentration, mg cm^{-3}
C_s is the total soil concentration, mg g^{-1}
K_{sw} is the total soil-water partition coefficient, cm^3 g^{-1}

5.2.3 Sorbed soil phase

The sorbed soil concentration is assumed to be the amount of chemical present in the soil after taking into account the solution and gas phases. It is estimated by subtracting the amount of chemical in pore water and pore gas from the total amount in a fixed volume of soil (see **Equation 5.8**). The total amount in soil is assumed to be equal to the sum of all the amounts in all three phases (Jury *et al*., 1990; Ryan *et al*., 1988).

Equation 5.8

$$C_{sb} = C_s - (C_w^* + C_{vap}^*)$$

Where: C_{sb} is the total amount of sorbed chemical in soil, mg g^{-1}
C_s is the total soil concentration, mg g^{-1}
C_w^* is the soil solution concentration on a mass basis, mg g^{-1}
C_{vap}^* is the soil gas concentration on a mass basis, mg g^{-1}

Equation 5.9 and **Equation 5.10** correct the concentration of a chemical in solution and in soil gas from a volumetric basis to the mass of soil respectively.

Equation 5.9

$$C_w^* = C_w \frac{\theta_w}{\rho_s}$$

Where: C_w^* is the soil solution concentration on a mass basis, mg g^{-1}
C_w is the soil solution concentration, mg cm^{-3}
θ_w is the water-filled soil porosity, cm^3 cm^{-3}
ρ_s is the dry soil bulk density, g cm^{-3}

Equation 5.10

$$C_{vap}^* = C_{vap} \frac{\theta_a}{\rho_s}$$

Where: C_{vap}^* is the soil gas concentration on a mass basis, mg g^{-1}
C_{vap} is the soil gas concentration, mg cm^{-3}
θ_a is the air-filled soil porosity, cm^3 cm^{-3}
ρ_s is the dry soil bulk density, g cm^{-3}

5.3 Saturated soil concentrations

The partitioning processes, as described in Section 5.2, depend on a number of limiting assumptions and are primarily based on linear behaviour observed at low chemical concentrations in soil (Environment Agency, 2002b; Jury *et al*., 1990). The CLEA model includes several checks to highlight when these boundary conditions have been exceeded while deriving SGVs, to help in the interpretation of results. However, media concentrations are not capped to any maximum value and the SGV will be based on worst-case assumptions. See the summary in Table 5.2 and the following discussion.

Table 5.2: Boundary conditions to partition calculations

Condition	Checks
Aqueous solubility cannot exceed the maximum aqueous solubility of the pure chemical under ambient conditions.	Does the generic assessment criterion exceed the saturated aqueous concentration? See Section 5.3.1.
Gas phase concentrations cannot exceed the saturated vapour concentration of the pure chemical under ambient conditions.	Does the generic assessment criterion exceed the saturated vapour concentration? See Section 5.3.2.
Sorbed concentrations cannot exceed the maximum surface capacity of the soil.	
Free phase contamination is not present such as a **NAPL** or a precipitated salt.	Is **free-phase** contamination present? See Section 5.3.3.

5.3.1 Saturated aqueous concentration

The calculated soil pore water concentration of a chemical may exceed the maximum aqueous solubility of the pure chemical in water at ambient temperature and pressure. This check is triggered at a soil concentration calculated using **Equation 5.11** for inorganic substances with no appreciable volatility and using **Equation 5.12** for organic chemicals (ASTM, 2000). Where a calculated generic assessment criterion exceeds the saturated aqueous soil concentration, C_{satw}, the risk assessor should consider whether uncertainty in the partitioning approach would affect the outcome of the assessment. For example, exceeding the maximum aqueous solubility limit may overestimate exposure via plant uptake and/or the inhalation of vapours.[27] In addition, the maximum aqueous solubility assumes only a single chemical is present in solution. Chemical solubility may be radically altered by other chemicals present in solution and by co-solvent effects arising from the presence of non-aqueous phase liquids (NAPL).

Equation 5.11

$$C_{satw} = S\,K_d \quad \times \quad 1000\,g\,kg^{-1} \quad \times \quad \frac{1}{1000} L\,cm^{-3}$$

Where: C_{satw} is the saturated soil concentration at the aqueous solubility limit, mg kg^{-1}
S is the maximum aqueous solubility of the pure chemical at ambient temperature and pressure, mg L^{-1}
K_d is the sorbed soil-water partition coefficient, cm^3 g^{-1}

Equation 5.12

$$C_{satw} = S\,K_{sw} \quad \times \quad 1000\,g\,kg^{-1} \quad \times \quad \frac{1}{1000} L\,cm^{-3}$$

Where: C_{satw} is the saturated soil concentration at the aqueous solubility limit, mg kg^{-1}
S is the maximum aqueous solubility of the pure chemical at ambient temperature and pressure, mg L^{-1}
K_{sw} is the total soil-water partition coefficient, cm^3 g^{-1}

5.3.2 Saturated vapour concentration

The calculated soil gas concentration of a chemical may exceed the saturated vapour concentration above the pure chemical at ambient temperature and pressure. The saturated vapour pressure is calculated using **Equation 5.13** and the soil concentration at which the check is triggered is calculated using **Equation 5.14** (ASTM, 2000). Where a calculated generic assessment criterion exceeds the saturated vapour soil concentration, C_{satv}, the risk assessor should consider whether uncertainty in the partitioning approach would affect the outcome of the assessment. For example, exceeding the saturated vapour pressure limit may overestimate exposure via the inhalation of vapours.

---

[27] Note that exceeding the aqueous solubility limit may not always over-predict plant uptake, since plants may actively scavenge chemicals from the soil solution and critically affect the soil-water equilibrium. The Environment Agency (2006) found better predictions of observed uptake behaviour for some chemicals when pore water concentration was not limited.

Equation 5.13

$$C_{sat\,vap} = P_v \frac{M}{RT_{amb}} \times 1000\,mg\,g^{-1}$$

Where: $C_{sat\,vap}$ is the saturated vapour concentration above the pure chemical at ambient temperature and pressure, mg m^{-3}
P_v is the saturated vapour pressure at ambient temperature and pressure, Pa
M is the chemical molecular weight, g mol^{-1}
R is the molar gas constant , Pa m^3 mol^{-1} K^{-1} [= 8.314472]
T_{amb} is the ambient temperature, K

Equation 5.14

$$C_{satv} = \frac{C_{sat\,vap}}{K_{aw}} K_{sw} \times \frac{1}{1000000} m^3\,cm^{-3} \times 1000\,g\,kg^{-1}$$

Where: C_{satv} is the saturated soil concentration at the saturated vapour limit, mg kg^{-1}
$C_{sat\,vap}$ is the saturated vapour concentration above the pure chemical at ambient temperature and pressure, mg m^{-3}
K_{aw} is the air-water partition coefficient at ambient temperature, cm^3 cm^{-3}
K_{sw} is the total soil-water partition coefficient, cm^3 g^{-1}

5.3.3 Non-aqueous phase liquids

The partitioning approach described in this chapter assumes that only three chemical phases are present in soil. Although it applies to a wide range of site conditions where chemicals are present in soil at low concentrations, it is not designed to consider situations where **residual phase contamination** may be present (ASTM, 2000; Environment Agency, 2002b; USEPA, 2003; Waitz *et al.*, 1996).

Residual phase contamination occurs when the sorbed phase, aqueous phase and gas phase have reached saturation for a pure chemical and therefore the saturated soil concentrations calculated in Sections 5.3.1 and 5.3.2 are useful indicators for this behaviour (ASTM, 2000; USEPA, 2003).[28] Residual phase contamination includes non-aqueous phase liquids and solids consisting of single chemicals or mixtures of two or more chemicals (USEPA, 2003). Using the approach described in this chapter will overestimate environmental concentrations of chemicals in the presence of residual phase contamination and alternative methods for risk assessment are recommended (Environment Agency, 2002b; Johnson *et al.*, 1990; Mackay, 2001; Robinson, 2003; USEPA, 2003; Waitz *et al.*, 1996).

---

[28] These equations are not applicable to situations where the residual contamination consists of a mixture of two or more chemicals (ASTM, 2000).

6 Ingestion of soil/dust

This exposure pathway includes direct ingestion from contact with contaminated soil and indoor dust, and indirect ingestion through consumption of fruit and vegetables with entrained dirt. In the case of non-volatile chemicals, this pathway often represents the most significant route of exposure. Although the calculation of chemical intake appears straightforward, the selection of default values for key parameters has been, and indeed continues to be, the subject of considerable scientific research and debate.

In the CLEA model, direct soil and dust ingestion is calculated separately from indirect ingestion of entrained dirt through consumption of fruit and vegetables and they are discussed separately below.

6.1 Direct soil and dust ingestion

Ingestion of soil and indoor dust, especially by children, is an important exposure pathway for non-volatile contaminants including polycyclic aromatic hydrocarbons (PAHs) and metals such as arsenic and lead (Paustenbach, 2000).

6.1.1 Child studies

All parents are aware that young children use their mouths as a means of exploration, with little or no sense of disgust or apprehension (Rozin and Fallon, 1987). Older children and adults can ingest soil inadvertently through casual hand-to-mouth contact, or by the careless act of eating food such as sweets that have been dropped on the ground. In adults, the amount of casual hand-to-mouth contact can be increased if the individual is a smoker or has a tendency to bite their nails. In relatively rare cases, children and adults may suffer from soil **pica**, a psychopathological condition that refers to the persistent and purposeful consumption of soil, often in relatively large quantities (World Health Organisation, 1990).

Early studies of soil ingestion by children used an activity-based approach to estimate the exposure rate (Ferguson and Marsh, 1993; Hawley, 1985). For example, Duggan and Williams (1977) coupled the observed frequency of hand-to-mouth events with measurements of dust and soil on children's hands. Subsequent studies used video observations and/or detailed questionnaires to identify links between soil ingestion and behaviour (Davis and Mirick, 2006; Davies *et al*., 1990).

Most recent studies have used a trace element methodology to quantify the amounts of soil and dust ingested by children (Binder *et al*., 1986; Clausing *et al*., 1987; Calabrese *et al*., 1989; Davis *et al*., 1990; van Wijnen *et al*., 1990; Calabrese *et al*., 1997b; Davis and Mirick, 2006). These methods compare analysis of persistent tracers (typically aluminium, silicon and titanium) in soils and dust with levels found in samples of excreta including faeces and urine (USEPA, 2006).

Such studies are few in number, and with relatively small sample sizes of limited duration (typically between one and two weeks); thus, considerable criticism has been levelled at much of the early work with tracers (Calabrese and Stanek, 1994; Paustenbach, 2000; USEPA, 2006). Re-analysis of existing data by several authors has improved the methodologies, identifying better techniques for taking into account food and non-food sources such as toothpaste, and the statistical interpretation of data (Calabrese and Stanek, 1995; Calabrese *et al*., 1996; Stanek and Calabrese, 1994, 1995, and 2000; Zartarian *et al*., 2005). Stanek and others noted that the distribution of estimated average daily soil ingestion over a short period is more spread out than the actual soil ingestion over a longer period (Stanek *et al*., 1999; Stanek and Calabrese, 2000). They observed that accounting for this effect (called "*regression to the mean*") in estimating long-term chronic ingestion rates in tracer studies resulted in lower values for the true 95th percentile soil ingestion rate from individual tracer studies (Table 6.1).

Table 6.1: Estimating long-term soil ingestion rates from tracer studies (Stanek and Calabrese, 2000)

Time period [1]	95th percentile of true average soil ingestion rate (mg day^{-1})
7 days	177
30 days	135
90 days	127
365 days	124

[1]Time period over which daily soil ingestion rate has been averaged

An important consideration in understanding soil ingestion by children is the prevalence of soil pica (USEPA, 2006). Early studies considered only inadvertent ingestion, regarding any form of deliberate soil eating as too rare a condition to warrant inclusion in an environmental exposure assessment (Ferguson and Marsh 1993). Recent studies have found that relatively short-term deliberate ingestion or exploratory mouthing is widespread among young children and a "*'normal' temporary phenomenon among some children*" (Calabrese *et al*., 1997a; Stanek *et al*., 1998; Paustenbach, 2000).

Few ingestion studies have drawn a clear distinction between childhood exploratory mouthing and pica (Ferguson and Marsh, 1993; Paustenbach, 2000). USEPA (2006) concluded that soil pica is characterised by the recurrent ingestion of unusually high amounts of soil (in the order of one to five g day^{-1}) and may be intentional or unintentional behaviour. Such behaviour appears to be rare, USEPA (2006) commenting that based on five key tracer studies[29], only one child out of more than 600 children involved ingested significantly higher amounts of soil than the rest. This child was found to have an overall mean ingestion rate of five to six g day^{-1} over a two-week period, although the daily rate was highly variable between 0.074 and 13.6 g day^{-1} (Calabrese *et al*., 1991). Spikes within individual studies have normally been considered as exploratory behaviour and have often been included in the derivation of many mean soil ingestion rates (USEPA 1997, 2006).

6.1.2 Adult studies

Far fewer tracer studies have determined soil ingestion rates for adults (Calabrese *et al*., 1989; Stanek *et al*., 1997; Davis and Mirick, 2006). Early studies had a limited number of participants, since the adults were included as controls for the experimental method for childhood studies (Calabrese *et al*., 1990; Stanek *et al*., 1997).

Calabrese *et al*. (1990) estimated soil ingestion rates in six adults as part of a mass balance experiment to support a larger study in children. Although the study was limited, they concluded that the adult soil ingestion rate was close to 50 mg day^{-1}. Stanek *et al*. (1997) carried out a similar study with ten adult volunteers using an

---

[29] These included the primary studies by Binder *et al*. (1986), Clausing *et al*. (1987), van Wijnen *et al*. (1990), Davis *et al*. (1990) and Calabrese *et al*. (1989).

improved experimental methodology and data analysis procedure. They observed that for half of the study period the volunteers ingested no soil, although over the four-week period the average soil ingestion rate was close to 10 mg day^{-1}.

Davis and Mirick (2006) studied the soil ingestion rates amongst 19 families in order to provide a meaningful comparison between parents and their children. They observed mean estimated soil ingestion rates for the parents comparable to their children, although the distribution was skewed towards much lower values. The average rate for adults including both parents and the results using the silicon and aluminium tracers was 52.5 mg day^{-1}. Davis and Mirick (2006) concluded that this was consistent with other small-scale studies and the default value of 50 mg day^{-1} recommended by the USEPA for risk assessments (USEPA, 1997b).

6.1.3 Distinguishing soil and dust

Many observers recognise the importance of house dust to human exposure from soil contaminants such as lead (Paustenbach *et al*., 1997). In assessing risks from lead, USEPA (1994 and 1999) used a combined soil and dust ingestion rate from 85 to135 mg day^{-1} (depending on the child's age) with the assumption that 55 per cent of lead exposure derived from indoor dust ingestion and 45 per cent from soil ingestion. The underlying basis of this decision was a further analysis of the tracer study by van Wijnen *et al*. (1990). Oomen and Lijzen (2004) concluded that although the evidence was limited, exposure of children to lead via ingestion of soil and of house dust was in the same order of magnitude.

Smith and Jones (2003) recommended a soil ingestion rate of 100 mg day^{-1} and 50 mg day^{-1} for an average child aged one and five respectively, and a house dust ingestion rate of 100 mg day^{-1} in radiological risk assessments. This corresponds to house dust contributing between 50 and 66 per cent of a combined soil and dust ingestion rate of between 150 and 200 mg day^{-1}. Paustenbach *et al*. (1997) concluded that dust contributes a substantial proportion to the combined dust and soil ingestion rate (from 50 to 90 per cent depending on the source or receptor behaviour), a view supported through examining the child tracer study data in Table 5-20 of USEPA (2006).

Stanek and Calabrese (1992) re-examined faecal tracer studies using a number of strategies to try to distinguish between soil and dust components in the combined ingestion rates reported in earlier studies. They concluded that such analyses were complicated by large variability in the data set and cautioned against attempting to generalise the results to other populations. The authors did not use this methodology again in their later work (Calabrese *et al*., 1997b; Stanek and Calabrese, 2000).

USEPA (2006) concluded that it was not possible to differentiate between soil and dust within the current recommended value for soil ingestion rate, although it acknowledged that indoor dust was likely to be an important component.

6.1.4 Selecting default soil and dust ingestion rates

In selecting a daily soil or dust ingestion rate, it is important to decide whether to include occasional deliberate ingestion and/or soil **pica** within the estimate. Most tracer studies do not distinguish between inadvertent and occasional deliberate ingestion of soil and such behaviour is considered normal behaviour for a proportion of young children (Calabrese *et al*., 1997a; USEPA, 2006). Pica behaviour is much rarer and is a psychopathological condition (USEPA, 2006; World Health Organisation, 1990). Although Kimbrough *et al*. (1984) took soil pica into account in their exposure assessment for dioxins at Times Beach, Missouri their assumptions were subsequently considered by several observers to be overly conservative (Paustenbach, 2000).

There are many types of psychopathological behaviour that can affect adults and children, and where it is considered that protective measures are necessary they are best decided upon and implemented on an individual basis. Soil pica has therefore not been included in the soil and dust ingestion rate for children or adults. However, where separate short-term effects from exposure to contamination are known, it is advisable for the risk assessor to consider a one-off high soil ingestion rate, when deriving site-specific assessment criteria (Calabrese *et al*., 1997a). USEPA (2006) concluded that an ingestion rate of 10 g day^{-1} may not be unreasonable in assessing risks to children with pica behaviour.

Almost all tracer studies have noted a high variability in the intra-child as well as inter-child soil ingestion rate (USEPA, 2006). This variability has been taken into account by some commentators though using a lognormal distribution function and Monte Carlo simulation (Thompson and Burmaster, 1991; Stanek *et al*., 1999; Zartarian *et al*., 2005). However, Stanek and Calabrese (2000) noted that over long-term exposure periods, the variability observed in short-term tracer studies would result in average soil ingestion rates tending to the mean values from these studies.

USEPA (2006) recommended 100 mg day^{-1} as the best estimate of mean combined soil and indoor dust ingestion rate for children under seven years of age, from consideration of all the key tracer studies. Otte *et al*. (2001) also concluded that 100 mg day^{-1} represented a good estimate of the average soil ingestion rate for children in a residential with garden scenario, and that a value between 150 and 200 mg day^{-1} represented a realistic worst case. The default value used in the CLEA model for the combined soil and dust ingestion rate by young children is 100 mg day^{-1}.

The evidence base for selecting a representative soil ingestion rate for adults is much smaller and studies such as that by Hawley (1985) are purely conjectural. USEPA (1997b) and Otte *et al*. (2001) both recommend an average soil and dust ingestion rate of 50 mg day^{-1}. USEPA (1997b) cautioned that the value is highly uncertain and based on a low level of confidence. Paustenbach (2000) concluded that a value between five and 25 mg day^{-1} for the rate of soil ingestion by most adults would be reasonable, although it appears that this is closer to the median value than the mean from the limited studies available. The default value used in the CLEA model for the combined soil and dust ingestion rate by adults is 50 mg day^{-1}.

Most tracer studies do not differentiate between soil and indoor dust (and in particular, the fraction of dust derived from soil sources). Although Stanek and Calabrese (1992) tried to distinguish between soil and dust components in earlier studies, they cautioned against attempting to generalise the results to other populations. In risk assessments for lead, several methods attempt to distinguish between soil and indoor dust ingestion rates; however, the justifications for doing so are often related to lead exposure and not specific media intakes (Oomen and Lijzen, 2004; USEPA, 1994). The default value used in the CLEA model is therefore a combined soil and dust ingestion rate, and the soil concentration is used in calculating intake.

6.1.5 Calculating the chemical intake rate

The chemical exposure rate for the direct ingestion of soil and indoor dust is calculated in the CLEA model using **Equation 6.1**. The soil and indoor dust ingestion rates are estimated from tracer study experiments and the default values used in the derivation of SGVs are summarised in Table 6.2.

Equation 6.1

$$IR_{direct\ soil\ and\ dust\ ingestion} = C_s\ S_{ING}$$

Where: IR is the chemical intake rate from direct soil and dust ingestion, mg day^{-1}
C_s is the total concentration of the chemical in soil, mg g^{-1}
S_{ING} is the direct soil and dust ingestion rate, g day^{-1}

Table 6.2: Default values for the combined soil and dust ingestion rate by age

Age class	Combined soil and dust ingestion rate (g day^{-1})	
	Residential/Allotment	Commercial
1	0.1	-
2	0.1	-
3	0.1	-
4	0.1	-
5	0.1	-
6	0.1	-
17	-	0.05

6.2 Indirect soil ingestion

Inadvertent ingestion of entrained soil on homegrown produce is likely to be an important component of adult exposure to non-volatile soil contaminants (Paustenbach, 2000). Fruit and vegetables grown in the garden or allotment may have fine-grained soil particles adhered to their skins or leaves through direct contact with soil or through aerial deposition onto leaves. Soil may remain in the skins of potatoes and carrots and in the leaves of cabbage and lettuce even after normal washing and cooking.

6.2.1 Available studies

There is very little quantitative information on soil loading of fruit and vegetable produce by direct contact or through dust deposition. Most studies have resulted from nuclear research and assessment of the impact from radioactive fallout. Paustenbach (2000) cited work by Russell in the 1960s carried out during nuclear weapon trials, noting that superficial dust deposition rarely resulted in contamination of plants by dirt due to the natural mechanical action of rainfall and the preparation and cooking of foodstuffs. However, such observations fail to consider the importance of direct contact between the soil and the growing vegetable, and localised rain splash of heavy particles and their entrainment between growing leaves (Trapp and Schwartz, 2000).

Kulhánek *et al*. (2005) cited experimental work by Li *et al*. (1994) that found soil loading rates for lettuce of 0.26 g g^{-1} dw lettuce from direct contact with soil. An experimental study on beet leaves by Sheppard and Evenden (1992) estimated the soil loading after thorough washing to be in the order of 0.03 g g^{-1} dw. These rates are much higher than the soil loading observed by Sheppard and Evenden (1995) who estimated soil loading for twelve vegetable and fruit crops, including bean leaves and pods, beet and chard leaves, cucumber and strawberry fruits and inner and outer leaves of cabbage. They estimated an average soil loading of 0.00002 g g^{-1} dw for leafy tissues and 0.000002 g g^{-1} for fruits.

The influence of food preparation on soil loading has also been investigated. Sheppard and Evenden (1995) found that washing vegetable and fruit crops decreased soil loading about 1.5 fold. Brunekreef (1996) investigated the soil content of washed leeks and found that washing the vegetables reduced the average soil loading by almost two-thirds. Samsøe-Petersen *et al*. (2002) investigated the contamination of fruit and vegetables grown in gardens and allotments in Denmark. They concluded that peeling root crops including potato and carrot significantly reduced the contaminant loading, indicating that uptake was the result of soil contact and from entrained soil.

Some researchers have suggested that most soil ingested from crops is likely to come from leafy vegetables (Paustenbach, 2000). However, there appears to be little or no information to support this. In the UK many people eat potato skin, increasing the potential for indirect soil ingestion from root vegetables. In addition, it is not known whether small soil particles that adhere to vegetables have elevated levels of contaminants, especially metals, from enrichment during soil contamination.[30]

The FARMLAND foodchain model, developed to simulate radionuclide transfer through terrestrial foods, included the resuspension of particles from the soil surface to the external parts of crops due to the action of wind and rain (Brown and Simmonds, 1995). The authors concluded that there is considerable uncertainty in assigning a representative soil loading to fruits and vegetables, but that a value of 0.1 per cent on a dry weight basis (0.001 g g^{-1} dw) would be representative of the literature. Oatway and Mobbs (2003) adopted the soil loading values for leafy vegetables in the FARMLAND model and extended this to root vegetables and fruit. They also included a correction factor for food preparation.

6.2.2 Calculating the chemical intake rate

The chemical exposure rate for the indirect ingestion of soil attached to homegrown produce is calculated in the CLEA model using **Equation 6.2**. The soil loading and preparation factors are based on Oatway and Mobbs (2003). Table 6.3 summarises the relevant values for each homegrown produce group.

Equation 6.2

$$IR_{indirect\ soil\ ingestion} = \sum_{all\ produce\, groups} C_s SL_x\, PF_x\, CR_x\, BW\, DW_x\, HF_x$$

Where:
IR is the chemical intake rate from indirect ingestion from attached soil, mg day^{-1}
C_s is the total chemical concentration in soil, mg g^{-1} dw
SL_x is the soil loading factor, g g^{-1} dw
PF_x is the food preparation correction factor, dimensionless
CR_x is the food consumption rate per unit body weight, g fw kg^{-1} bw day^{-1}
BW is the body weight, kg
DW_x is the fresh plant weight to dry plant weight conversion factor, g dw g^{-1} fw
HF_x is the homegrown fraction, dimensionless

x represents the six produce groups described in Table 4.16

---

[30] Finer particles such as clays and silts are known to concentrate metal contamination in soil because of their surface charge and high surface area.

Table 6.3: Default values for entrained soil according to produce category

Produce category	Soil loading (SL) g g^{-1} dw	Preparation factor (PF) dimensionless	Dry weight conversion factor (DW) [1] g dw g^{-1} fw
Green vegetables	0.001	0.2	0.096
Root vegetables	0.001	1.0	0.103
Tuber vegetables	0.001	1.0	0.210
Herbaceous fruit	0.001	0.6	0.058
Shrub fruit	0.001	0.6	0.166
Tree fruit	0.001	0.6	0.157

[1] See Chapter 7 for derivation.

7 Ingestion of fruit/vegetables

This exposure pathway considers the potential transfer of chemicals in soil to fruit and vegetables grown in contaminated ground. Families eating such contaminated produce from a home garden or allotment are potentially exposed to such chemicals through their diet. In the case of mobile and non-volatile chemicals, this often represents the most significant route of exposure.

In this chapter, the approach to predicting plant uptake of chemicals from soil is discussed. See also Chapter 4 for information on the amount of homegrown fruit and vegetables that people are assumed to consume.

7.1 Overview

7.1.1 Plant uptake processes

Plants accumulate chemicals from soil via a number of different pathways, although the most important is through the root system and translocation within the plant by the xylem (Environment Agency, 2006; Kabata-Pendias, 2001). Uptake can also result from the absorption of chemical vapour from ambient air by shoots during respiration, mediated by gaseous exchange rather than through aqueous solution (Bell, 1992; Environment Agency, 2006). The vapour pathway is important not just for highly volatile pollutants but also those with a strong preference to partition to air rather than water, including PAHs, PCBs and dioxins (Bell, 1992).[31]

Root uptake of chemicals occurs predominantly from the soil solution; direct uptake of material sorbed on soil surfaces or on organic matter is small (Alloway, 1995). Not all root uptake processes are passive and several plant species can increase the soil availability of contaminants through the release of simple organic acids (such as malates and citrates), which chelate trace elements needed by the plant and promote desorption from soil (Kabata-Pendias, 2001). For example, some species of *Astragalus* can scavenge up to 10,000 mg of selenium per kg^{-1} dw of plant from the surrounding soil (Kabata-Pendias, 2001). In soils and sediments where the clay content is relatively low, the availability of organic contaminants is often strongly related to the fraction of organic carbon present in the soil (Environment Agency, 2006).

Uptake behaviour differs markedly between plant species and individual cultivars (John and van Laerhoven, 1976; Kabata-Pendias, 2001). Jopony and Young (1993) studied lead uptake by radish and red fescue grown in soils contaminated by mine spoil, observing a linear response for the latter and a markedly non-linear response for the former. Transport within plant tissues involves many processes that depend on plant species and the specific contaminant (Environment Agency, 2006; Thorne *et al*., 2005). In the case of organic contaminants, the complex chemistry of the plant system offers many pathways for their generation, transformation and destruction (Bell, 1992).

---

[31] It is recognised that airborne deposition of pollution, particularly in an urban setting, is a significant additional source of plant uptake. However, because such pollution derives from non-soil sources it has not been included in the exposure model.

Other dietary intakes

The CLEA model estimates the chemical intake rate of soil contaminants from the consumption of fruit and vegetables only. It does not take account of other intakes from contaminated food such as meat, dairy produce including eggs and, in the case of infants, breast milk. However, many of these factors are considered as background intakes when deriving the TDSI (Environment Agency, 2009a).

Where site-specific circumstances suggest that produce other than fruits and vegetables are being grown on contaminated soils and consumed locally, the generic assumptions in the standard land uses may not be health protective.

7.1.2 Soil-to-plant concentration factors

Ideally, the concentration of chemicals in homegrown fruits and vegetables would be measured directly on a site-specific basis. However, this is often impractical for a number of reasons including the time and cost associated with such investigations, analytical complexity and statistical variability, and the availability of fresh produce. More commonly, chemical concentrations in the edible portions of fruits and vegetables are predicted from the relationship between soil and plant. This is known as the soil-to-plant concentration factor (CF) and is shown in **Equation 7.1**.

Equation 7.1

$$CF = \frac{C_{plant}}{C_s}$$

Where: CF is the soil-to-plant concentration factor, mg g^{-1} fw plant per mg g^{-1} dw soil
C_{plant} is the chemical concentration in edible plant tissues, mg g^{-1} fw plant
C_s is the total soil concentration, mg g^{-1} dw soil

In the CLEA model, CF is required in units of fresh weight (fw) plant concentration to compare with the fresh weight consumption data described in Section 4.4.4. However many literature studies report the plant concentration and/or *CF* value on a dry weight (dw) basis. It is important to correct such values to fresh weight because the water content of some plants, such as leafy salads, are typically more than 95 per cent water (Alloway *et al*., 1988; Gebhardt and Thomas, 2002). This relationship is shown in **Equation 7.2** and the dry weight conversion factors for individual fruits/vegetables and produce categories are summarised in Table 7.1.

Equation 7.2

$$CF = \frac{C^{*}_{plant} DW_c}{C_s} \quad or \quad CF^{*}\ DW_c$$

Where: CF is the soil-to-plant concentration factor, mg g^{-1} fw plant per mg g^{-1} dw soil
C^{*}_{plant} is the chemical concentration in edible plant tissues, mg g^{-1} dw plant
C_s is the total soil concentration, mg g^{-1} dw soil
DW_c is the dry weight to fresh weight conversion factor, g dw g^{-1} fw plant
CF^{*} is the soil-to-plant concentration factor, mg g^{-1} dw plant per mg g^{-1} dw soil

Table 7.1: Dry weight conversion factors used in the CLEA model (Alloway *et al.*, 1988; Gebhardt and Thomas, 2002; FSA, 2005)

	Water content (per cent weight)	Dry matter content (per cent weight)	Dry weight conversion factor (g dw g^{-1} fw)
Green vegetables	**90.4**	**9.6**	**0.096**
Beans[1]	86.9	13.1	0.131
Brussels sprout	90.5	9.5	0.095
Cabbage[2]	89.5	10.5	0.105
Cauliflower	92.4	7.6	0.076
Lettuce	96.0	4.0	0.040
Spinach	93.7	6.3	0.063
Peas	82.2	17.8	0.178
Fresh herbs[3]	88.7	11.3	0.113
Other fresh green vegetables[4]	92.0	8.0	0.080
Stem vegetables[5]	92.1	7.9	0.079
Root vegetables	**89.7**	**10.3**	**0.103**
Carrot	90.3	9.7	0.097
Fresh turnips and swede	90.6	9.4	0.094
Fresh onions and leeks	90.3	9.7	0.097
Fresh rhubarb	91.3	8.7	0.087
Other[6]	86.2	13.8	0.138
Tuber vegetables	**79.0**	**21.0**	**0.210**
Potato	79.0	21.0	0.210
Herbaceous fruit	**94.2**	**5.8**	**0.058**
Cucumber	96.0	4.0	0.040
Marrow, courgettes, aubergine and pumpkin	94.2	5.8	0.058
Tomato	94.7	5.3	0.053
Other fruit (strawberries)	92.0	8.0	0.080
Shrub fruit	**83.4**	**16.6**	**0.166**
Other soft fruit[7]	83.4	16.6	0.166
Tree fruit	**84.3**	**15.7**	**0.157**
Fresh apples	84.0	16.0	0.160
Fresh pears	84.0	16.0	0.160
Fresh stone fruit[8]	85.0	15.0	0.150

[1] Includes broad, French, runner beans
[2] Includes cabbage and kale
[3] Includes mint and parsley
[4] Includes okra and endives
[5] Includes broccoli, celery and asparagus
[6] Includes beetroot, parsnip, radish, Jerusalem artichoke
[7] Includes blackcurrant, gooseberry, raspberry
[8] Includes apricots, cherries, peaches and plums

7.2 Estimating concentration factors

Given the large variations in reported uptake of contaminants by different plants and under various soil conditions, a cautious approach has been adopted in the CLEA model to review plant uptake on a substance-by-substance basis, using literature data and generic modelling methods. The procedure includes the following elements:

- review of literature on soil chemistry and plant uptake to identify trends in behaviour related to soil properties and sources of contamination;
- review of literature to identify soil-to-plant concentration factors (CF) for the key fruits and vegetables outlined in Table 4.16;
- comparison of generalised relationships for plant uptake behaviour with literature values (if any);

Although there is a wealth of literature on plant uptake for many contaminants including lead, cadmium, zinc, and agricultural chemicals such as herbicides, pesticides and growth regulators, little or no uptake data are available for many common industrial chemicals (Bell, 1992; Environment Agency, 2006; Martin and Ferguson, 1996). Soil-to-plant concentration factors (CF) obtained from the literature should be carefully evaluated before being used in generic risk assessments (see text box).

Generalised relationships for plant uptake fall into two broad categories:

- Use of simple empirical relationships from the literature relating reported data to one or more factors including K_d and chemical lipophilicity (for example, Baes *et al*., 1984; Travis and Arms, 1988).
- Semi-empirical and mechanistic models from the literature, which are often validated against a limited data set (Environment Agency, 2006; Samsøe-Petersen *et al*., 2003; Bell, 1992).

The CLEA model uses a different approach for inorganic and organic chemicals, see Section 7.2.1 and 7.2.2 respectively.

Reviewing plant uptake studies

The Environment Agency (2006) sets out guidelines for evaluating plant uptake studies from the scientific literature for inorganic and organic chemicals. These guidelines included the article quality (track record of researchers, publication source, detailed method description), scale of study (bench-scale, pot experiments, glass house and field studies), and other factors that might affect the usability of the data (source of contamination, soil type, plant type). Surprisingly, many studies can be rejected because the experimental methodology is unclear and crucial information such as the soil concentration is not reported. Pot experiments, in a growth chamber or indoor greenhouse, are often seen by researchers as a compromise between control and realism. However, pot experiments have a number of known limitations including restricted soil volumes, increased leaching and/or vaporisation under optimum conditions, and potential cross contamination.

7.2.1 Approach for inorganic chemicals

The generic model used to estimate uptake of inorganic chemicals by fruit and vegetables is consistent with the approach used by the Food Standards Agency (FSA) within PRISM Version 2.0 (Thorne *et al*., 2004, 2005). The PRISM model is designed to model the transport of radionuclides in the terrestrial foodchain, in order to assess the potential impacts on food quality of routine or accidental contaminant releases to the atmosphere. It comprises interlinked soil, plant and animal modules (Thorne *et al*., 2005). The model distinguishes between broad categories of plants rather than between individual species or varieties (Thorne *et al.,* 2004).

Equation 7.3 describes the calculation of the soil-to-root concentration factor (CR). This model assumes that the root concentration of an inorganic element is directly proportional to its concentration in soil solution. The chemical concentration in soil solution is determined by the soil-water partition coefficient (K_d) and depends on soil type and pH (see also Chapter 5). The proportionality constant (δ) accounts for a number of variable factors found in plant uptake pot experiments and includes the total plant density (including roots), the depth of pot soil, the duration of the experiment, and an empirical calibration parameter. Generic CR values are adopted for each inorganic element across all crops of interest, on the basis that the range of uncertainty in the CR value for a particular plant is not significantly different from the total range of uncertainty across all plants (Thorne *et al*., 2005).

Equation 7.3

$$CR = \frac{\delta}{(\theta_w + \rho_s K_d)}$$

Where: CR is the soil-to-root concentration factor, mg g^{-1} fw plant per mg g^{-1} dw soil
δ is the soil-plant availability correction, dimensionless
θ_w is the water-filled soil porosity, $cm^3\ cm^{-3}$
ρ_s is the dry soil bulk density, g cm^{-3}
K_d is the soil-water partition coefficient, $cm^3\ g^{-1}$

Note that in Thorne *et al*. (2005), CR is presented in units of Bq kg^{-1} fw plant per Bq kg^{-1} dw soil to estimate the radiation dose.

Table 7.2: Assigning values to δ (Thorne *et al*., 2005)

Category	δ
Very low uptake potential elements (for example, lanthanides and higher actinides)	0.5
Essential to metabolic plant processes or chemically similar to such elements (for example, most common heavy metals including arsenic, cadmium, lead, mercury, and nickel)	5
Unusually high uptake potential elements (for example, selenium)	50

Further analysis of data for 17 elements including lead, nickel and selenium led Thorne *et al*. (2005) to conclude that the inorganic elements considered in the PRISM model could be largely separated into groups of consistent behaviour based on considerations of soil chemistry, plant kinetics and uncertainty. The authors proposed guidelines for determining the value of δ for any inorganic element (see Table 7.2). The CLEA model has adopted these guidelines.

Thorne *et al*. (2005) also considered the transport of inorganic elements within the plant from the root zone to edible fruits, leaves, root storage organs and tubers. They concluded that elements transported within the xylem through passive transpiration should be treated separately from those transported by the **phloem** (which interacts with storage organs like fruits and tubers). The calculated value of *CR* in **Equation 7.3** is corrected to account for the fraction reaching the internal plant system (f_{int}) to derive a soil-to-plant concentration factor (CF) representative of edible plant parts (see **Equation 7.4**). For elements transported by the xylem such as lead and mercury, f_{int} was based on a review of the available uptake literature and is categorised for each produce group using the information in Table 7.3. Therefore in the CLEA model, there are potentially four different f_{int} values to account for the different internal plant partitioning behaviour. For elements transported in the phloem such as arsenic and cadmium, f_{int} was assumed to be 0.5 for any internal plant compartment, to account for their rapid and highly distributed behaviour (Thorne *et al*., 2005).

Equation 7.4

$$CF = CR\, f_{\mathrm{int}}$$

Where:
CF is the soil-to-plant concentration factor for edible fractions, mg g^{-1} fw plant per mg g^{-1} dw soil
CR is the soil-to-root concentration factor, mg g^{-1} fw plant per mg g^{-1} dw soil
f_{int} is the fraction of chemical in the root system reaching edible plant parts including root store, tubers, fruits and shoots [between 0 and 1]

Table 7.3: Correction factors (f_{int}) for root system to edible plant parts

Produce group	Correction factor (f_{int}) between
Green vegetables	Root system to shoot concentration
Root vegetables	Root system to root store concentration
Tuber vegetables	Root system to tuber concentration
Herbaceous fruit	Root system to fruit concentration
Shrub fruit	Root system to fruit concentration
Tree fruit	Root system to fruit concentration

If available, contaminant-specific correction factors for both phloem and xylem transport processes, based on a literature review, will be provided in individual SGV reports.

7.2.2 Approaches for organic chemicals

As part of the ongoing evaluation of the science that underpins the CLEA model, the Environment Agency (2006) reviewed research on screening approaches to plant uptake of organic chemicals from soil. Throughout the study, the pattern of empirical data suggested that organic chemicals behave in a predictable pattern with respect to plant uptake, although the overall performance of screening models was highly inconsistent (Environment Agency, 2006). These findings have been supported by similar authoritative reviews (Samsøe-Petersen *et al*., 2003; Rikken *et al*., 2001).

The Environment Agency (2006) recommended that the CLEA model continue to view generic predictions of plant uptake cautiously and to evaluate results on a substance-by-substance basis. However, for many industrial organic chemicals there have been very few uptake studies and generic models are the only available mechanism for making predictions. In terms of models, Environment Agency (2006) concluded that:

- Ryan *et al*. (1988) could be used for predicting shoot concentrations, provided that aqueous solubility should not be subject to theoretical limits.
- Crop-specific models should be evaluated for estimating root concentrations.
- Crop-specific models should be evaluated for tuber and fruit concentrations, although it was recognised that this is an area for further research.

Further review by the Environment Agency has identified crop-specific models for key fruits and vegetables including carrots (Trapp, 2002), potatoes (Samsøe-Petersen *et al*., 2003; Trapp *et al*., 2007), and tree fruit (Trapp *et al,*. 2003). The allocation of model outputs to the produce groups is summarised in Table 7.4. No suitable models were identified for herbaceous or shrub fruits.

Advice for handling uptake by herbaceous and shrub fruit will be considered on a substance-by-substance basis. Typically, these two produce groups make up about 20 per cent by weight of the fruit and vegetables grown and consumed in residential and allotment settings (see data from Table 4.17 and Table 4.19). In most circumstances, these two groups will make only a small contribution to overall exposure; however, risk assessors should exercise caution when dealing with sites where these fruits constitute a much higher than average proportion of the total fruit and vegetables consumed.

Green vegetables

Ryan *et al*. (1988) set out a screening model for assessing the uptake of non-ionic chemicals from soil. This was intended to provide a simple approach to identifying those chemicals for which plant uptake may be an important pathway for human exposure. The model built on the experimental work of Briggs *et al*. (1982 and 1983) by applying a correction for the reduced availability of chemicals from soil compared to an **aqueous nutrient solution**. It was the best performing model for predicting shoot concentrations across five different case studies (Environment Agency, 2006).[32] The soil-to-plant concentration factor (CF) for green vegetables is calculated using **Equation 7.5**, which is based on the soil-to-plant stem concentration factor (SCF) in the original Ryan *et al*. paper. Care should be taken when applying this approach to chemicals outside of a working range of *log* K_{ow} from zero to four (Environment Agency, 2006b).

Table 7.4: Generic models for predicting soil-to-plant concentration factors according to produce groups

Produce group	Generic model
Green vegetables	Ryan *et al*. (1988)
Root vegetables	Trapp (2002)
Tuber vegetables	Trapp *et al*. (2007)
Herbaceous fruit	See text
Shrub fruit	See text
Tree fruit	Trapp *et al*. (2003)

---

[32] The soil correction term used by Ryan *et al*. (1988) does not take into account the potential partitioning into the vapour phase that is accounted for by the total soil-water partition coefficient (K_{sw}) described in Chapter 5. However, this appeared to have no detrimental impact on the performance of the model for the substances reviewed by Environment Agency (2006).

Equation 7.5

$$CF_{Green\,Vegetables} = (10^{0.95\log K_{ow}-2.05} + 0.82)(0.784 \times 10^{-0.434(\log K_{ow}-1.78)^2/2.44})\left(\frac{\rho_s}{\theta_w + \rho_s K_{oc} f_{oc}}\right)$$

where CF is the calculated soil-to-plant concentration factor for green vegetables, mg g^{-1} fw plant over mg g^{-1} dw soil

K_{ow} is the octanol-water partition coefficient for the chemical, dimensionless

ρ_s is the dry soil bulk density, g cm^{-3}

θ_w is the soil-water content by volume, cm^3 cm^{-3}

K_{oc} is the organic carbon-water partition coefficient for the contaminant, cm^3 g^{-1} dw

f_{oc} is the fraction of organic carbon in the soil, dimensionless

Root vegetables

The Environment Agency (2006) consistently observed that equilibrium-based plant uptake models over-predicted observed uptake in a number of case studies. Trapp (2002) proposed a dynamic root uptake model to address this, noting that for thicker roots and those chemicals with high K_{ow} values, real root concentrations could be far below those observed at chemical equilibrium. The model proposes that uptake by roots is due to diffusion through the peel and by preferential partitioning of organic chemicals in the xylem stream to cell lipids. The partitioning coefficient for a chemical between root and water (K_{rw}) can be estimated using **Equation 7.6** and is similar to that used by the *Technical Guidance Document for Risk Assessment* (ECB, 2003).

The bulk of the carrot core will be contaminated from the xylem stream and the dynamic (steady-state) root concentration will be a balance of **transpiration rate** and growth rate using **Equation 7.7** (Trapp, 2002). Figure 7.1 shows a comparison between the outputs of Trapp (2002) with the equilibrium partitioning model by Trapp and Matthies (1995) using case study data from uptake of different chemicals by carrot (Environment Agency, 2006). Trapp (2002) significantly reduces the over-predicted uptake as the chemical lipophilicity increases.

Equation 7.6

$$K_{rw} = \frac{W}{\rho_p} + \frac{L}{\rho_p} a K_{ow}^{b}$$

Where: K_{rw} is the equilibrium partition coefficient between root and water, cm^3 g^{-1} fw
W is the root water content, g g^{-1} [0.89]
ρ_p is the plant root density, g cm^{-3} [1]
L is the root lipid content on a mass basis, g g^{-1} [0.025]
a is the density correction factor between water and octanol, unitless [1.22]
K_{ow} is the octanol-water partition coefficient, dimensionless
b is the correction coefficient for roots, unitless [0.77]

Note that the original equation presented in Trapp (2002) neglects plant root density.

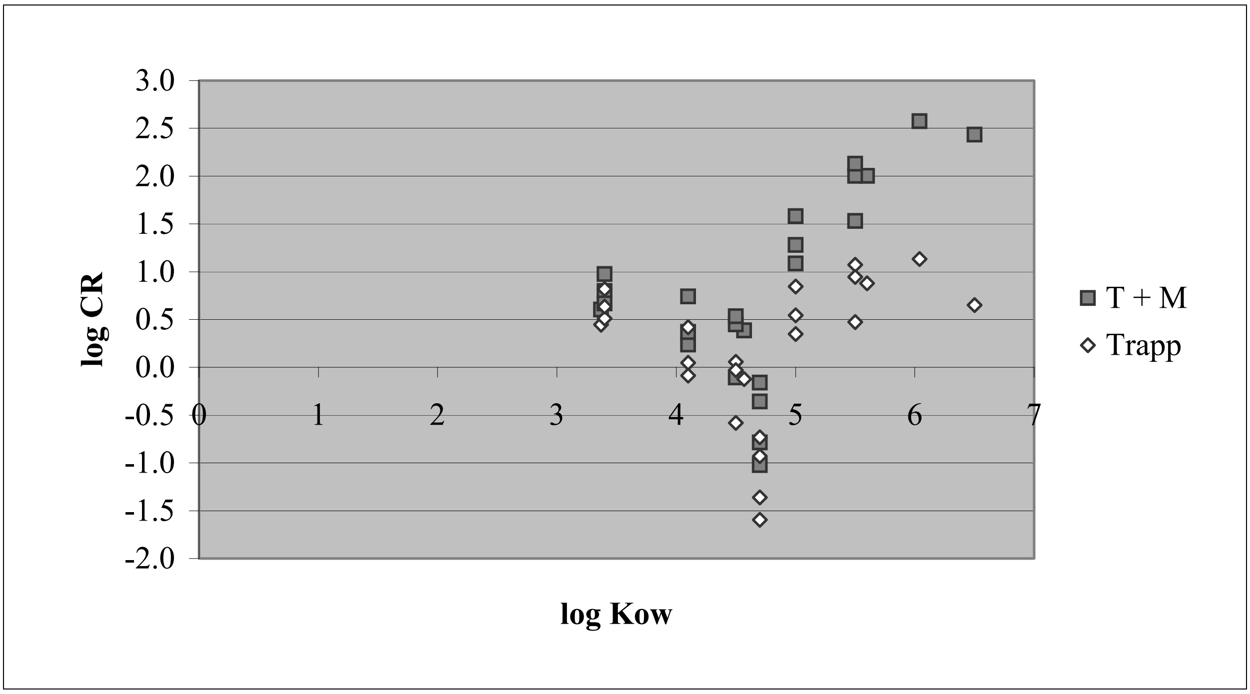


Figure 7.1: Comparison of predicted versus observed plant uptake of various chemicals by carrot using the Trapp and Matthies (1995) and Trapp (2002) models. Log CR is the logarithm of the ratio of predicted to observed plant concentration (Environment Agency, 2006)

Equation 7.7

$$CF = \frac{(Q/K_d)}{\frac{Q}{K_{rw}} + (k_g + k_m)\rho_p V}$$

Where: CF is the calculated soil-to-plant concentration factor for root vegetables, mg g^{-1} fw plant over mg g^{-1} dw soil
K_d is the sorbed soil-water partition coefficient, cm^3 g^{-1} dw
K_{rw} is the equilibrium partition coefficient between root and water, cm^3 g^{-1} fw
Q is the transpiration stream flow rate, cm^3 day^{-1} [1,000]
ρ_p is the plant root density, g fw cm^{-3} [1]
V is the root volume, cm^3 [1,000]
k_g is the first order growth rate constant, day^{-1} [0.1]
K_m is the first order metabolism rate constant, day^{-1} [0]

Note that the original equation presented in Trapp (2002) neglects plant root density.

Tuber vegetables

The potato is the most important vegetable grown in Europe and is a major component of the European diet (Samsøe-Petersen *et al.*, 2003; Trapp, 2002). The potato is a tuber, which is a storage organ of the stem, and not part of the root system (Trapp *et al.*, 2007). Generalised root uptake models are not applicable to the potato, which receives contamination either through the phloem or by diffusion through the skin

(Environment Agency, 2006; Samsøe-Petersen *et al*., 2003). Trapp *et al*. (2007) concluded that for lipophilic organic chemicals, transport in the phloem is negligible.

There have been two crop-specific models proposed for potato based on diffusion of contamination into the tuber through the skin (Samsøe-Petersen *et al*., 2003; Trapp *et al*., 2007). Trapp *et al*. (2007) considered the potato to be a sphere with the soil-to-plant concentration factor (CF) described as the dynamic equilibrium point where chemical diffusion into and out of the potato is balanced. Chemical diffusion is assumed to occur only in the water-filled pore spaces within the potato (that is, diffusion through the solid material and air-filled pores is taken to be negligible).

Equation 7.8 calculates the potato to water partition coefficient (K_{pw}) based on the lipid and carbohydrate content of the plant matter (Trapp *et al*., 2007). The carbohydrate water partition coefficient (K_{ch}) is calculated from chemical lipophilicity according to Chiou *et al*. (2001) as shown in Table 7.5.

Table 7.5: Values for the carbohydrate to water partition coefficient (K_{ch}) after Chiou *et al*. (2001)

Chemical *Log* K_{ow}	Chemical K_{ch}
< 0	0.1
≥ 0 but < 1	0.2
≥ 1 but < 2	0.5
≥ 2 but < 3	1
≥ 3 but < 4	2
≥ 4	3

Equation 7.8

$$K_{pw} = \frac{W}{\rho_p} + (f_{\mathrm{ch}} K_{ch}) + \frac{L}{\rho_p} a K_{ow}^{b}$$

Where: K_{pw} is the equilibrium partition coefficient between potato and water, $cm^3\ g^{-1}$ fw
W is the water content of potato, $g\ g^{-1}$ [0.79][33]
ρ_p is the plant tuber density, $g\ cm^{-3}$ [1]
f_{ch} is the fraction of carbohydrates in the potato, unitless [0.209][34]
K_{ch} is the carbohydrate-water partition coefficient, $cm^3\ g^{-1}$ fw
L is the lipid content of potato on a mass basis, $g\ g^{-1}$ [0.001]
a is the density correction factor between water and octanol, unitless [1.22]
K_{ow} is the octanol-water partition coefficient for the chemical, dimensionless
b is the correction coefficient for roots, unitless [0.77]

Note that the original equation presented in Trapp (2007) neglects plant root density.

The steady-state soil-to-potato concentration factor (CF) is the balance of the rate of diffusion into the potato (k_1) and out of the potato (k_2), correcting for dilution due to plant growth (k_g), and is shown in **Equation 7.9**. Using a radial diffusion model, the rate constants into and out of the potato can be estimated from an assumed potato radius, the effective rate of diffusion through the plant matrix, and the equilibrium partitioning between the plant matrix and soil pore water (see **Equation 7.10** and

---

[33] The value used is consistent with the value for tuber vegetables in Table 7.1.

[34] The value in Trapp *et al.* (2007) has not been used, as this is based on the carbohydrate content of barley. Instead, it is assumed that the carbohydrate content is the remaining content after subtraction of the water and lipid content.

Equation 7.11). Trapp *et al*. (2007) found good agreement between model predictions and the observed experimental concentrations of several PAHs.

Equation 7.9

$$CF_{Tuber\ Vegetables} = \frac{k_1}{k_2 + k_g}$$

Where: CF is the calculated soil-to-plant concentration factor for tuber vegetables, mg g^{-1} fw plant over mg g^{-1} dw soil
k_1 is the rate of chemical flux into the potato, $hour^{-1}$ [see Equation 7.11]
k_2 is the rate of chemical flux out of the potato, $hour^{-1}$ [see Equation 7.10]
k_g is the exponential rate of growth of the potato, $hour^{-1}$ [0.0014] [35]

Equation 7.10

$$k_2 = \frac{23\left(\dfrac{3600 D_{water} (W^{7/3}/\rho_p)}{K_{pw}}\right)}{R^2}$$

Where: k_2 is the rate of chemical flux out of the potato, $hour^{-1}$
D_{water} is the chemical diffusion coefficient in water, $m^2\ s^{-1}$
W is the water content of potato, g g^{-1} [0.79]
ρ_p is the potato tissue density, g cm^{-3} [1]
R is the radius of the potato, m [0.04]
K_{pw} is the equilibrium partition coefficient between potato and water, $cm^3\ g^{-1}$ fw

Note, the original equation presented in Trapp (2007) neglects potato tissue density.

Equation 7.11

$$k_1 = k_2\left(\frac{K_{pw}}{K_{sw}}\right)$$

Where: k_1 is the rate of chemical flux into the potato, $hour^{-1}$
k_2 is the rate of chemical flux out of the potato, $hour^{-1}$
K_{pw} is the equilibrium partition coefficient between potato and water, $cm^3\ g^{-1}$ fw
K_{sw} is the total soil-water partition coefficient, $cm^3\ g^{-1}$

Tree fruit

Many studies on the uptake of organic chemicals into plants have focused on accumulation within the leaf (Environment Agency, 2006; Trapp *et al*., 2003). However, there are several features of fruit trees that suggest that persistent organic chemicals may accumulate in the fruit, including the increased size and depth of the root system and the longevity of the trees themselves (Trapp *et al*., 2003). Fruit are often eaten with little or no preparation and their smaller surface-to-volume ratios restrict loss mechanisms including volatilisation.

---

[35] Calculated from a half-life of 20 days using the growth curve data for potato plants used in the PRISM model (Thorne *et al*., 2004b)

Trapp *et al*. (2003) proposed a fruit tree model based on chemical equilibrium partitioning between wood and water. The ratio between a chemical's concentration in wood and water (K_{wood}) is correlated to chemical lipophilicity using **Equation 7.12**. The steady-state concentration of the chemical within the woody stem is the mass balance of the flux into the stem via the **xylem** and out of the stem after equilibration, also taking into account dilution due to growth (Trapp *et al*., 2003). Exchange with the air and the bark and flow through the phloem are neglected. The chemical concentration in the xylem (C_{Xy}) flowing into the stem is calculated using **Equation 7.13** and the steady-state concentration in the stem (C_{stem}) using **Equation 7.14**.

Equation 7.12

$$\log K_{wood} = -0.27 + 0.632 \log K_{ow}$$

Where: K_{wood} is the wood-water partition coefficient, mg g^{-1} dw wood per mg cm^{-3} water
K_{ow} is the octanol-water partition coefficient, unitless

Equation 7.13

$$C_{Xy} = \left(\frac{C_s}{K_{sw}}\right) 0.756 e^{\frac{-(\log K_{ow}-2.50)^2}{2.58}}$$

Where: C_{Xy} is the chemical concentration in the xylem sap, mg cm^{-3}
C_s is the total soil concentration, mg g^{-1} dw
K_{sw} is the total soil-water partition coefficient, cm^3 g^{-1}
K_{ow} is the octanol-water partition coefficient, unitless

Equation 7.14

$$C_{stem} = \frac{C_{Xy}\dfrac{Q}{M}}{\dfrac{Q}{K_{wood}M} + k_e + k_g}$$

Where: C_{stem} is the chemical concentration in the woody stem, mg g^{-1} dw
C_{Xy} is the chemical concentration in the xylem sap, mg cm^{-3}
Q is the transpiration stream flow rate, cm^3 $year^{-1}$ [25,000,000] [35]
M is the mass of the woody stem, g dw [50,000] [36]
K_{wood} is the wood-water partition coefficient, mg g^{-1} dw wood per mg cm^{-3} water
k_e is the rate of chemical metabolism, $year^{-1}$ [0]
k_g is the rate of dilution due to wood growth, $year^{-1}$ [0.01]

Transport from the stem into the fruit can occur via the phloem and xylem sap and with the exception of very polar compounds, the chemical concentrations in each stream are assumed to be similar (Trapp *et al*., 2003). Phloem flow rate into the fruit is assumed to be ten times the dry matter content of the fruit, since the phloem consists of about ten per cent dry matter. Xylem flow rate is about the same as that of the phloem to replace water lost through the skin of the fruit through evaporation. The chemical flow into the fruit can then be estimated by assuming a chemical equilibrium between the concentration in the woody stem (C_{stem}) and the concentration in the xylem

---

[36] Based on empirical measurements of water uptake by a mature apple tree (Green *et al*., 2003) and the density of apple wood (Simetric, 2007)

and phloem (Trapp *et al.*, 2003). The resulting soil-to-tree fruit concentration factor (CF) can then be calculated using **Equation 7.15**.

Equation 7.15

$$CF_{Tree\ Fruit} = \frac{\left(\left(M_f Q_{fruit} DM_{fruit} \right) \frac{C_{stem}}{K_{wood}} \right) / M_f}{C_s}$$

Where: *CF* is the calculated soil-to-plant concentration factor for tree fruit, mg g^{-1} fw plant over mg g^{-1} dw soil
M_f is the mass of fruit, g fw [1]
Q_{fruit} is the water flow rate per unit mass of fruit, cm^3 g^{-1} fw [20]
DM_{fruit} is the dry matter content of fruit, g g^{-1} [0.16] [36]
C_{stem} is the chemical concentration in the woody stem, mg g^{-1} dw
K_{wood} is the wood-water partition coefficient, mg g^{-1} dw wood per mg cm^{-3} water
C_s is the total chemical concentration in soil, mg g^{-1} dw

7.2.3 Calculating the chemical intake rate

The chemical exposure rate for the consumption of homegrown produce is calculated in the CLEA model using **Equation 7.16**. The soil-to-plant concentration factors are described in Sections 7.1 and 7.2 above. The relevant exposure characteristics are described in Section 4.4. Note that **Equation 7.16** assumes that CF is calculated on a fresh weight plant basis.

Equation 7.16

$$IR = \sum_{all\ produce\ groups} C_s CF_x CR_x\ BW\ HF_x$$

Where: IR is the chemical intake rate from consumption of homegrown produce, mg day^{-1}
C_s is the total concentration of the chemical in soil, mg g^{-1} dw
CF_x is the soil-to-plant concentration factor for each produce group, mg g^{-1} fw per mg g^{-1} dw
CR_x is the food consumption rate per unit body weight for each produce group, g fw kg^{-1} bw day^{-1}
BW is the body weight, kg
HF_x is the homegrown fraction for each produce group, dimensionless

x represents the six produce groups described in Table 4.16

8 Skin uptake from soil/dust

This exposure pathway considers the dermal uptake of chemicals from soil and indoor dust during and following contact with contaminated media. Dermal exposure to chemicals is normally a more significant problem for occupational health than it is for environmental health, because of the frequency with which workers come into contact with pure chemicals and strong aqueous solutions. However, it may be an important exposure pathway for persistent and highly lipophilic chemicals in soil. In contrast to the other pathways considered in the CLEA model, this exposure route is measured as uptake rather than intake (see Section 2.1).

8.1 Overview

This pathway considers the potential transfer of soil contaminants to adults and children through skin contact with contaminated soil and dust. Estimating exposure by this route depends on three elements (Paustenbach, 2000; USEPA, 1992, 2006):

- exposed skin area and the degree of contact with soil or dust;
- amount of soil adhering to the skin;
- amount of contamination absorbed through the skin.

Exposed skin area depends on the total body surface area minus the assumed clothing coverage, taking into account the typical amount of contact with dirty surfaces during different activities. This exposure characteristic is described in Section 4.4.2.

In Section 8.1.1 and 8.1.2, the remaining factors are discussed based on a review of the available literature. The CLEA model does not consider skin contact with contaminated water (such as swimming in a lake or pond or washing with a contaminated private water supply).

8.1.1 How much soil adheres to the skin?

Exposure to soil contamination via the dermal pathway is particularly sensitive to the amount of soil adhered to, or in intimate contact with, the skin over the contact period. Despite a number of recent studies, there is still considerable uncertainty in the soil-to-skin adherence factors used to assess dermal exposure (USEPA, 2004a). Not surprisingly, soil loading is found to be highly variable. USEPA (2004a and 2006) have undertaken a further review of soil-to-skin adherence factors and have revised their opinion on the recommendations made in USEPA (1992).

Studies on soil adherence have shown that it varies with soil properties (especially texture and moisture content), the parts of the body examined, and the types of activities undertaken with each study (USEPA, 2004a and 2006). The CLEA model uses the soil-to-skin adherence factors (AF) in Table 8.1 as default values in generic exposure assessments. They have been calculated as a weighted average of the experimental values found for different parts of the body described in USEPA (2004a) and based on the exposed body areas in Table 4.8 and Table 4.11 according to age and land use. That is, the average AF for children and adults reflects the average of the experimental factors determined for each body part (for example, hands, face, lower leg) taking into account the proportion of exposed area accounted for by each body part. All AF values are significantly lower than estimates of **monolayer saturation** for different soil types (USEPA, 2004a).[37]

For children up to the age of sixteen, the default AF values distinguish between indoor and outdoor exposure activities in a residential land use scenario. The indoor AF of 0.06 mg cm^{-2} is based on the 95th percentile of experimental studies (Holmes *et al*., 1999). This value is consistent with the recommendation in USEPA (2004a).

USEPA (2004a) noted that establishing a reasonable worst-case activity for children in a residential setting was more difficult than for adults. An outdoor AF of 1 mg cm^{-2} is consistent with the recommendations in USEPA (1992); however, it is higher than the value chosen in 2004 of 0.2 mg cm^{-2}, which is the geometric mean of observed soil adherence factors (USEPA, 2004a). An AF of 1 mg cm^{-2} lies between the 95th percentile adherence for dry soil (0.4 mg cm^{-2}) and the 95th percentile for wet soil (3.3 mg cm^{-2}) and is considered reasonably protective of soil conditions throughout the year. In using the geometric mean and not the 95th percentile value of 3.3 mg cm^{-2} from the same study, USEPA concludes that this is at the high end of soil contact activity (USEPA, 2004a).

For adults in an outdoor residential or allotment setting, an AF value of 0.3 mg cm^{-2} has been selected from an experimental study of gardeners (Holmes *et al*., 1999). This value is higher than the default value chosen by USEPA (2004a) of 0.07 mg cm^{-2}, because in the land use scenarios described in Chapter 3 the assumption is that gardening is a typical activity and therefore the 95th percentile value from Holmes *et al*. (1999) has been used. USEPA (2004a) concluded that gardening is an unusual high-end activity and therefore chose a central tendency weighted value.

No indoor studies for adults have been identified other than for specialist groups such as those undertaking Tae Kwon Do (Kissel *et al.,* 1996). Therefore, the child indoor AF values have been applied to adults, although it is recognised that this is likely to be a conservative assumption for adults.

Table 8.1: Default values for soil-to-skin adherence factors by age and land use

		Soil-to-skin adherence factors (mg soil cm^{-2} skin)	
Land use		**Child**	**Adult**
Residential			
	Indoor	0.06	0.06
	Outdoor	1	0.3
Allotments		1	0.3
Commercial		-	0.14

For the commercial and industrial land use, an adult AF value of 0.14 mg cm^{-2} is used for both indoor and outdoor exposure, which is the geometric mean of weighted adherence factors (excluding feet) from a study of groundskeepers by Kissel *et al.* (1996). There is an absence of data for the typical office worker who may spend their lunch hour outdoors, and it is unlikely that the activities undertaken by groundskeepers in campus grounds or an arboretum are typical scenarios. However, it is considered more prudent to use the 95th percentile of this data, since Kissel *et al.* (1996) reported that those studied only “intermittently used gloves”. Again, it is recognised that this assumption is tentative and almost certainly conservative.

---

[37] Monolayer saturation assumes that the skin is covered with a single layer of tightly packed soil particles. In the case of soil applications of less than a monolayer, the space between particles increases and the incomplete coverage results in a lower diffusive flux of contamination from the soil to the skin (USEPA, 1992).

8.1.2 How much contamination can the skin absorb?

Skin is composed of two layers: the ***epidermis***, a non-vascular layer about 100 μm thick, and the ***dermis***, a highly vascularised layer about 500-3,000 μm thick. The outermost layer of the *epidermis*, the *stratum corneum* is about 10-40 μm thick. This layer is thought to provide the major barrier to the absorption of chemicals into the systemic circulation from skin contact (USEPA, 1992).

The simplest way to describe the process of chemical absorption is by diffusion from the soil in contact with the skin through the *stratum corneum* and into the underlying body tissue (USEPA, 1992). The concentration gradient from the soil adjacent to the skin to the body tissue beneath the *stratum corneum* is the driving force for dermal absorption. Since for most contaminants, the concentration in body tissues is negligible, the rate of absorption is approximately proportional to the soil concentration in the adhered layer (USEPA, 1992; Paustenbach, 2000).

A number of factors affect the bioavailability of soil and indoor dust contaminants to skin absorption, including ageing, soil type and lipophilicity of the contaminant (Shu *et al*., 1988). Some researchers have suggested that the contaminants most likely to be absorbed through the *stratum corneum* are those with a high solubility in both fats and water (USEPA, 1992). The absorption process is clearly complicated by a number of competing factors; for example, although lipophilic compounds more readily penetrate through the *stratum corneum*, they are also more likely to be strongly adsorbed within the soil (McKone, 1990). Lighter organic compounds may diffuse away from the skin surface through the soil layer and be lost by volatilisation (USEPA, 1992).

There are major uncertainties in our understanding of the extent to which a chemical is absorbed by the skin and the extent to which it partitions from soil to skin (USEPA, 1992, 2004a). USEPA (2004a) recognises the need for simplified calculations at the generic screening level for soil and acknowledges the lack of underpinning experimental data to adequately quantify the variation in soil-to-skin permeability rates for many chemicals and soil properties. An absorbed fraction per event approach provides a good balance to these two factors.

The dermal absorption fraction (ABS_d) is chosen on a contaminant-by-contaminant basis, based on a review of the scientific literature. The approach to estimating human dermal exposure to contaminants in soil using the $\mathrm{ABS_d}$ does not explicitly use contact time. However, contact time is clearly important in establishing the $\mathrm{ABS_d}$ according to the reported experimental conditions. Ideally, there should be close agreement between the contact time used in the exposure assessment scenario and in the experimental work. If good time-dependent data is available, the $\mathrm{ABS_d}$ value for a contact time of 12 hours is chosen as the default for that chemical.

USEPA (2004a, 2004b) recommends an $\mathrm{ABS_d}$ value for only a limited number of substances based on a review of experimental data. This reflects a wider paucity of data for many organic and inorganic chemicals. The CLEA model therefore uses a generic default $\mathrm{ABS_d}$ value of 0.1 for all organic chemicals and zero for inorganic chemicals in the absence of a literature value. This approach is broadly consistent with the USEPA view, although it applies to both volatile and semi-volatile compounds (USEPA, 2004a). The available $\mathrm{ABS_d}$ values are summarised in Table 8.2.

Table 8.2: Experimentally derived values for the dermally absorbed fraction (ABS_d) from USEPA (2004a, 2004b)

Chemical	**ABS_d (dimensionless)**
Arsenic	0.03
Cadmium	0.001
Benzo(a)pyrene and other PAHs	0.13
Aroclors 1254/1242 and other PCBs	0.14
Pentachlorophenol	0.25
Chlordane	0.04
2,4-Dichlorophenoxyacetic acid	0.05
DDT	0.03
TCDD and other dioxins	0.03
(where soil organic content is above 10%)	0.001
Lindane	0.04
Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)	0.0015
Thiodiglycol	0.0075
Trinitrobenzene	0.019
2,4-Dinitrotoluene (2,4-DNT)	0.102
2,6-Dinitrotoluene (2,6-DNT)	0.099
2-Amino-4,6-dinitrotoluene (2A, 4,6-DNT)	0.006
4-Amino-2,6-dinitrotoluene (4A, 2,6-DNT)	0.009
2,4-Diamino-6-nitrotoluene (2,4-DA-6-NT)	0.011
2,6-Diamino-4-nitrotoluene (2,6-DA, 4-NT)	0.005
Trinitrotoluene (TNT)	0.032
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	0.006
Tetryl (N-methyl-N, 2,4,6-tetranitrobenzamine)	0.00065

8.2 Calculating the chemical uptake rate

The chemical uptake rate for dermal contact with soil and dust is calculated in the CLEA model for outdoor and indoor exposure using **Equation 8.1** and **Equation 8.2** respectively. The exposed skin area is described in Section 4.4.2. The soil-to-skin adherence factor (AF) and the dermal absorption fraction (*ABS_d*) are discussed in Section 8.1. Transport factor (TF) is discussed in Section 4.3.2. In deriving SGVs, the number of daily soil contact events is assumed to be one.

Equation 8.1

$$IR = C_s \; n \; AF \; ABS_d \; A_{skin} \quad \times \quad \frac{1}{1000} g \, mg^{-1} \quad \times \quad 10000 \, cm^2 m^{-2}$$

Where: IR is the chemical uptake rate from outdoor dermal contact with soil, mg day^{-1}
C_s is the total concentration of the chemical in soil, mg g^{-1} dw
AF is the soil-to-skin adherence factor, mg cm^{-2}
ABS_d is the dermal absorption fraction, dimensionless
A_{skin} is the exposed skin area, m^2
n is the number of daily soil contact events, day^{-1}

Equation 8.2

$$IR = C_s \; TF \; n \; AF \; ABS_d \; A_{skin} \quad \times \quad \frac{1}{1000} g \, mg^{-1} \quad \times \quad 10\,000 \; cm^2 m^{-2}$$

Where: IR is the chemical uptake rate from indoor dermal contact with soil, mg day^{-1}
C_s is the total concentration of the chemical in soil, mg g^{-1} dw
TF is the soil to indoor dust transport factor, g g^{-1} dw
AF is the soil-to-skin adherence factor, mg cm^{-2}
ABS_d is the dermal absorption fraction, dimensionless
A_{skin} is the exposed skin area, m^2
n is the number of daily soil contact events, day^{-1}

9 Inhalation of dusts

This exposure pathway considers the inhalation of respirable dust from contaminated soils by children and adults in both ambient and indoor air. Long-term background air concentrations of localised soil-derived dust are typically low in most residential and commercial settings because of the degree of land cover (either vegetative or hard standing). However, it may be an important pathway for metal and persistent highly lipophilic chemicals where the main risk to health arises from the inhalation route.

This pathway considers long-term exposure levels arising principally from wind action. It does not take into account short-term events such as mechanical erosion, although these may be important when evaluating short-term or acute risks to health.

9.1 Overview

Dust is a complex and highly heterogeneous mixture of components including local soil particles, clothing fibres, ambient particulate emissions (from vehicles and stacks), hair, fibres, moulds, pollen, bacteria, and skin (Oomen and Lijzen, 2004; Paustenbach *et al*., 1997). In assessing exposure from land contamination, the CLEA model only considers the component arising from local soil including mineral components, organic matter, and free products such as powders or loose fibrous materials. See Section 4.3.2 for a discussion about the fraction of outdoor soil contributing to indoor dust.

Not all dust particles are considered to be biologically relevant to assessing adverse health effects. It is generally assumed that although particles less than 150 μm in diameter can be breathed in by adults and children, virtually all particles greater than 10 μm will be captured in the nose or throat and thus not transferred to the lung (Paustenbach, 2000).[38] Most authoritative bodies consider the particulate matter concentration in air with a cut-off diameter of either 10 μm, or even lower at 2.5 μm, as important indicators of dust exposure (Oomen and Lijzen, 2004; USEPA, 1996). Chemicals within the finer fractions are likely to be more bioavailable than coarser particles, because of the length of time they remain trapped in the lung wall (Paustenbach, 2000).

Dust can be generated from bare soil surfaces by a variety of activities including wind erosion, mechanical attrition such as the movement of vehicles across open ground, by localised working of soil such as digging or raking and by the actions of walking or running (Cowherd *et al*., 1985; Simmonds *et al*., 1995; Oatway and Mobbs, 2003). Emissions from bare soil depend on many factors such as the source area, its surface roughness, soil erodibility (itself depending on factors such as moisture content), wind speed and the degree of building or vegetative cover (Cowherd *et al*., 1985; Simmonds *et al*., 1995; USEPA, 1996). Once lifted by disturbance, particles less than 50 μm in diameter can remain suspended for significant periods of time (Simmonds *et al*., 1995).

It is very difficult to assess dust emission and deposition rates from generic site conditions and activities, leading to the introduction of considerable uncertainties into subsequent modelling (Cowherd *et al*., 1985; Simmonds *et al*., 1995). Simmonds *et al*. (1995) concluded that there is insufficient data to develop detailed models for man-made resuspension of soil dust, although a higher dust concentration in air (the **dust loading**) could result from localised activities such as vehicle movements and

---

[38] Although not transferred to the lung, these particles are likely to be entrained in mucus and ingested. Such particles therefore contribute to the amount of soil ingested by an adult or child and are taken into account in the setting of soil ingestion rates (see Chapter 6).

ploughing. The authors suggested a value of 10,000 μg m^{-3} as a representative dust loading value for estimating individual exposure during man-made surface disturbances although such exposures would be for limited time periods (Simmonds *et al*., 1995). Oatway and Mobbs (2003) suggested generic dust loading values for man-made disturbances of 500 μg m^{-3} and 10,000 μg m^{-3} for a residential and school land use and an agricultural land use respectively. These concentrations are higher than indoor and outdoor data reviewed by Oomen and Lijzen (2004) for residential, commercial and school land uses (mean PM_{10} concentrations between 12.6 and 157 μg m^{-3}).

Van den Berg (1994) applied dust loading factors of 53 and 70 μg m^{-3} for indoor and outdoor air respectively in the generic model C-SOIL; the values are based on the assumptions of Hawley (1985). Paustenbach *et al*. (1997) recommended an indoor dust level of 50 μg m^{-3} in the absence of site-specific information. Oomen and Lijzen (2004) recommended a mean PM_{10} concentration of 60 μg m^{-3} for inside homes and moderately crowded places and 100 μg m^{-3} for very crowded places such as classrooms.

Transport of particulates in the atmosphere can be described by factors including the plume properties, wind speed and direction, the particle size composition and the degree of atmospheric turbulence (Cowherd *et al*., 1985). The conventional approach is to estimate firstly the plume rise and then the dispersion in three dimensions using approximations such as the **Gaussian distribution** (LaGrega *et al*., 1994). However, this technique is mainly applicable to point source emissions and is not valid for large area sources such as contaminated soils. According to some commentators, this exposure pathway has amongst the lowest level of modelling uncertainty (Paustenbach, 2000). However, while dispersion models for stack emissions take into account ever-increasingly complex computer representations of wind patterns and landscape features, there remains doubt over their reliability for receptors close to and/or living on the source site (LaGrega *et al*., 1994).

9.2 Estimating ambient dust concentrations

Soil-derived dust concentrations in ambient air are estimated in the CLEA model using the generic approach proposed by Cowherd *et al*. (1985) for wind erosion. The US Environmental Protection Agency, in the development of soil screening levels, has adopted a similar approach (USEPA, 1996 and 2002a).

Equation 9.1 shows the calculation of the **particle emission factor** (PEF), which represents an estimate of the relationship between the concentration of a contaminant in soil and its concentration in air as a consequence of dust resuspension (USEPA, 2002a). Dust particles are assumed to be less than 10 μm in diameter. Generic values for the **air dispersion factor** (Q/C_{wind}) and the PM_{10} **emission flux** (J_w) are discussed in Section 9.2.1 and 9.2.2 respectively.

Equation 9.1

$$PEF = Q / C_{wind} \times \frac{1}{J_w}$$

Where: PEF is the particulate emission factor, m^3 kg^{-1}
Q/C_{wind} is the air dispersion factor, g m^{-2} s^{-1} per kg m^{-3}
J_w is the PM_{10} emission flux, g m^{-2} s^{-1}

9.2.1 Air dispersion factors for UK cities

The Environment Agency's Air Quality Modelling and Assessment Unit (AQMAU) has estimated generic air dispersion factors (Q/C_{wind}) for thirteen UK cities and the data is presented in Table 9.1. The cities considered were: Aberdeen, Belfast, Birmingham, Cardiff, Edinburgh, Glasgow, Ipswich, London, Manchester, Newcastle, Nottingham, Plymouth and Southampton. Cities were selected to provide a good geographical spread around the UK and to potentially represent different climate zones.

The USEPA dispersion model AERMOD PRIME (07026) was used to model an emission of contaminants at a rate of 1 g m^{-2} s^{-1} from an area source. Annual mean air concentrations (kg m^{-3}) of contaminants at two receptor heights (0.8 m and 1.6 m) were predicted at a grid of receptors over four different sizes of source area (from 0.01 to two hectares). Five years of hourly meteorological data at weather stations nearest to these cities were used for the modelling. The following assumptions were made:

- each contaminant area source was assumed to be square;
- hourly sequential meteorological data for the period 1992-1997 is representative of typical conditions;
- contaminant emission was modelled as a ground level release of neutrally buoyant gas and emission rates were constant across the source area;
- no terrain effect, nor building downwash effect, was considered;
- surface roughness of 0.1 m was used for the thirteen cities (representative of a suburban location).

Table 9.1: Estimated mean annual air dispersion factors (Q/C_{wind}) for thirteen UK cities and different source areas at 0.8 m and 1.6 m above the ground

	Mean annual air dispersion factor (g m^{-2} s^{-1} per kg m^{-3})							
	Receptor height (0.8 m)				Receptor height (1.6 m)			
	Source area (ha)				Source area (ha)			
City	**0.01**	**0.05**	**0.5**	**2**	**0.01**	**0.05**	**0.5**	**2**
Aberdeen	3.1E+03	6.4E+02	1.7E+02	1.0E+02	2.8E+04	2.5E+03	3.6E+02	1.7E+02
Belfast	3.0E+03	6.7E+02	1.9E+02	1.2E+02	2.8E+04	2.5E+03	3.8E+02	1.9E+02
Birmingham	2.8E+03	6.1E+02	1.7E+02	1.1E+02	2.6E+04	2.3E+03	3.5E+02	1.7E+02
Cardiff	3.4E+03	7.7E+02	2.3E+02	1.4E+02	3.2E+04	2.7E+03	4.5E+02	2.3E+02
Edinburgh	3.1E+03	6.7E+02	1.9E+02	1.1E+02	2.8E+04	2.5E+03	3.8E+02	1.8E+02
Glasgow	3.0E+03	6.4E+02	1.7E+02	1.0E+02	2.7E+04	2.4E+03	3.6E+02	1.7E+02
Ipswich	3.3E+03	7.8E+02	2.4E+02	1.5E+02	3.2E+04	2.7E+03	4.6E+02	2.4E+02
London	2.5E+03	5.1E+02	1.3E+02	7.8E+01	2.3E+04	2.1E+03	2.9E+02	1.3E+02
Manchester	2.9E+03	6.1E+02	1.6E+02	9.7E+01	2.8E+04	2.4E+03	3.4E+02	1.6E+02
Newcastle [1]	2.4E+03	5.0E+02	1.2E+02	6.8E+01	1.9E+04	2.0E+03	2.8E+02	1.2E+02
Nottingham	3.2E+03	7.6E+02	2.3E+02	1.4E+02	3.0E+04	2.6E+03	4.4E+02	2.3E+02
Plymouth	3.5E+03	8.4E+02	2.7E+02	1.7E+02	3.2E+04	2.8E+03	5.0E+02	2.7E+02
Southampton	2.2E+03	4.9E+02	1.3E+02	7.1E+01	1.8E+04	1.9E+03	2.8E+02	1.3E+02

[1] Values used for the derivation of SGVs

In the derivation of SGVs, the mean annual Q/C_{wind} data for Newcastle has been used. Newcastle was selected because its data is close to the 10th percentile value for mean values of all thirteen UK cities modelled. Considering the mean dispersion factors for each city across five years and for each area source, the standard deviation about the mean was typically five per cent and in extreme cases approximately ten per cent.

A receptor height of 0.8 m is representative of young children (aged zero to six years) and a height of 1.6 m is representative of older children and adults. All dispersion factors decrease with increased source area. According to the generic land use descriptions in Chapter 3, the source area equals 0.01, 0.5, and 2 ha for the residential, allotment and commercial scenarios respectively.

9.2.2 PM_{10} emission fluxes for generic soil types

Cowherd *et al*. (1985) described an approach to characterising wind erosion potential for contaminated surfaces and this is set out in **Equation 9.2** for surfaces with unlimited erosion potential. Only wind erosion is considered in the calculation of the PM_{10} emission flux for generic assessment in the CLEA model.

The fraction of outdoor surface cover (V) depends on land use and includes grass and other vegetation and hard standing. According to the standard land use descriptions in Chapter 3, V equals 0.75 for the residential scenario, 0.5 for the allotment scenario, and 0.8 for the commercial scenario.

Equation 9.2

$$J_w = 0.036\,(1-V)\,(\frac{u}{u_t})^3\;F(x) \quad \times \quad \frac{1}{3600} hr\,s^{-1}$$

Where: J_w is the PM_{10} emission flux, g m^{-2} s^{-1}
V is the fraction of outdoor surface cover (equals zero for bare soil), dimensionless [0.5 to 0.8]
u is the mean annual wind speed at height of 10 m, m s^{-1} [5]
u_t is the threshold value of wind speed at height of 10 m, m s^{-1} [7.2]
$F(x)$ is an empirical function of x , dimensionless [1.22]

Annual mean wind speeds (*u*) in the UK are normally in the range of eight to 18 knots at a height of 10 m (that is, 4.1 to 9.3 m s^{-1}), with the highest values reported for the Scottish Highlands (Fullwood, *personal communication*, 2001). Generally the least windy areas are London, Birmingham, Nottingham and the Thames Valley, where parts of the region fall below 4.1 m s^{-1}. In the CLEA model, 5.0 m s^{-1} is used as a generic default value.

Equation 9.2 is most sensitive to the **threshold friction velocity**, which is a measure of how much wind is needed to generate dust at a given site from an erodible surface (USEPA, 1996); it is used to calculate the threshold value of wind speed at a height of 10m (u_t). Cowherd *et al*. (1985) proposed a site-specific method to estimate the threshold friction velocity from the mode of the dry aggregate size distribution using hand sieving and the relationship derived by Gillette (1980). In the absence of site-specific data, USEPA (1996) proposed a mode soil aggregate size of 500 μm as a generic default value, indicating that this choice was "*conservative*". This value has also been adopted in the CLEA model and corresponds to an uncorrected threshold friction velocity of 0.5 m s^{-1} using Figure 3.4 in Cowherd *et al.* (1985).

If a soil contains non-erodible elements, these must be taken into account by increasing the threshold velocity (Cowherd *et al*., 1985). Non-erodible elements include clumps of grass or stones (larger than about one cm) that absorb energy from the wind, preventing its transfer to the erodible surface. Assuming no non-erodible elements in soil is roughly equivalent to modelling "*coal dust on a concrete pad*" (USEPA, 1996). The generic correction factor used in the CLEA model is 1.25 and is based on the recommendation of USEPA (1996) that this is "*a reasonable number that would be at the more conservative end of the range.*" If we assume that the corrected to uncorrected ratio is 1.25, an uncorrected threshold friction velocity of 0.5 m s^{-1} results in a corrected value of 0.625 m s^{-1}. This value is consistent with that proposed by the soil screening levels (USEPA 1996).

Equation 9.3 taken from Cowherd *et al*. (1985) is used to convert wind speeds at ground level to values at a height of 10 m above the ground. An important parameter in this equation is the assumed roughness height, which is related to the size and spacing of ground elements that will disrupt the airflow above the ground. The surface roughness found in a suburban location lies in the range five to 50 cm (Cowherd *et al*., 1985). The default value used in **Equation 9.3** is 10 cm, which is equivalent to an open but residential setting. Using **Equation 9.3**, the threshold wind speed at a height of 10 m above the ground is 7.2 m s^{-1}.

Equation 9.3

$$\frac{u_t}{u_*} = \frac{1}{0.4} LN(\frac{z_t}{z_0})$$

Where: u_t is the threshold value of wind speed at height of 10 m, m s^{-1}
u_* is the corrected threshold friction velocity at 0 m, m s^{-1} [0.625]
z_t is the height above the ground, cm [1000]
z_0 is the roughness height, cm [10]

The empirical constant *x* in **Equation 9.2** is calculated using **Equation 9.4** after Cowherd *et al*. (1985). The function of *x* (that is, $F_{(x)}$) is estimated from Figure 9.1 and Appendix B of Cowherd *et al*. (1985). Using the default mean average wind speed at 10 m of 5 m s^{-1} and the threshold value of wind speed at 10 m of 7.2 m s^{-1}, results in a generic default $F_{(x)}$ value of 1.22.

Equation 9.4

$$x = 0.886 \frac{u_t}{[u]}$$

Where: *x* is the empirical parameter, dimensionless
u_t is the threshold value of wind speed at 10 m, m s^{-1} [7.2]
[u] is the mean annual wind speed at 10 m, m s^{-1} [5]

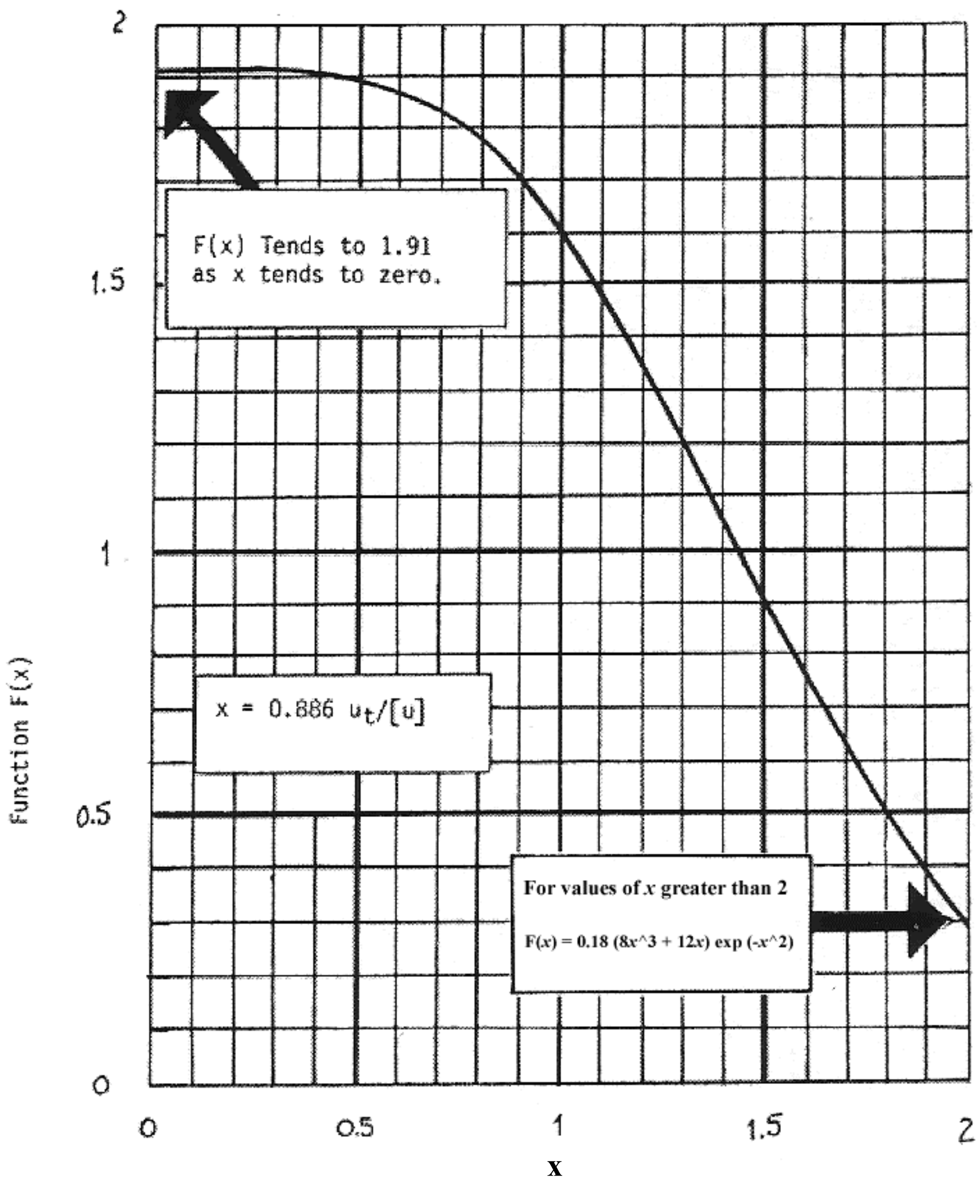


Figure 9.1: Graph of function *F(x)* versus *x* [after Cowherd *et al*., 1985] used in Equation 9.2, where *x* is calculated from the ratio of the mean annual wind speed (*u*) and the threshold value of wind speed (u_t)

9.3 Calculating the chemical intake

The chemical exposure rate for the inhalation of contamination from soil-derived airborne dust is presented in **Equation 9.5** for ambient air. The particulate emission factor (PEF), the daily inhalation rate (V_{inh}) and the site occupancy period (T_{site}) are discussed in Section 9.2, Section 4.4.3 and Chapter 3 respectively.

Equation 9.5

$$IR = C_s \left(\frac{1}{PEF}\right) V_{inh} \left(\frac{T_{site}}{24}\right) \quad x \quad 1000\, g\, kg^{-1}$$

Where:
IR is the chemical intake rate from inhalation of dust from ambient air, mg day^{-1}
C_s is the total concentration of the chemical in soil, mg g^{-1} dw
PEF is the particulate emission factor, m^3 kg^{-1}
V_{inh} is the daily inhalation rate, m^3 day^{-1}
T_{site} is the outdoor site occupancy period, hour day^{-1}

The chemical exposure rate for the inhalation of contaminated indoor dust is presented in **Equation 9.6**. The intake rate is based on the sum of the ambient air dust concentration plus a representative indoor dust loading factor (DL) for the resuspension of indoor dust. Based on the available literature, a reasonable estimate of DL for a residential property is 50 μg m^{-3} and for a commercial property is 100 μg m^{-3} (Oatway and Mobbs 2003, Oomen and Lijzen 2004, Simmonds *et al*. 1995). These are the generic values used in the CLEA model.

Indoor dust concentrations are assumed to equilibrate with those found in ambient air through natural **building ventilation**. This is a reasonable assumption in the summer months because of the higher airflow through open doors and windows. However, it is likely to be much more conservative for buildings in winter because of lower airflow, and especially so for offices that use air conditioning all year round, because filtration reduces the dust concentration in indoor air.

TF is described in Section 4.3.2.

Equation 9.6

$$IR = \left[C_s \left(\frac{1}{PEF}\right) x\, 1000\, g\, kg^{-1} + \left(C_s\, TF\ DL\right) \right] V_{inh} \left(\frac{T_{site}}{24}\right)$$

Where:
IR is the chemical intake rate from inhalation of dust from indoor air, mg day^{-1}
C_s is the total concentration of the chemical in soil, mg g^{-1} dw
TF is the soil-to-dust transport factor according to soil type, g g^{-1} dw [0.7]
PEF is the particulate emission factor, m^3 kg^{-1}
DL is the indoor dust loading factor, g m^{-3}
V_{inh} is the daily inhalation rate, m^3 day^{-1}
T_{site} is the indoor site occupancy period, hour day^{-1}

10 Inhalation of vapours

This pathway considers exposure to chemical vapours released from soil into ambient and indoor air. It is often the critical exposure route for volatile organic compounds including BTEX, the lighter petroleum bands, and chlorinated solvents. However, it can also be the only exposure pathway for subsurface contamination and is therefore important for a wider range of semi-volatile compounds in specific scenarios.

10.1 Overview

Estimating the fate and transport of volatile chemicals in soil has been the subject of considerable scientific review and only a summary of the issues relevant to generic modelling are presented in this report (see also text box). A more comprehensive overview can be found in CIRIA (in press), Environment Agency (2002b), and other documents such as ITRC (2007), and NJDEP (2005).

Ambient and indoor air concentrations of chemical pollutants are often modelled differently although they share two principles in common. Firstly, the degree to which the sources of contamination in soil partition into the relevant mobile phases (that is, the dissolved and the gaseous phases), and secondly, the transport of chemicals from the subsurface soil to the surface. Migration in the soil gas phase occurs by diffusion and advection processes (Environment Agency, 2002b).

Vapour intrusion into buildings

"**Vapour intrusion**" is the generic term used to describe the migration of volatile chemicals in soil gas from the subsurface into overlying buildings (ITRC, 2007). Since the publication of the original CLR10 (Defra and Environment Agency, 2002c), this pathway has continued to generate considerable technical debate in the UK and internationally, and its investigation and risk assessment remains a highly uncertain scientific area (Davis *et al*., 2004; ITRC, 2007; NJDEP, 2005; USEPA, 2002; van Wijnen and Lijzen, 2006).

This chapter presents an approach to the modelling of these pathways as part of the derivation of SGVs. As noted in Chapter 2, SGVs are a starting point for the assessment of risks to health from soil contamination and this is especially true for volatile contaminants. It is strongly recommended that in any risk evaluation involving vapour intrusion, assessors take account of the limitations to modelling identified in this report and use additional lines of evidence. Further guidance on investigating and assessing this pathway can be found in *The VOCs Handbook* (CIRIA, in press).

10.1.1 Predicting the soil gas concentration at source

Many environmental models, including the CLEA model (see Chapter 5), predict chemical partitioning in soil systems using Henry's Law constant. Relatively few peer-reviewed papers have compared predicted and measured gas concentrations in soil and groundwater systems from real sites (Baker, *personal communication*, 2008), although those that have suggest they are poorly correlated (Fitzpatrick and Fitzgerald

1996; Hartman, 2002). In particular, Hartman (2002) noted that "*results of published studies comparing measured soil vapour [gas] concentrations to soil vapour [gas] values calculated from groundwater using Henry's constants indicate that calculated values are often overestimated by factors of 10 to 100.*" However, such an over-prediction has not been observed at all sites and may be more of an issue for petroleum hydrocarbons and not chlorinated solvents (Baker, *personal communication*s, 2008).

There are several possible reasons for the difference between modelled and measured soil gas concentrations including limitations in the above approach and difficulties with gas investigation and sampling techniques. In an open soil system, it is highly unlikely that the soil, water and gas phases within interconnected pores achieve equilibrium or that the gas gradient through the soil has reached steady state. In addition, biodegradation within the migrating plume is an important mechanism for reducing observed concentrations of chemicals in soil gas over relatively short distances from the source zone, although this depends on chemical type and may in part explain the field data for petroleum hydrocarbons (NJDEP, 2005). Considerable research has been undertaken to show that biodegradation of petroleum hydrocarbons in the unsaturated zone occurs regularly (Fischer *et al*., 1996; Fitzpatrick and Fitzgerald, 1996; Roggemans et al., 2001; Lahvis, 2006). However, in some cases the practical constraints on targeting and measuring soil gas concentrations *in situ*, without unduly disturbing the system, may have exaggerated the differences between predicted and measured concentrations (ITRC, 2007).

The degree of conservatism when using the above approach to predict the soil gas concentration in the subsurface varies considerably according to site conditions and the types of volatile chemical investigated. However, as a general rule of thumb, it is recognised that this approach will estimate gas concentrations from dissolved and sorbed phase contamination by petroleum hydrocarbons at least a factor of ten higher than are likely to be measured on site.

10.1.2 Soil gas transport processes

Diffusion is often a slow process, where the rate of diffusive transport is a function of chemical gradient, temperature, and the viscosity of the transporting medium (Environment Agency, 2002b). For example, air has a much lower viscosity than water and so chemical diffusion coefficients in air are often several orders of magnitude higher than in water. While diffusion is a random process, over time there will be a net chemical movement from zones of high concentration to those of lower concentration (along a so-called **chemical gradient**).

Diffusion in soil occurs primarily through interconnecting pore spaces, which in the unsaturated zone will contain water and air in highly varying amounts. The degree to which these pore spaces interconnect and the effective distance that a chemical molecule must diffuse through the pore network is measured by the tortuosity factor (Millington and Quirk, 1961).[39] Therefore, the effective diffusion rate for a chemical in soil is the sum of the rate of diffusion of the chemical in soil and air modified by the soil tortuosity and is calculated as shown in **Equation 10.1** (ASTM, 2000; USEPA, 2003). Several commentators have observed through empirical study that the Millington-Quirk relationship generally under-predicts chemical diffusivity and that this difference increases with increasing soil moisture content (Environment Agency, 2002b).

---

[39] Granular media such as soil contain a variety of different shaped grains that compact together, leaving pore spaces between them. The diffusion pathway is rarely a straight line but rather it is dictated by the connectivity of these pore spaces. To travel from one point to another in a straight line, a molecule of vapour or gas must actually travel a much further distance and therefore a correction to laboratory-determined diffusion rates is required to account for this.

Equation 10.1

$$D_{eff} = D_{air}\frac{\theta_a^{3.33}}{\theta_T^2} + D_{water}\frac{\theta_w^{3.33}}{K_{aw}\theta_T^2} \times 10000\, cm^2 m^{-2}$$

Where:
D_{eff} is the effective chemical diffusion coefficient in soil, $cm^2\ s^{-1}$
D_{air} is the diffusion coefficient in air at ambient temperature, $m^2\ s^{-1}$
D_{water} is the diffusion coefficient in water at ambient temperature, $m^2\ s^{-1}$
θ_a is the air-filled soil porosity, $cm^3\ cm^{-3}$
θ_w is the water-filled soil porosity, $cm^3\ cm^{-3}$
θ_T is the total air- and water-filled soil porosity, $cm^3\ cm^{-3}$
K_{aw} is the air-water partition coefficient at ambient temperature, $cm^3\ cm^{-3}$

Advection can often be a much quicker transport process and involves chemical transport as part of the bulk movement of air and water under the influence of differences in pressure, temperature and density between adjacent locations (Environment Agency, 2002b). For example, the net upward transport of contaminant gas from depth has been reported for a number of cases and is an accepted phenomenon for landfill gas movement (Attenborough *et al.*, 2002).

In quantifying vapour transport in the unsaturated zone, many models distinguish between advective soil transport within the zone of influence of a building or gas generation zone and that found in the bulk soil environment. In a critical review of radon ingress into buildings, Nazaroff and Nero (1984) observed that precipitation and atmospheric pressure changes may also play a significant role in controlling chemical transport in soils, by providing a driving force for advective flow. The mechanisms that could induce a pressure gradient in the soil profile include fluctuations in the water table (a so-called “pumping effect”), precipitation, atmospheric pressure changes, and/or temperature gradients caused by daily fluctuations in temperature (Barraclough, *personal communication*, 2003; Nazaroff and Nero, 1984).

Fluctuations in water table, precipitation and atmospheric pressure are likely to be highly site-specific and their effects are likely to be very difficult to apply in a generic model. Soil temperature fluctuations are only likely to be important in the top 50 cm of the soil and theoretical considerations of such gradients are that they are likely to be either insignificant or will tend to drive the vapour downwards from the surface into deeper soil layers (Barraclough, *personal communication*, 2003; Davis *et al.*, 2004).

Undoubtedly, even a modest upward pressure gradient of 2 Pa over a short distance in soil (such as one metre) would significantly increase rates of chemical transport compared to a diffusion-only approach. However, a literature review has found no reported studies of pressure gradients in soil (Barraclough, *personal communication*, 2003). On balance, the inclusion of advective flow in soil transport modelling is not recommended at this time, because there is a need for stronger evidence that the driving force for such flow exists and that any observed difference could be sustained long enough to have an effect.

10.1.3 Ambient air modelling

Jury *et al*. (1983) proposed a model to describe the combined effects of volatilisation, leaching, and biological/chemical degradation of organic chemicals applied to soil such as pesticides. Jury *et al*. (1990) further developed this model to consider the scenario where volatile organic chemicals polluted soil from surface spills or leaking pipes and tanks. Volatilisation of chemical vapour to the atmosphere was assumed to occur by vapour diffusion through a stagnant air boundary layer of finite thickness, above which the chemical concentration is zero.

Jury *et al*. (1990) observed that soil type had a significant effect on predicted volatilisation from a near surface source. In a sandy soil, the flux of volatilised benzene rose quickly to a maximum rate after about 30 days and remained high thereafter. In contrast, the flux from the clay soil did not reach a maximum during the first year and was more than two orders of magnitude less than the flux from the sandy soil after the first year. Soil moisture content appeared to be a critical factor in reducing the volatile flux rate because of the much lower diffusion rates for a chemical in water compared to air (Jury *et al*., 1990; USEPA, 1996). Jury *et al*. (1990) also found that the depth to source of contamination delayed volatile chemicals from reaching the surface, but was only effective longer-term if other factors such as degradation were taken into account to reduce the overall source term. USEPA (1996) undertook to validate the Jury models under bench and field conditions using studies from the literature. They found a good agreement between the models and measured data for the chemicals studied.

Johnson *et al*. (1990) proposed several models for assessing vapour transport from both surface and buried contamination, using assumptions similar to the work of Jury and co-workers. ASTM (2000) incorporated this model within the RBCA guidance.

Despite a confusing similarity in terminology, USEPA (1996) and ASTM (2000) are similar models for predicting ambient air concentrations from surface and subsurface soil contamination. The key difference is the approach to modelling air dispersion. ASTM (2000) proposes a ‘box model’ to predict conservative ambient concentration estimates for receptors located on the downwind edge of the area source at a height of two metres. USEPA (1996) estimates dispersion within the well-mixed box using calculated air dispersion factors for major US cities at ground level (see Section 9.2.1). Within CSOIL, outdoor vapour concentrations are also calculated using the Jury model with parameters for typical Dutch weather conditions (van den Berg, 1994).

The approach adopted by the CLEA model is discussed in Section 10.2.

10.1.4 Indoor air modelling

As noted in Section 10.1, there are sizeable uncertainties in assessing the vapour intrusion pathway, including the gas concentration in the subsurface source and the extent of attenuation from the source zone into the building. Many generic models have limited or no validation data under UK conditions and across the varied UK housing stock (Environment Agency, 2002b). Although there are high profile studies in the US and the UK that show that vapour modelling can under-predict the flux of vapour into the building (Denver Post, 2002; McAlary *et al*., 2002), there is also considerable evidence that such models can overestimate the risk if used without taking into account additional lines of evidence (ITRC, 2007).

Important site-specific factors that affect the suitability of vapour intrusion models to predict indoor air concentrations include the depth to source and whether biological/ chemical degradation is likely to be significant. Models may under-predict intrusion where the contamination is at shallow depths in the unsaturated zone and over-predict where the chemical is highly degradable and the site conditions support biodegradation (Hers *et al*., 2003; Hartman, 2002; USEPA, 2002b).

The Environment Agency (2002b) reviewed ten generic models for vapour intrusion into buildings including Johnson and Ettinger (1991), Ferguson *et al*. (1995), Krylov and Ferguson (1998), and Waitz *et al*. (1996). More recent publications include work on vapour modelling in Australian homes (Turczynowicz and Robinson, 2001; Robinson, 2003; Robinson and Turczynowicz, 2005), development of a three-dimensional numerical model (Abreu and Johnson, 2005, 2006), and further validation of the Dutch VOLASOIL model (van Wijnen and Lijzen 2006). There are many common features between the models and some significant differences, principally in the design and parameterisation of building structures, specifying the location of the source term, and the inclusion or exclusion of chemical and biological degradation.

Vapour intrusion into buildings, through its foundations, occurs as a result of diffusion through dust-filled cracks and bulk building layers such as concrete slabs and by advection through drains, service penetrations, expansion joints and floor and perimeter cracks (Environment Agency 2002b). In most cases, advection is considered the dominant mechanism for vapour entering a building (Johnson and Ettinger, 1991; Waitz *et al*., 1996). Advection through cracks and openings occurs because of the negative indoor air pressure (relative to atmospheric pressure) created by building construction, temperature differences between inside and outside, wind loading on walls and mechanical circulation such as the use of air conditioning (Environment Agency, 2005). Advective air movement of chemicals within unsaturated soils is controlled by its effective air permeability, which depends on its properties including porosity, hydraulic conductivity, and water content (Environment Agency, 2002b).

The Environment Agency (2002b) concluded that in choosing a model for vapour intrusion into buildings, the "*most important factor is that the CLEA model should provide a simple screening process that in most cases will provide conservative predictions and that requires the least amount of data collection*." The recommended approach was based on the Johnson and Ettinger model and is consistent with that used by USEPA and several other countries (Johnson and Ettinger, 1991; USEPA 2002b, 2003). Johnson and Ettinger (1991) assume the building has a solid slab foundation, a type of construction found in about half of all residential properties in the UK irrespective of age and between 70 and 75 per cent of houses built since the late 1960s (see Section 4.5). However, many new build properties comprise suspended floors over a void, which is generally ventilated to avoid damp and the floors are sealed with plastic membranes to minimise gas ingress (Krylov *et al*., 1998; CIRIA, 2006). In such circumstances, the Johnson and Ettinger model could significantly overestimate vapour ingress into the building.

The original work of Johnson and Ettinger (1991) is one of the most widely applied models for estimating vapour ingress into buildings (Johnson, 2002). It is a screening model with a number of simplifying assumptions regarding contaminant distribution and occurrence, subsurface characteristics, transport mechanisms and building construction and design (USEPA 2002b, 2003). It calculates an **attenuation factor** that relates steady-state gas concentrations at the source to indoor air concentration based on soil and building characteristics.

Figure 10.1 is a simplified diagram showing how soil vapour intrusion is modelled in CLEA. At the top boundary of contamination, molecular diffusion moves the chemical in soil gas towards the soil surface until it reaches the zone of influence of the building. Convective air movement within the soil column transports the gas through cracks between the foundation and the basement slab floor (a simple foundation design similar to a ground-bearing slab is considered) as vapour intrusion. This advective sweep effect is induced by a negative pressure within the structure caused by wind and stack effects due to building heating and mechanical ventilation.

The Johnson and Ettinger model uses a one-dimensional analytical solution to diffusive and advective transport of vapours (Johnson and Ettinger, 1991; USEPA, 2003), and makes the following critical assumptions:

- The source of contamination is homogeneously distributed within the ground and lies directly beneath the building. The chemicals present are assumed to be at a concentration below their aqueous solubility limit, their soil saturation concentration, and/or their pure component vapour concentration.

- No account of spatial horizontal variation in subsurface stratigraphy. Vertical stratigraphy can be described as one or more horizontal soil layers with isotropic properties.
- Diffusion through soil moisture is considered to be insignificant relative to diffusion through air. Vapour flow is described by **Darcy's Law**, that is, flow through a porous media and does not take into account the presence of **dual porosity** systems and preferential flow channels.
- Vapour migration is through cracks and openings in the walls and foundations and this in turn is affected by the number of cracks or openings within the building foundations including floor and wall slabs. Advection through the building floor-slab is modelled assuming that vapour flow can only occur through an edge crack between the wall and the edge of the floor slab (that is, the perimeter of a building basement or ground floor slab). Preferential flow through service ducts, open drains or other pathways is not modelled.
- Indoor air concentration depends not only on the rate of vapour intrusion, but on the structure and ventilation performance of the building, as dilution with "cleaner" outdoor air reduces the contaminant concentration. Johnson and Ettinger (1991) assume a simple 'box' model with uniform and instantaneous mixing and dilution of chemicals within the air inside the building. The height and footprint of the building define the dimensions of the box and the air exchange rate controls the dilution of the contaminant entering into it with ambient air (Hers *et al.,* 2003). It does not take into account potential building "hot spots". No contaminant sources or sinks in the building are considered. Neither sorption nor biodegradation is accounted for in vapour transport through the soil and into the building.

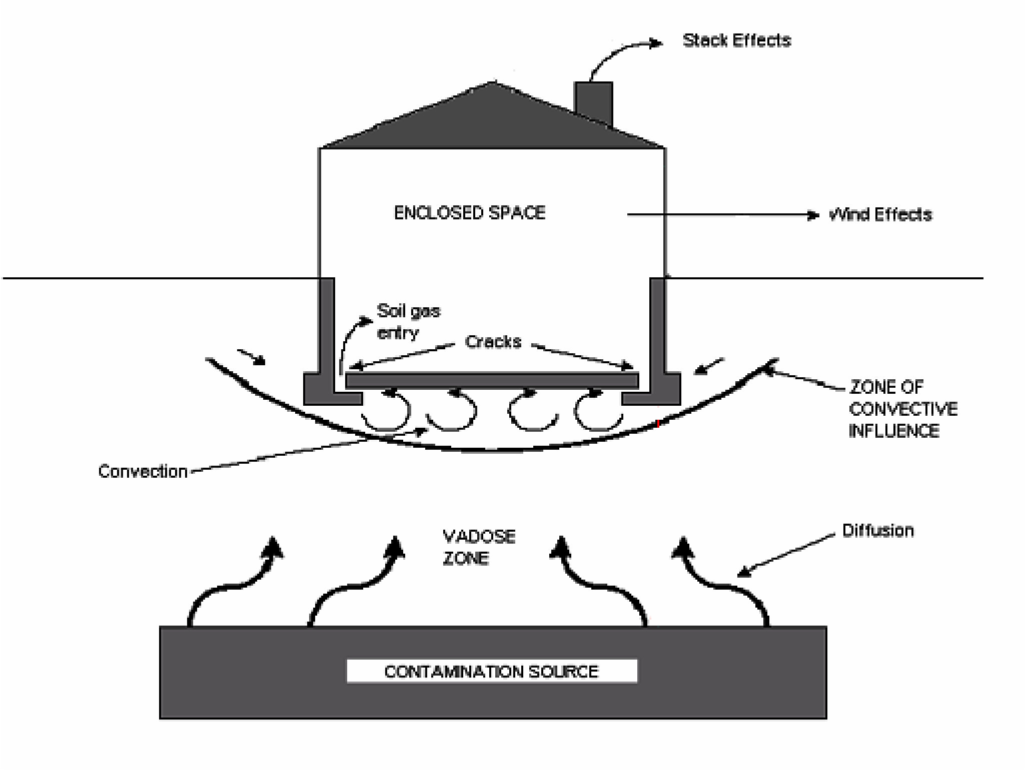


Figure 10.1: Conceptual model for vapour intrusion [after USEPA 2003]

Because of its popularity as a screening tool, the Johnson and Ettinger model has been the subject of several sensitivity studies (Environment Agency, 2002b; Hers *et al*. 2003; Johnson, 2002; USEPA, 2002b, 2003). The objective of these reviews has been to target those parameters that have the greatest influence on the estimated indoor air concentration, to enable better targeted data collection and more meaningful comparison between predicted concentrations and those observed at a number of case study sites. For example, Hers *et al*. (2003) reviewed the Johnson and Ettinger model, evaluating the sensitivity and uncertainty in the model from both a theoretical basis and through comparison with several published case studies of petroleum hydrocarbon and chlorinated solvent contaminated sites.

The relative sensitivity of the soil, building and chemical parameters used in the Johnson and Ettinger model depend on the scenario being conceptualised (Hers *et al*., 2003; Johnson, 2002; USEPA, 2002b). Scenarios can be defined on the basis of:

- depth below ground to source (that is, a shallow or deep source);
- whether the contamination is in the unsaturated zone or at the water table (that is, a soil or a groundwater source);
- whether building depressurisation is assumed (that is, flow into the building is based on advective and diffusion flow rather than diffusion only).

For the purpose of generic modelling, a reasonable worst-case scenario assumes a shallow source term less than one metre beneath the surface in the unsaturated zone above the water table (that is, 0.5 m below the bottom of the floor).[40] The building is subject to depressurisation (see Section 4.5). On the basis of this type of conceptual model, the relative sensitivity of parameters in the Johnson and Ettinger model (as observed by Hers *et al*., 2003; Johnson, 2002; USEPA, 2002b) is shown in **Table 10.1**.

It is important to distinguish the basic equations described in Johnson and Ettinger (1991) from their subsequent application in practice (Johnson 2002). In many cases such as USEPA (2003) and ASTM (2000), the initial approach has been supplemented with additional guidance on factors including source zone partitioning and estimation methods for soil characteristics. Johnson (2002) and USEPA (2002b) expressed reservations that these additional characteristics can be estimated using generic assumptions and are best investigated on a site-specific basis. Use of the Johnson and Ettinger model in the derivation of SGVs recognises that generic predictions of the volumetric soil gas ingress rate can be problematic (USEPA, 2002b; Johnson, 2002).

The approach adopted by the CLEA model is discussed in Section 10.3.

10.2 Ambient air concentrations

The generic CLEA model assumes that the source of outdoor air contamination is present as a continuous layer from the surface to a depth of 100 cm. This is broadly consistent with the conceptual model for the other direct contact exposure pathways including soil ingestion and dermal contact. The default approach is also to assume that the contamination is not depleted by volatilisation nor reduced by chemical or biological degradation. Chemical transport within the soil is assumed to occur via diffusion within unsaturated pore spaces and not as a result of water evaporation. USEPA (1996) and ASTM (2000) propose similar approaches to model ambient concentrations, although they adopt different and somewhat confusing nomenclature. For example, the volatilisation factor (VF) proposed by ASTM (2000) is the inverse of the same named parameter in USEPA (1996).

---

[40] Equivalent to 0.65 m below the ground surface for a foundation thickness of 0.15 m (see Table 4.21)

Table 10.1: Relative sensitivity of parameters in the Johnson and Ettinger model for a shallow source in the unsaturated zone (Hers *et al.*, 2003; Johnson, 2002; USEPA, 2002b)

Parameter		Relative sensitivity
Soil		
	Fraction of organic carbon	Moderate to high
	Total porosity	Low
	Water-filled porosity	Low to moderate
	Soil bulk density	Low
	Pressure driven gas flow rate	Moderate to high
	Soil air permeability	Moderate to high
Building		
	Air depressurisation	Moderate
	Air exchange rate	Moderate
	Height	Moderate
	Foundation area	Low to moderate
	Depth to base of foundation	Low
	Floor to wall crack ratio	Low
	Crack moisture content	Low
	Foundation slab thickness	Low
Chemical		
	Henry's Law constant	Low to moderate
	Air diffusion coefficient	Low

[1]Sensitivity of these parameters will vary if another conceptual model is used (for example, the source is close to the water table)

The approach adopted by the CLEA model is shown in **Equation 10.2** and is based on the infinite source calculation for surface soils recommended by ASTM (2000). However, the model has been adapted to include the generic air dispersion factors (Q/C_{wind}) described in Section 9.2.1 and which more accurately reflect both UK climate conditions and the source dimensions set out in the standard land use scenarios.[41] The volatilisation factor from surface soils to ambient air (VF) is used to calculate an ambient air concentration at the receptor breathing height (C_{air}) using

Equation 10.3.

Equation 10.2

$$VF = \frac{\rho_s}{\frac{1}{10} \times Q/C_{wind}} \sqrt{\frac{4D_{eff}}{\pi\,\tau \times 31536000\,s\,yr^{-1}} \times \frac{K_{aw}}{K_{sw}\,\rho_s}}$$

Where: VF is the volatilisation factor from surface soil to ambient air, g cm^{-3}
ρ_s is the dry bulk soil density, g cm^{-3}
Q/C_{wind} is the air dispersion factor, g m^{-2} s^{-1} per kg m^{-3}
D_{eff} is the effective diffusion coefficient for unsaturated soils, cm^2 s^{-1}
τ is the averaging time for surface emission vapour flux, year
K_{aw} is the air-water partition coefficient at ambient temperature, cm^3 cm^{-3}
K_{sw} is the total soil-water partition coefficient, cm^3 g^{-1}

---

[41] Equation 10.2 replaces the original dispersion factor for ambient air (DF_{amb}) in ASTM (2000) with Q/C_{wind} adjusting for the unit differences between the two factors (1/10).

Equation 10.3

$$C_{air} = C_s \, VF \quad \times \quad 1000000 \; cm^3 m^{-3}$$

Where: C_{air} is the ambient air concentration at the receptor height, mg m^{-3}
C_s is the total soil concentration, mg g^{-1}
VF is the volatilisation factor from surface soil to ambient air, g cm^{-3}

10.3 Indoor air concentrations

The generic CLEA model assumes that the source of indoor air contamination is present at a depth of 0.5 m below the bottom of the building floor or foundation. The default approach is also to assume that the contamination is not depleted by volatilisation nor reduced by chemical or biological degradation. Chemical transport within the soil is assumed to occur via diffusion within unsaturated pore spaces until the zone of influence of the building is reached. The principal route of entry into the building is assumed to be through cracks within the foundation and between the wall and the edge of the foundation slab.

The attenuation factor between soil and indoor air concentration (alpha) is estimated using **Equation 10.4** and is used to calculate the indoor air concentration (C_{air}) in **Equation 10.6**. The building ventilation rate (Q_b) is calculated using **Equation 10.5**. Generic values for the volumetric flow rate of soil gas into the enclosed space (Q_s) are based on a combination of a sandy loam soil with a worst-case building type using the data presented in Table 4.4 and Table 4.21, and the calculations set out here and in Appendix 1. The generic flow rates used in the derivation of SGVs are 25 and 150 cm^3 s^{-1} for the residential and commercial land use respectively.[42] These values lie within the range of values for soil ingress rate observed by Hers *et al*. (2003) of between 17 cm^3 s^{-1} and 167 cm^3 s^{-1}.

---

[42] Default values selected from a comparison of calculated soil gas ingress rates for all residential and commercial building types with data for a sandy loam soil. Residential and commercial default values were based on the detached house and the post-1970 warehouse respectively.

Equation 10.4

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

Where: α is the steady-state attenuation coefficient between soil and indoor air, dimensionless
D_{eff} is the effective diffusion coefficient for unsaturated soils, $cm^2\ s^{-1}$
A_B is the area of enclosed floor and walls below ground, cm^2
Q_b is the building ventilation rate, $cm^3\ s^{-1}$
L_T is the source-building separation, cm
Q_s is the volumetric flow rate of soil gas into the enclosed space, $cm^3\ s^{-1}$ [25 to 150]
L_{crack} is the foundation slab thickness, cm
A_{crack} is the floor crack area, cm^2
D_{crack} is the effective diffusion coefficient through the cracks, $cm^2\ s^{-1}$ [= D_{eff}]
Note: Appendix 1, Equation A10 where the Peclet number approaches infinity

Equation 10.5

$$Q_b = \left(H \times A_{foot} \times Ex\right) \times 1000000\, cm^3\ m^{-3} \quad \frac{1}{3600}\ s\ hr^{-1}$$

Where: Q_b is the building ventilation rate, $cm^3\ s^{-1}$
H is height of living space, m
A_{foot} is the building footprint, m^2
Ex is the building air exchange rate, $hour^{-1}$

Equation 10.6

$$C_{air} = \alpha\ C_{vap} \times 1000000\, cm^3 m^{-3}$$

Where: C_{air} is the indoor air concentration, mg m^{-3}
α is steady-state attenuation coefficient between soil and indoor air, dimensionless
C_{vap} is the soil vapour concentration, mg cm^{-3}

10.4 Calculating the chemical intake

The chemical exposure rate for the inhalation of contamination from soil-derived vapours is presented in **Equation 10.7** for ambient air. The ambient air vapour concentration is described in Section 10.2; the daily inhalation rate (V_{inh}) and the site occupancy period (T_{site}) are discussed in Section 4.4.3 and Chapter 3 respectively.

Equation 10.7

$$IR = C_{air}\ V_{inh}\left(\frac{T_{site}}{24}\right)$$

Where: IR is the chemical intake rate from inhalation of vapour from ambient air, mg day^{-1}
C_{air} is the ambient air concentration of the chemical, mg m^{-3}
V_{inh} is the daily inhalation rate, m^3 day^{-1}
T_{site} is the outdoor site occupancy period, hour day^{-1}

The chemical exposure rate for the inhalation of contamination from soil-derived vapours is presented in **Equation 10.8** for indoor air. The indoor air vapour concentration is described in Section 10.3; the daily inhalation rate (V_{inh}) and the site occupancy period (T_{site}) are discussed in Section 4.4.3 and Chapter 3 respectively.

Equation 10.8

$$IR = C_{air}\ V_{inh}\left(\frac{T_{site}}{24}\right)$$

Where: IR is the chemical intake rate from inhalation of vapour from indoor air, mg day^{-1}
C_{air} is the indoor air concentration of the chemical, mg m^{-3}
V_{inh} is the daily inhalation rate, m^3 day^{-1}
T_{site} is the indoor site occupancy period, hour day^{-1}

11 References

ABREU, L.D., JOHNSON, P.C., 2006. Simulating the effect of aerobic biodegradation on soil vapour intrusion into buildings: influence of degradation rate, source concentration and depth. *Environmental Science and Technology*, 40, 2304-2315.

ABREU, L.D., JOHNSON, P.C., 2005. Effect of vapor source – building separation and building construction on soil vapour intrusion as studied with a three-dimensional numerical model. *Environmental Science and Technology*, 39, 4550-4561.

ALLISON, J.D., BROWN, D.S., NOVO-GRADAC, K.J., 1991. *MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems*. Report EPA 600-3-91-021. Washington: United States Environmental Protection Agency.

ALLOWAY, B.J., 1995. *Heavy Metals in Soils*. Second edition. London: Blackie Academic & Professional.

ALLOWAY, B.J., THORNTON, I., SMART, G.A., SHERLOCK, J.C., QUINN, M.J., 1988. Metal Availability. Special Issue: The Shipham Report: An Investigation into Cadmium Contamination and its Implications for Human Health. *Science of the Total Environment*, 75, 41-70.

ASTM, 2000. *Standard Guide for Risk-Based Corrective Action*. Report E2081-00. West Conshohocken: American Society for Testing and Materials.

ATTENBOROUGH, G.M., HALL, D.H., GREGORY, R.G., MCGOOCHAN, L., 2002. Development of a landfill gas risk assessment model: GasSim. In: *Proceedings of the 25th Annual Landfill Gas Symposium*, Solid Waste Association of North America, held between March 25-28 2002 in Monterey, California, 207-220.

BAES, C.F., SHARP, R.D., SJOREEN, A.L., SHOR, R.W., 1984. A *Review and Analysis of Parameters for Assessing Transport of Environmentally Released Radionuclides Through Agriculture*. ORNL-5786. Oak Ridge National Laboratory, Oak Ridge, TN.

BELL, R. M, 1992. *Higher plant accumulation of organic pollutants from soils*. Report EPA 600-R-92-138. Washington: United States Environmental Protection Agency.

BERNY, P.J., COTE, L.M., BUCK, W.B., 1994. Relationship between soil lead, dust lead, and blood lead concentrations in pets and their owners: evaluation of soil lead threshold values. *Environmental Research*, 67, 84-97.

BINDER, S., SOKAL, D., MAUGHAN, D., 1986. Estimating soil ingestion: the use of tracer elements in estimating the amount of soil ingested by young children. *Archives of Environmental Health*, 41, 341-345.

BIRMINGHAM CITY COUNCIL, 2007. *Allotments*. [online] http://www.birmingham.gov.uk/GenerateContent?CONTENT_ITEM_ID=3040&CONTENT_ITEM_TYPE=0&MENU_ID=1758 [Accessed March 2007]

BISHOP, K., 2004. Working time patterns in the UK, France, Denmark, and Sweden. *Labour Market Trends*, 113-122.

BOETHLING, R., MACKAY, D., 2000. *Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences*. Boca Raton: CRC Press.

BOURG, A., 1982. ADSORP, a chemical equilibria computer program accounting for adsorption processes in aquatic systems. *Environmental Technology Letters*, 3, 305-310.

BRADY, N., WEIL, R., 1990. *The Nature and Properties of Soils*. Eleventh edition. London: Prentice Hall International.

BRIGGS, G.G., BROMILOW, R.H., EVANS, A.A., 1982. Relationships between lipophilicity and root uptake and translocation of non-ionised chemicals by barley. *Pesticide Science*, 13, 495-504.

BRIGGS, G., BROMILOW, R., EVANS, A., WILLIAMS, M., 1983. Relationships between lipophilicity and the distribution of non-ionised chemicals in barley shoots following uptake by the roots. *Pesticide Science*, 14, 492-500.

BRITISH COUNCIL OF OFFICES, 2000. *BCO Guide*. Reading: British Council of Offices.

BROWN, J., SIMMONDS, J., 1995. *FARMLAND. A dynamic model for the transfer of radionuclides through terrestrial foodchains*. NRPB-R273. Didcot: National Radiological Protection Board.

BROWN, F., RICKABY, P., BRUHNS, H., STEADMAN, P., 2000. *Surveys of non-domestic buildings in four English towns*. Environment and Planning B: Planning and Design, 27, 11.

BRUNEKREEF, C., 1996. *An investigation of soil-loading on leeks using two experimental methodologies*. Paper submitted to Hogeschool van Utrecht. Unpublished.

BURGESS, S., REES, H., 1996. Job tenure in Britain 1975-92. *Economic Journal*, 106 (435), 334-344.

CALABRESE, E.J., BARNES, R., STANEK, E.J., PASTIDES, H., GILBERT, C.E., VENEMAN, P., WANG, X., LASZTITY, A., KOSTECKI, P., 1989. How much soil do young children ingest: an epidemiologic study. *Regulatory Toxicology and Pharmacology*, 10, 123-137.

CALABRESE, E.J., STANEK, E.J., 1995. Resolving intertracer inconsistencies in soil ingestion estimates. *Environmental Health Perspectives*, 103, 454-457.

CALABRESE, E.J., STANEK, E.J., 1994. Soil ingestion issues and recommendations. *Journal of Environmental Science and Health*, A29(3), 517-530.

CALABRESE, E.J., STANEK, E.J., 1992. What proportion of household dust is derived from outdoor soil? *Journal of Soil Contamination*, 1, 253-263.

CALABRESE, E.J., STANEK, E.J., BARNES, R., 1997a. Soil ingestion rates in children identified by parental observation as likely high soil ingesters. *Journal of Soil Contamination*, 6, 271-279.

CALABRESE, E.J., STANEK, E.J., BARNES, R., 1996. Methodology to estimate the amount and particle size of soil ingested by children: implications for exposure assessment at waste sites. *Regulatory Toxicology and Pharmacology*, 24, 264-268.

CALABRESE, E.J., STANEK, E.J., GILBERT, C.E., 1991. Evidence of soil-pica behaviour and quantification of soil ingested. *Human and Experimental Toxicology*, 10, 245-249.

CALABRESE, E., STANEK, E., GILBERT, C., 1990. Adult soil ingestion estimates. In: *Petroleum Contaminated Soils, Volume 3*. KOSTECKI, P., CALABRESE, E., editors., Chelsea: Lewis Publishers, 349-356.

CALABRESE, E.J., STANEK, E.J., PEKOW, P., BARNES, R., 1997b. Soil ingestion estimates for children residing on a Superfund site. *Ecotoxicology and Environmental Safety*, 36, 258-268.

CENTRE FOR CHEMICALS MANAGEMENT, 2007. Chemical Physico-Chemical Properties Database [online]. Available from: http://www.lec.lancs.ac.uk/ccm/research/database/index.htm [accessed February 2008]

CHIOU, C.T., SHENG, G.Y., MANES, M., 2001. A partition-limited model for the plant uptake of organic contaminants from soil and water. *Environmental Science and Technology*, 35, 1437-1444.

CHUANG, J.C., CALLAHAN, P.J., MENTON, R.G., GORDON, S.M., LEWIS, R.G., WILSON, N.K., 1995. Monitoring methods for polycyclic aromatic hydrocarbons and their distribution in house dust and track-in soil. *Environmental Science and Technology*, 29, 494-500.

CIRIA, in press. *The VOCs Handbook: Investigating, assessing and managing risks from inhalation of VOCs at land affected by contamination*. Unpublished Project No. RP766. London: Construction Industry Research and Information Association.

CIRIA, 2006. *Assessing risks posed by hazardous ground gases to buildings*. Report C659. London: Construction Industry Research and Information Association.

CLAUSING, P., BRUNEKREEF, B., VAN WIJNEN, J.H., 1987. A method for estimating soil ingestion by children. *International Archives of Occupational and Environmental Health*, 59, 73-82.

COTTER-HOWELLS, J., THORNTON, I., 1991. Sources and pathways of environmental lead to children in a Derbyshire mining village. *Environmental Geochemistry and Health*, 13, 127-135.

COWHERD, C., MULESKI, G.E., ENGLEHART, P.J., GILLETTE, D.A., 1985. *Rapid Assessment of Exposure to Particulate Emissions from Surface Contamination Sites*. Report EPA/600/8-85/002. Washington: United States Environmental Protection Agency.

CROUCH, D., 1997. *English Allotments Survey. Report of the Joint Survey of Allotments in England*. Corby: National Society of Allotment and Leisure Gardeners Ltd.

CSTEE, 2001. *Exposure Data in Risk Assessment of Organic Chemicals*. Report EXPASSESS20072001/D(01). Brussels: European Commission.

CULBARD, E.B., THORNTON, I., WATT, J., WHEATLEY, M., MOORCROFT, S., THOMPSON, M., 1988. Metal contamination in British urban dusts and soils. *Journal of Environmental Quality*, 17, 226-234.

DATAMONITOR, 2000. Changing Lunch Occasions. London: Datamonitor Ltd.

DAVIES, D.J.A., THORNTON, I., WATT, J.M., CULBARD, E.B., HARVEY, P.G., DELVES, H.T., SHERLOCK, J.C., SMART, G.A., THOMAS, J.F.A., QUINN, M.J., 1990. Lead intake and blood lead in two-year-old UK urban children. *Science of the Total Environment*, 90, 13-29.

DAVIS, G.B., TREFRY, M.G., PATTERSON, B.M., 2004. *Petroleum and Solvent Vapours: Quantifying their Behaviour, Assessment and Exposure*. Victoria, Australia: Commonwealth Scientific and Industrial Research Organisation.

DAVIS, S., MIRICK, D.K., 2006. Soil ingestion in children and adults in the same family. *Journal of Exposure Science and Environmental Epidemiology*, 16, 63-75.

DAVIS, S., WALLER, P., BUSCHOM, R., BALLOU, J., WHITE, P., 1990. Quantitative estimates of soil ingestion in normal children between the ages of two and seven years: population-based estimates using aluminium, silicon, and titanium as soil tracer elements. *Archives of Environmental Health*, 45, 112-122.

DAYCARE TRUST, 2005. *Childcare is Everyone's Business*. [online] http://www.bbc.co.uk/health/awareness_campaigns/jun_childcare.shtml [Accessed June 2006]

DCLG, 2006a. *Housing in England 2004/05. A Report Principally from the 2004/05 Survey of English Housing*. London: Department for Communities and Local Government.

DCLG, 2006b. *English House Condition Survey 2003*. Annual Report. London: Department for Communities and Local Government.

DCLG, 2006c. *English House Condition Survey 2004*. Annual Report. London: Department for Communities and Local Government.

DCLG, 2006d. *Survey of Allotments, Community Gardens and City Farms, Urban Research Summary 23*. London: Department for Communities and Local Government.

DCLG, 2006e. *Land Use Change in England to 2005, Additional Tables LUCS 21A*. London: Department for Communities and Local Government.

DCLG, 2001. *English House Condition Survey 2001*. London: Department for Communities and Local Government.

DEFRA, 2008a. *Improvements to contaminated land guidance. Outcome of the "Way Forward" exercise on soil guideline values.* Defra: London.

DEFRA, 2008b. *Guidance on the legal definition of contaminated land*. Defra: London.

DEFRA, 2007. *UK Purchases and Expenditure on Food and Drink and derived Energy and Nutrient Intakes in 2005-06*. Defra: London.

DEFRA, 2006. *Environmental Protection Act 1990: Part 2A*. Contaminated Land, Circular 01/2006. Defra: London.

DEFRA, ENVIRONMENT AGENCY, 2004. *Model Procedures for the Management of Land Contamination, Contaminated Land Report 11*. Bristol: Environment Agency.

DEFRA, ENVIRONMENT AGENCY, 2002a. *Contaminants in Soil: Collation of Toxicological Data and Intake Values for Humans. Lead*. R&D Publication TOX 6. Bristol: Environment Agency.

DEFRA, ENVIRONMENT AGENCY, 2002b. *Contaminants in Soil: Collation of Toxicological Data and Intake Values for Humans. Nickel*. R&D Publication TOX 8. Bristol: Environment Agency.

DEFRA, ENVIRONMENT AGENCY, 2002c. *The Contaminated Land Exposure Assessment Model (CLEA): Technical Basis and Algorithms*. R&D Publication CLR10. Bristol: Environment Agency.

DEPARTMENT OF HEALTH, 1991. *Dietary Reference Values for Food Energy and Nutrients for the UK*. London: The Stationary Office

DEPARTMENT OF HEALTH, 2006. *Birth to five*. London: Department of Health.

DETR, ENVIRONMENT AGENCY, INSTITUTE FOR ENVIRONMENT AND HEALTH, 2000. *Guidelines for Environmental Risk Assessment and Management*. London: The Stationery Office.

DETR, 2001. *Our Towns and Cities: The Future – Delivering an Urban Renaissance*. London: The Stationery Office.

DETR, 2000. *The State of English Cities*. London: The Stationery Office.

DENVER POST 2002. *Toxic test model unreliable*. Editorial comment 13th January 2002 [on-line] http://www.denverpost.com [January 2007]

DUBOIS, D., DUBOIS, E.F., 1916. A formula to estimate the approximate surface area if height and weight be known. *Archives of Internal Medicine*, 17, 863-871.

DUGGAN, M., WILLIAMS, S., 1977. Lead in dust in city streets. *Science of the Total Environment*, 7, 91-97.

EATON, R.S., SCOTT, A.G., 1984. Understanding radon transport into houses. *Radiation Protection Dosimetry*, 7, 251-253.

ECB, 2003. *Technical Guidance Document on Risk Assessment*. Brussels: European Commission.

ENVIRONMENT AGENCY, 2009a. *Human Health Toxicological Assessment of Contaminants in Soil*. Report Final SC050021/SR2. Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2009b. *CLEA Software (Version 1.04) Handbook*, Report SC050021/SR4. Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2008c. *Compilation of Data for Priority Organic Pollutants for Derivation of Soil Guideline Values*, Report SC050021/SR7. Bristol: Environment Agency.

ENVIRONMENT AGENCY, in preparation. *Sensitivity Analysis of the CLEA Model: Critical Input Parameters and Areas of Uncertainty*. Unpublished Report SC050021/SR5. Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2006a. *Science Update on the Use of Bioaccessibility Testing in Risk Assessment of Contaminated Land*. September 2006. Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2006b. *Evaluation of Models for Predicting Plant Uptake of Chemicals from Soil.* Report SC050021/SR. Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2005a. *Review of Building Parameters for Development of a Soil Vapour Intrusion Model.* Report P5-079/PR. Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2005b. *Update on the Dermal Exposure Pathway, CLEA Briefing Note 1, Version 1.1.* Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2005c. *An Update on Deriving Soil Guideline Values Based on Combined Intake from Individual Routes of Exposure, CLEA Briefing Note 4, Version 1.0.* Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2005d. *The UK Approach for Evaluating Human Health Risks from Petroleum Hydrocarbons in Soil*. Report P5-080/TR3. Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2004a. *Update on Estimating Vapour Intrusion into Buildings, CLEA Briefing Note 2, Version 1.1.* Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2004b. *Update of Supporting Values and Assumptions Describing UK Building Stock, CLEA Briefing Note 3, Version 1.1.* Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2003. *Review of the Fate and Transport of Selected Contaminants in the Soil Environment.* Draft Technical Report P5-079/TR1. Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2002a. *Collation of Toxicological Data and Development of Guideline Values for Explosive Substances*. R&D Project Record P5-036/01. Bristol: Environment Agency.

ENVIRONMENT AGENCY, 2002b. *Vapour Transfer of Soil Contaminants*. R&D Technical Report P5-018/TR. Bristol: Environment Agency.

FERGUSON, C.C., KRYLOV, V.V., MCGRATH, P.T., 1995. Contamination of indoor air by toxic soil vapours: a screening risk assessment model. *Building and Environment*, 30, 375-383.

FERGUSON, C., MARSH, J., 1993. Assessing human health risks from ingestion of contaminated soil. *Land Contamination and Reclamation*, 1, 177-185.

FISCHER, M.L., BENTLEY, A.J., DUNKIN, K.A., HODGSON, A.T., NAZAROFF, W.W., SEXTRO, R.G., DAISEY, J.M., 1996. Factors affecting indoor air concentrations of volatile organic compounds at a site of subsurface gasoline contamination. *Environmental Science and Technology*, 30, 10, 2948-2957.

FITZPATRICK, N.A., FITZGERALD, J.J., 1996. *An evaluation of vapour intrusion into buildings through a study of field data*. Presented at the 11th Annual Conference on Contaminated Soils, University of Massachusetts at Amherst, October 1996.

FSA, 2005. *A multi-element survey of allotment produce*. Report C02043. Food Standards Agency.

GEBHARDT, S.E., THOMAS, R.G., 2002. *Nutritive Value of Foods, Home and Garden* Bulletin No. 72. Maryland: US Department of Agriculture.

GEHAN, E.A., GEORGE, S.L., 1970. Estimation of human body surface area from height and weight. *Cancer Chemotherapy Reports*, 54, 225-235.

GERSHUNY, J., 2000. *Changing Times: Work and Leisure in Post-industrial Societies*. Oxford: Oxford University Press.

GERSHUNY, J., MILES, I., JONES, S., MULLINGS, C., THOMAS, G., WYATT, S., 1986. Time budgets: preliminary analysis of a national survey, *Quarterly Journal of Social Affairs*, 2(1), 13-19.

GILLETTE, D.A., ADAMS, J., ENDO, A., SMITH, D., KIHL, R., 1980. Threshold velocities for input of soil particles into the air by desert soils. *Journal of Geophysical Research*, 85, 5621-5630.

GLA, 2006. *A lot to lose: London's disappearing allotments*. London: Greater London Authority

GREGORY, J., LOWE, S., NATES, C., PRENTICE, A., JACKSON, L., SMITHERS, G., WENLOCK, R., FARON, M., 2000. *National Diet and Nutrition Survey: Young People Aged 4 – 18 Years, Volume 1*. Norwich: The Stationery Office.

GREGORY, J., COLLINS, D., DAVIES, P., HUGHES, J., CLARKE, P., 1995. *National Diet and Nutrition Survey: Children Aged 1½ - 4½ Years, Volume 1*. Norwich: The Stationery Office.

GREEN, S.R., VOGELER, I., CLOTHIER, B.E., MILLS, T.M., VAN DEN DIJSSEL, 2003. Modelling water uptake by a mature apple tree. *Australian Journal of Soil Research*, 41, 365-380.

HALL, D.G.M., REEVE, M.J., THOMASSON, A.J., WRIGHT, V.F., 1977. *Water Retention, Porosity and Density of Field Soils. Technical Monograph No.9*. Silsoe: National Soil Resources Institute.

HARTMAN, B., 2002. Re-evaluating the upward vapour migration risk pathway. *LUSTLine Bulletin*, 41, June 2002.

HAWLEY, J.K., 1985. Assessment of health risk from exposure to contaminated soil. *Risk Analysis*, 5, 289-302.

HAYCOCK, G.B., SCHWARTZ, G.J., WISOTSKY, D.H., 1978. Geometric method for measuring body surface area: a height-weight formula validated in infants, children and adults. *Journal of Paediatrics*, 93, 62-66.

HEALTH PROMOTION ENGLAND, 2001. *Weaning Your Baby*. London: Health Promotion England.

HENDERSON, L., GREGORY, J., SWAN, G., 2002. *National Diet and Nutrition Survey: Adults Aged 19 – 64 Years, Volume 1*. Norwich: The Stationery Office.

HERS, I., ZAPF-GILJE, R., JOHNSON, P.C., LI, L., 2003. Evaluation of the Johnson and Ettinger model for prediction of indoor air quality. *Ground Water Monitoring and Remediation*, 23, 62-76.

HODGSON, J.M., 1997. *Soil Survey Field Handbook, Technical Monograph No.5.* Silsoe: National Soil Resources Institute.

HOLMES, K.K., SHIRAI, J.H., RICHTER, K.Y., KISSEL, J.C., 1999. Field measurement of dermal soil loadings in occupational and recreational activities. *Environmental Research*, 80, 148-157.

HOUSE OF COMMONS, 1950. *The Allotments Act, Section 12*. London: The Stationery Office.

HOUSE OF COMMONS, 1922. *The Allotments Act, Section 22*. London: The Stationery Office.

HUNT, A., JOHNSON, D., GRIFFITH, D., 2006. Mass transfer of soil indoors by track-in on footwear. *Science of the Total Environment*, 370, 360-371.

ICRP, 1975. *Reference Man: Anatomical, Physiological and Metabolic Characteristics*. ICRP Publication 23. Amsterdam: Elsevier Science.

IGHRC, 2006. *Guidelines on route-to-route extrapolation of toxicity data when assessing health risks of chemicals, cr12*. Bedfordshire: Institute of Environment and Health.

IPCS, 2005. *Principles of Characterizing and Applying Human Exposure Models*. Harmonization Project Document No.3. Geneva: World Health Organisation.

IPCS, 2004. *Report of the First Meeting of the IPCS Working Group on Uncertainty in Exposure Assessment in conjunction with a Scoping Discussion on Exposure Data Quality*. 19-20 August 2004. Geneva: World Health Organisation.

IPCS, 2000. *Human Exposure Assessment. Environmental Health Criteria 214*. Geneva: World Health Organisation.

ITRC, 2007. *Vapour Intrusion Pathway: A Practical Guideline*. Washington DC: The Interstate Technology and Regulatory Council.

IUPAC-NIST, 2006. IUPAC-NIST Solubility Database, NIST Standard Reference Database 106 (Updated 2006) [online]. Available from: http://srdata.nist.gov/solubility/index.asp [Accessed in January 2007]

JEFFRIES, J., 2009. *A review of body weight and height data used within the Contaminated Land Exposure Assessment model (CLEA).* Project SC050021/ Final Technical Review 1. Bristol: Environment Agency.

JOHN, M., VAN LAERHOVEN, C., 1975. Cadmium, lead and zinc accumulation in soil near a smelter complex. *Environmental Letters*, 10, 25.

JOHNSON, P.C., 2002. *Identification of Critical Parameters for the Johnson and Ettinger (1991) Vapor Intrusion Model*. API Bulletin No. 17. Washington: American Petroleum Institute.

JOHNSON, P., ETTINGER, R., 1991. Heuristic model for predicting the intrusion rate of contaminant vapours in buildings. *Environmental Science and Technology*, 25, 1445-1452.

JOHNSON, P., HERTZ, M., BYERS, D., 1990. Estimates for hydrocarbon vapor emissions resulting from service station remediations and buried gasoline-contaminated soils. In: *Petroleum Contaminated Soils, Volume 3*. KOSTECKI, P., CALABRESE, E., editors., Chelsea: Lewis Publishers, 295-326.

JOPONY, M., YOUNG, S.D., 1993. Assessment of lead availability in soils contaminated by mine spoil. *Plant and Soil*, 151, 273-278.

JURY, W., RUSSO, D., STREILE, G., EL ABD, H., 1990. Evaluation of volatilisation by organic chemicals residing below the soil surface. *Water Resources Research*, 26, 13-20.

JURY, W., SPENCER, W., FARMER, W., 1983. Behaviour assessment model for trace organics in soil: I. Model description. *Journal of Environmental Quality*, 12, 558-564.

KABATA-PENDIAS, A., 2001. *Trace elements in soils and plants*. London: CRC Press.

KEENAN, R., ALGEO, E., EBERT, E., PAUSTENBACH, D., 1993. Taking a risk assessment approach to RCA corrective action. In: *Developing Cleanup Standards for Contaminated Soil, Sediment, and Groundwater: How Clean is Clean?* Alexandria: Water Environment Federation, 225–275.

KIMBROUGH, R.D., FALK, H., STEHR, P., 1984. Health implications of 2,3,7,8-tetrachlorodibenzodioxin (TCDD) contamination of residential soil. *Journal of Toxicology and Environmental Health*, 14, 47-93.

KISSEL, J.C., RICHTER, K.Y., FENSKE, R.A., 1996. Field measurement of dermal soil loading attributable to various activities: implications for exposure assessment. *Risk Analysis*, 16, 115-125.

KRYLOV, V.V., FERGUSON, C.C., 1998. Contamination of indoor air by toxic soil vapours: the effects of subfloor ventilation and other protective measures. *Building and Environment*, 33, 331-347.

KULHANEK, A., TRAPP, S., SISMILICH, M., JANKU, J., ZIMOVA, M., 2005. Crop-specific human exposure assessment for polycyclic aromatic hydrocarbons in Czech soils. *Science of the Total Environment*, 339, 71-80.

LAGREGA, M.D., BUCKINGHAM, P.L., EVANS, J.C., 1994. *Hazardous Waste Management*. New York: McGraw-Hill Publishers.

LAHVIS, M., 2006. Alternative model-based approach for assessing vapor intrusion at petroleum hydrocarbon sites. Geological Society of America *Abstracts with Programs*, 38, 7, 373.

LAYTON, D.W., 1993. Metabolically consistent breathing rates for use in dose assessments. *Health Physics*, 64, 23-36.

LIDE, D.R., 2008. *CRC Handbook of Chemistry and Physics*. 88th Edition. Boca Raton, Florida: CRC Press.

LIJZEN, J., BAARS, A., OTTE, P., RIKKEN, M., SWARTJES, F., VERBRUGGEN, E., VAN WEZEL, A., 2001. *Technical Evaluation of the Intervention Values for Soil/Sediment and Groundwater*. RIVM Report 711701023. Bilthoven: National Institute of Public Health and the Environment.

LIOY, P.J., FREEMAN, N.C.G., MILLETTE, J.R., 2002. Dust: a metric for use in residential and building exposure assessment and source characterization. *Environmental Health Perspectives*, 110, 969-983.

LORDO, B., SANFORD, J., MOHNSON, M, 2006. *Revision of the Metabolically-Derived Ventilation Rates Within the Exposure Factors Handbook*. Battelle Institute, Columbus, OH. Prepared for USEPA/ORD, Contract No. EP-C-04-027. 18

LOUEKARI, K., MROUEH, U., MAIDELL-MUNSTER, L., VALKONEN, S., TUOMI, T., SAVOLAINEN, K., 2004. Reducing the risks of children living near the site of a former lead smelter. *The Science of the Total Environment*, 319, 65-75.

LYMAN, W.J., REEHL, W.F., ROSENBLATT, D.H., 1990. *Handbook of Chemical Property Estimation Methods.* Washington: American Chemical Society.

MAFF, 1999. *Exposure of Non-Target Organisms to Pesticides in Gardens*. Report PN0916. London: Department for Environment, Food and Rural Affairs.

MACKAY, D., 2001. *Multimedia Environmental Models: The Fugacity Approach*. Second Edition. Boca Raton: Lewis Publishers.

MACKAY, D., SHIU, W., MA, K., LEE S., 2006. *Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals*. Second Edition. Boca Raton: Taylor Francis LLC.

MAERTENS, R.M., BAILEY, J., WHITE, P.A., 2004. The mutagenic hazards of settled dust: a review. *Mutation Research*, 567, 401-425.

MAFF, 1974. *Infiltration Rates and Hydraulic Conductivity, Field Drainage Experimental Unit Technical Bulletin 74/4.* London: The Stationery Office.

MARTIN, I., FERGUSON, C., 1996. A robust risk assessment approach for predicting trace metal uptake by vegetables grown in contaminated soil. In: *Proceedings of the Third International Conference on the Biogeochemistry of Trace Metals*, Paris, France, 15-19 May 1995. (Note that paper is only available electronically on the CD accompanying the written proceedings.)

McKONE, T.E., 1990. Dermal uptake of organic chemicals from a soil matrix. *Risk Analysis*, 10, 407-419.

McKONE, T.E., DANIELS, J. I., 1991. Estimating human exposure through multiple pathways from air, water and soil. *Regulatory Toxicology and Pharmacology*, 13, 36-61.

McALARY, T., DOLLAR, P., DEHAVEN, P., WILKINSON, G., MOSS, R., LLEWELLYN, J., CRUMP, D., 2002. Assessment of subsurface vapour transport through Triassic sandstone and quarry fill into indoor air in Weston village, Runcorn, UK. In *Proceedings of Indoor Air 2002*, Monterey, California, 30th June – 5th July 2002, 902 – 907.

MERCK, 2006. *The MERCK Index*. Fourteenth Edition. (Editors) O'NEIL, M.J., HECKELMAN, P.E., KOCH, C.B., ROMAN, K.J. Whitehouse Station, New Jersey: MERCK & Co., Inc.

MET OFFICE, 2007. England [online]. Available from: http://www.metoffice.gov.uk/climate/uk/averages/index.html [Accessed January 2007]

MILLINGTON, R.J., QUIRK, J.M., 1961. *Permeability of porous solids*. Transactions of the Faraday Society, 57, 1200-1207.

MILLS, A., TYLER, H., 1992. *Food and Nutrient Intakes of British Infants Aged 6 – 12 Months.* Norwich: The Stationery Office.

MINISTRY OF HOUSING AND LOCAL GOVERNMENT, 1969. *Departmental Committee of Inquiry into Allotments [Thorpe Report].* Norwich: The Stationery Office.

MOBBS, P., 2003. *Grow Your Own Food, Free Range Practice Guide No.5* [online] Available from: http://www.fraw.org.uk [Accessed December 2006]

MONTGOMERY, J.H., 2007. *Groundwater Chemicals Desk Reference*. Fourth Edition. Boca Raton, Florida: CRC Press.

NATIONAL AUDIT OFFICE, 2004. *Early Years: Progress in Developing High Quality Childcare and Early Education Accessible to All*. HC 268. London: The Stationery Office.

NAZAROFF, W.W., NERO, A.V., 1984. Transport of radon from soil into residences. In: *Indoor Air Number 2*, BERGLUND, B., LINDVALL, T., SUNDELL, J., editors., 15-21. Stockholm: Swedish Council for Building Research.

NCSR, UCL, 2003. *Department of Epidemiology and Public Health, Health Survey for England, 2003.* March 2005. SN:5098. [computer file]. Colchester: UK Data Archive [distributor].

NIST, 1995. *Guide for the Use of the International System of Units (SI)*. NIST Special Publication 811. Washington: National Institute of Standards and Technology.

NJDEP, 2005. *Vapor Intrusion Guidance*. Trenton, NJ: New Jersey Department of Environmental Protection.

OATWAY, W.B., MOBBS, S.F., 2003. *Methodology for Estimating the Doses to Members of the Public from the Future Use of Land Previously Contaminated with Radioactivity*. NRPB-W36. Didcot: National Radiological Protection Board.

ODPM, 2004a. *Planning Policy Statement 23: Planning and Pollution Control*. London: Office of the Deputy Prime Minister.

ODPM, 2004b. *Planning Policy Statement 23: Planning and Pollution Control. Annex 2: Development on Land Affected by Contamination.* London: Office of the Deputy Prime Minister.

OFFICE OF NATIONAL STATISTICS, 2006a. *Data from the Time Use Survey 2000*. [online] Available from: http://www.statistics.gov.uk [Accessed July 2006]

OFFICE OF NATIONAL STATISTICS, 2006b. *Regional Trends No. 39.* London: The Stationery Office. Available from: http://www.statistics.gov.uk [Accessed January 2007]

OFFICE OF NATIONAL STATISTICS, 2006c. *Data from the Annual Business Inquiry, Whole Economy Statistics for Sectors A-O*, 22nd November 2006 as Excel spreadsheet. [online] Available from: http://www.statistics.gov.uk [Accessed January 2007]

OFFICE OF NATIONAL STATISTICS, 2003. *Length of Service of Employees 2002: Social Trends 33.* [online] Available from http://www.statistics.gov.uk [Accessed January 2007]

OFFICE OF NATIONAL STATISTICS, 2002a. *UK Standard Industrial Classification of Economic Activities 2003*. Report UK SIC (2003). London: The Stationery Office.

OFFICE OF NATIONAL STATISTICS, 2002b. *Length of Service of Employees 1986 – 2000: Social Trends 31.* [online] Available from: http://www.statistics.gov.uk [Accessed July 2006]

OFFICE OF NATIONAL STATISTICS, 2002c. *Holidays taken by Great Britain residents: by number taken per year 1971-1998: Social Trends 31.* [online] Available from: http://www.statistics.gov.uk [Accessed July 2006]

OOMEN, A.G., LIJZEN, J.P.A., 2004. *Relevancy of human exposure via house dust to the contaminants lead and asbestos*. RIVM Report 711701037/2004. Bilthoven: National Institute of Public Health and the Environment.

OTTE, P., LIJZEN, J., OTTE, J., SWARTJES, F., VERSLUIJS, C., 2001. Evaluation *and revision of the CSOIL parameter set*. RIVM Report 711701021. Bilthoven: National Institute of Public Health and the Environment.

PAUSTENBACH, D.J., 2000. The practice of exposure assessment: a state of the art review. *Toxicology and Environmental Health*, Part B, 3, 179-291.

PAUSTENBACH, D.J., FINLEY, B.L., LONG, T.F., 1997. The critical role of house dust in understanding the hazards posed by contaminated soils. *International Journal of Toxicology*, 16, 339-362.

POLLOCK, M., 2002. *Royal Horticultural Society: Fruit and Vegetable Gardening*. London: DK Publishing.

POUT, C., MACKENZIE, F., BETTLE, R., 1998. *Non-Domestic Building Energy Fact File*. January 1998. London: CRC Press.

RASMUSSEN, P.E., 2004. Can metal concentrations in indoor dust be predicted from soil geochemistry? *Canadian Journal of Analytical Sciences and Spectroscopy*, 49, 166-174.

RASMUSSEN, P.E., SUBRAMANIAN, K.S., JESSIMAN, B.J., 2001. A multi-element profile of house dust in relation to exterior dust and soils in the city of Ottawa, Canada. *The Science of the Total Environment*, 267, 125-140.

REED CONSULTING, 2005. *Employee Attrition. Causes, Effects and Retention Strategies.* [online] Available from: http://reed.co.uk/consulting [Accessed July 2006]

RIKKEN, M.G.J., LIJZEN, J.P.A., CORNELESE, A.A., 2001. *Evaluation of model concepts on human exposure. Proposals for updating the most relevant exposure routes of CSOIL*. RIVM Report 711701022. Bilthoven: National Institute of Public Health and the Environment.

RIEUWERTS, J.S., SEARLE, P., BUCK, R., 2006. Bioaccessible arsenic in the home environment in south west England. *Science of the Total Environment*, 371, 89-98.

ROBERTS, J.W., CAMANN, D.E., SPITTLER, T.M., 1990. Monitoring and controlling lead in house dust in older homes. In: *Proceedings of the Fifth International Conference on Indoor Air*, held in Toronto, Canada.

ROBINSON, N.I., TURCZYNOWICZ, L., 2005. One- and three-dimensional soil transportation models for volatiles migrating from soils to house interiors. *Transportation in Porous Media*, 59, 301-323.

ROBINSON, N., 2003. *Modelling the migration of VOCs from soils to dwelling interiors*. In: Proceedings of the Fifth National Workshop on the Assessment of Site Contamination, LANGLEY, A., GILBEY, M., KENNEDY, B., editors., Adelaide: National Environment Protection Council, 47-71.

ROGGEMANS, S., BRUCE, C.L., JOHNSON, P.L., JOHNSON, R.L., 2001. Vadose zone natural attenuation of hydrocarbon vapors: an empirical assessment of soil gas vertical profile data. *American Petroleum Institute Bulletin*, 15, 12.

ROZIN, P., FALLON, A., 1987. A perspective on disgust. *Psychological Review*, 94, 23-41.

ROWELL, D.L., 1994. *Soil Science Methods and Applications*. Harlow: Longman Scientific and Technical

RYAN, J.A., BELL, R.M., DAVIDSON, J.M., OCONNOR, G.A., 1988. Plant uptake of non-ionic organic chemicals from soils. *Chemosphere*, 17, 2299-2323.

SALTELLI, A., TARANTOLA, S., CAMPOLONGO, F., RATTO, M., 2004. *Sensitivity analysis in practice: A guide to assessing scientific models*. London: John Wiley & Sons Ltd.

SAMSØE-PETERSEN, L., LARSEN, E.H., LARSEN, P.B., BRUUN, P., 2002. Uptake of trace elements and PAHs by fruit and vegetables from contaminated soils. *Environmental Science and Technology*, 36, 3057-3063.

SAMSØE-PETERSEN, L., RASMUSSEN, D., TRAPP, S., 2003. *Modellering af optagelse af organiske stoffer i grøntsager og frugt*. Report 765. In Danish with extended English summary. Copenhagen: Danish Environmental Protection Agency.

SAUNDERS, P., 1993. *Towards Allotments 2000, National Survey of Allotment Gardeners Views in England and Wales*. Corby: National Society of Allotment and Leisure Gardeners Ltd.

SCETRA, 1998. *The Future for Allotments*. Fifth Report of the House of Commons Select Committee on Environment, Transport and Regional Affairs. London: The Stationery Office.

SHELDRAKE, S., STIFELMAN, M., 2003. A case study of lead contamination cleanup effectiveness at Bunker Hill. *The Science of the Total Environment*, 303, 105-123.

SHEPPARD, S.C., 1995. A model to predict concentration enrichment of contaminants on soil adhering to plants and skin. *Environmental Geochemistry and Health*, 17, 13-20.

SHEPPARD, S.C., EVENDEN, W.G., 1994. Contaminant enrichment and properties of soil adhering to skin. *Journal of Environmental Quality*, 23, 604-613.

SHEPPARD, S.C., EVENDEN, W.G., 1992. Concentration enrichment of sparingly soluble contaminants (U, Th, and Pb) by erosion and by soil adhesion to plants and skin. *Environmental Geochemistry and Health*, 14, 121-131.

SHEPPARD, M., THIBAULT, D., 1990. Default soil solid/liquid partition coefficients, K_dS, for four major soil types: a compendium. *Health Physics*, 59, 471-482.

SHU, H., PAUSTENBACH, D., MURRAY, F.J., MARPLE, L., BRUNCK, B., DEI ROSSI, D., TEITELBAUM, P., 1988. Bioavailability of soil-bound TCDD: dermal bioavailability in the rat. *Fundamentals of Applied Toxicology*, 10, 648-654.

SIMMONDS, J.R., LAWSON, G., MAYALL, A., 1995. *Methodology for Assessing the Radiological Consequences of Routine Releases of Radionuclides to the Environment*. Report EUR 15760. Brussels: European Commission.

SMALL BUSINESS SERVICE, 2006a. *A Government Action Plan for Small Business. Making the UK the Best Place in the World to Start and Grow a Business. The Evidence Base.* [online] Available from http://www.sbs.gov.uk [Accessed January 2007]

SMALL BUSINESS SERVICE, 2006b. *SME statistics 2005*. [online] Available from http://www.sbs.gov.uk [Accessed April 2007]

SMITH, K.R., JONES, A.L., 2003. *Generalised habit data for radiological assessments*. NRPB-W41. Didcot: National Radiological Protection Board.

STANEK, E.J., CALABRESE, E.J., BARNES, R., PEKOW, P., 1997. Soil ingestion in adults – results of a second pilot study, *Ecotoxicology and Environmental Safety*, 36, 249-257.

STANEK, E.J., CALABRESE, E.J., 2000. Daily soil ingestion estimates for children at a Superfund site. *Risk Analysis*, 20, 627-635.

STANEK, E.J., CALABRESE, E.J., 1995. Daily estimates of soil ingestion in children. *Environmental Health Perspectives*, 103, 276-285.

STANEK, E.J., CALABRESE, E.J., 1994. Bias and the detection limit model for soil ingestion. *Journal of Soil Contamination*, 3, 183-189.

STANEK, E.J., CALABRESE, E.J., 1992. Soil ingestion in children: outdoor soil or indoor dust? *Journal of Soil Contamination*, 1, 1-28.

STANEK, E.J., CALABRESE, E.J., MUNDT, K., PEKOW, P., YEATTS, K.B., 1998. Prevalence of soil mouthing/ingestion among healthy children aged one to six. Journal of *Soil Contamination*, 7, 227-242.

STANEK, E.J., CALABRESE, E.J., ZORN, M., 1999. *Development of Exposure Distribution Parameters for Use in Monte Carlo Risk Assessment of Exposure Due to Soil Ingestion*. Final Report. Denver: United States Environmental Protection Agency Region 8.

THATCHER, T.L., LAYTON, D.W., 1995. Deposition, resuspension, and penetration of particles within a residence. *Atmospheric Environment*, 29, 1487-1497.

THOMPSON, K.M., BURMASTER, D.E., 1991. Parametric distributions for soil ingestion by children. *Risk Analysis*, 11, 339-342.

THORNE, M., MAUL, P., ROBINSON, P., 2004. *The PRISM Foodchain Modelling Software, Model Structures for PRISM 2, QRS-1198A-1.* London: Food Standards Agency.

THORNE, M., MAUL, P., ROBINSON, P., 2005. *The PRISM Foodchain Modelling Software, Parameter Values for the Soil/Plant Model, QRS-1198A-3, version 1.1.* London: Food Standards Agency.

TPHCWG, 1999. *Human Health-Based Risk Evaluation of Petroleum Release Sites*. Total Petroleum Hydrocarbon Criteria Working Group, Volume 5. Amherst: Amherst Scientific Publishers.

TRAPP, S., CAMMARANO, A., CAPRI, E., REICHENBERG, F., MAYER, P., 2007. Diffusion of PAH in potato and carrot slices and application for a potato model. *Environmental Science and Technology*, 41, 3103-3108.

TRAPP, S., RASMUSSEN, D., SAMSØE-PETERSEN, L., 2003. Fruit tree model for uptake of organic compounds from soil. *Environmental Research*, 14, 17-26.

TRAPP, S., 2002. Dynamic root uptake model for neutral lipophilic organics. *Environmental Toxicology and Chemistry*, 21, 203-206.

TRAPP, S., SCHWARTZ, S., 2000. Proposals to overcome limitations in the EU chemical risk assessment scheme. *Chemosphere*, 41, 965-971.

TRAVIS, C.C., ARMS, A.D., 1988. Bioconcentration of organics in beef, milk, and vegetation. *Environmental Science and Technology*, 22, 271-274.

TURCZYNOWICZ, L., ROBINSON, N., 2001. A model to derive soil criteria for benzene migrating from soil to dwelling interior in homes with crawl spaces. *Human and Ecological Risk Assessment*, 7, 387-415.

URBAN TASK FORCE, 1999. *Towards an Urban Renaissance*. Final Report of the Urban Task Force. London: Taylor and Francis.

USEPA, 2007. Diffusion Coefficient Estimation, EPA On-line Tools for Site Assessment Calculation. [on-line] Available from http://www.epa.gov/athens/learn2model/part-two/onsite/estdiffusion.htm [Accessed January 2007]

USEPA, 2006. *Child-Specific Exposure Factors Handbook (External Review Draft.* September 2006, Report EPA/600/R/06/096A. Washington: United States Environmental Protection Agency.

USEPA, 2004a. *Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment),* Final Report EPA/540/R/99/005. Washington: United States Environmental Protection Agency.

USEPA, 2004b. *Additional and current dermal absorption fraction values for soil (ABS_d)* (Supplementing Exhibit 3-4 of Part E) [online]. Available from www.epa.gov/oswer/riskassessment/ragse/index.htm [Accessed 15 January 2007].

USEPA, 2003. *User's Guide for Evaluating Subsurface Vapour Intrusion into Buildings*. Report PN 030224.0001. Washington: United States Environmental Protection Agency.

USEPA, 2002a. *Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites*. Report OSWER 9355.4-24. Washington: United States Environmental Protection Agency.

USEPA, 2002b. *OSWER Draft Guidance for Evaluating the Vapour Intrusion to Indoor Air Pathway from Groundwater and Soils (Subsurface Vapour Intrusion Guidance).* Report EPA 530-D-02-004. Washington: United States Environmental Protection Agency.

USEPA, 2000. *TRW Recommendations for Sampling and Analysis of Soil at Lead (Pb) Sites*. EPA 540-F-00-010. Washington: United States Environmental Protection Agency.

USEPA, 1999. *Overview of the IEUBK model for lead in children.* Guidance document EPA 540-R-99-015. Washington: United States Environmental Protection Agency.

USEPA, 1998. *IEUBK model mass fraction of soil in indoor dust (M_{sd}) variable.* Guidance document EPA 540-F-00-008. Washington: United States Environmental Protection Agency.

USEPA, 1997a. *Guiding Principles for Monte Carlo Analysis*. Report EPA/630/R-97/001. Washington: United States Environmental Protection Agency.

USEPA, 1997b. *Exposure Factors Handbook*. August 1997. Washington: United States Environmental Protection Agency.

USEPA, 1996. *Soil Screening Guidance: Technical Background Document*. Report EPA/540/R95/128. Washington: United States Environmental Protection Agency.

USEPA, 1994. *Guidance Manual for the Integrated Exposure Uptake Biokinetic Model for Lead in Children*. Report EPA/540/R-93/081. Washington: United States Environmental Protection Agency.

USEPA, 1992. *Dermal Exposure Assessment: Principles and Applications*. Report EPA/600/8-9/011B. Interim Report. Washington: United States Environmental Protection Agency.

USEPA, 1985. *Development of Statistical Distributions or Ranges of Standard Factors Used in Exposure Assessments*. Report EPA/600/8-85/010. Washington: United States Environmental Protection Agency.

VAN DEN BERG. R., 1994. *Human Exposure to Soil Contamination: A Qualitative and Quantitative Analysis Towards Proposals for Human Toxicological Intervention Values*. RIVM Report 725201011. Bilthoven: National Institute of Public Health and the Environment.

VAN GENUCHTEN, M.T., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Journal of the American Soil Science Society*, 44, 892-898

VAN GENUCHTEN, M.T., LEIJ, F.J., YATES, S.R., 1991. *The RETC Code for Quantifying the Hydraulic Functions of Unsaturated Soils*. EPA/600/2-91/065. Oklahoma: United States Environmental Protection Agency

VAN WIJNEN, J.H., CLAUSING, P., BRUNEKREEF, B., 1990. Estimated soil ingestion by children. *Environmental Research*, 51, 147-162.

VAN WIJNEN, H., LIJZEN, J., 2006. *Validation of the VOLASOIL Model Using Air Measurements from Dutch Contaminated Sites: Concentrations of Four Chlorinated Compounds*. RIVM Report 711701041/2006. Bilthoven: National Institute of Public Health and the Environment.

VON LINDERN, I.H., SPALINGER, S.M., BERO, B.N., PETROSYAN, V., VON BRAUN, M.C., 2003. The influence of soil remediation on lead in house dust. *Science of the Total Environment*, 303, 59-78.

WAITZ, M., FREIJER, J., KREULE, P., SWARTJES, F., 1996. *The VOLASOIL Risk Assessment Model Based on CSOIL for Soils Contaminated with Volatile Compounds*. RIVM Report 715810014. Bilthoven: National Institute of Public Health and the Environment.

WORLD HEALTH ORGANISATION, 1990. *International Classification of Diseases*. Tenth Revision. Available from: http://www.who.int/classifications/apps/icd/icd10online/ [Accessed 14 February 2007]

ZARTARIAN, V.G., XUE, J., OZKAYNAK, H., DANG, W., GLEN, G., SMITH, L., STALLINGS, C., 2005. *A Probabilistic Exposure Assessment for Children Who Contact CCA-Treated Playsets and Decks*. Washington: United States Environmental Protection Agency.

List of abbreviations

ABS	Dermal absorption fraction
AC	Assessment criteria
ach	Air exchanges per hour
ADE	Average Daily Exposure
AERMOD PRIME	Air dispersion model developed by the US Environmental Protection Agency
AF	Soil-to-skin adherence factor
ALARP	As low as reasonably practicable
AQMAU	Air Quality Modelling and Assessment Unit (Environment Agency)
ASTM	American Society for Testing and Materials
AT	Averaging time
BRE	Building Research Establishment
BTEX	Benzene, toluene, ethylbenzene and xylene
bw	Body weight
C-SOIL	Dutch model for estimating human exposure to chemicals in soil
CF	Soil-to-plant concentration factor
CIRIA	Construction Industry Research and Information Association
CLEA	Contaminated Land Exposure Assessment
CODATA	Committee on Data for Science and Technology for international use
CSTEE	Scientific Committee on Toxicity, Ecotoxicity and the Environment
DCLG	Department for Communities and Local Government
DEFRA	Department for Environment, Food and Rural Affairs

DETR	Department of Environment, Transport and the Regions
DL	Dust loading
DQRA	Detailed Quantitative Risk Assessment
dw	Dry weight
ECB	European Chemicals Bureau
ED	Exposure duration
EF	Exposure frequency
EHCS	English House Condition Survey
FARMLAND	Food Activity from Radionuclide Movement on LAND
FSA	Food Standards Agency
fw	Fresh weight
GAC	Generic Assessment Criteria
GLA	Greater London Authority
HCV	Health Criteria Value(s)
HI	Hazard Index
HLC	Henry’s Law constant
HPA	Health Protection Agency
HQ	Hazard Quotient
ICRP	International Commission on Radiological Protection
ID	Index Dose
IGHRC	Interdepartmental Group on Health Risks from Chemicals
IPCS	International Programme on Chemical Safety (World Health Organisation)

IR	Chemical intake/uptake rate
ITRC	Interstate Technology and Regulatory Council
IUPAC	International Union for Pure and Applied Chemistry
MAFF	Ministry of Agriculture, Fisheries and Food
MDI	Mean Daily Intake
NAPL	Non-aqueous phase liquid
NCSR	National Centre for Social Research
NDNS	National Diet and Nutrition Survey
NIST	National Institute of Standards and Technology
NJDEP	New Jersey Department of Environmental Protection
NRPB	National Radiological Protection Board
NSRI	National Soil Resources Institute
ODPM	Office of the Deputy Prime Minister
PAH	Polycyclic aromatic hydrocarbons
PCB	Polychlorinated biphenyls
PEF	Particulate Emission Factor
PRISM	Foodchain model used by the Food Standards Agency
QSAR	Quantitative Structure Activity Relationships
RBCA	Risk-Based Corrective Action
RIVM	National Institute for Public Health and the Environment
SCETRA	Select Committee on Environment, Transport and Regional Affairs
SCF	Soil-to-plant stem concentration factor

SEH	Survey of English Housing
SGV	Soil Guideline Value
SI	International System of Units
SOM	Soil organic matter
SSAC	Site-Specific Assessment Criteria
TDI	Tolerable Daily Intake
TDSI	Tolerable Daily Soil Intake
TOX	TOX guidance report (Environment Agency)
TPH	Total Petroleum Hydrocarbons
TPHCWG	Total Petroleum Hydrocarbons Criteria Working Group
UCL	University College London
UK	United Kingdom
USEPA	United States Environmental Protection Agency
VOC	Volatile organic compounds
VOLASOIL	Dutch model for assessing vapour intrusion into buildings

Glossary

Activity patterns	Time-use studies explore how children and adults spend their time and the types, duration and location of activities including eating, sleeping, working, and playing. Such activities that occur regularly according to discrete boundaries such as land use can be grouped together to form a pattern of behaviour that can be used to predict likely exposure.
Advection	The movement of a fluid (liquid, gas) as part of the bulk movement of air and water, under the influence of differences in pressure, temperature and density between locations.
Adverse effect	A change in morphology, physiology, growth, development, reproduction, or lifespan of an organism which results in impairment of functional capacity or impairment of capacity to compensate for additional stress or increase in susceptibility to the harmful effects of other environmental influences. Decisions on whether or not any effect is adverse require expert judgement.
Age classes	System used by the CLEA model to divide human exposure into discrete time periods, where exposure characteristics change over a human lifetime. There are eighteen age classes, sixteen covering childhood from birth to sixteen years old, and two covering the working and retirement periods of adult life.
Air dispersion factor	Describes the dispersion of fugitive dusts emitted from soils and is defined as the inverse of the ratio of geometric mean air concentration to the emission/flux at the centre of the source
ALARP principle	The ALARP principle ensures that, irrespective of whether a health-based guideline is being breached or not, exposures must be kept 'as low as reasonably practicable'.
Algorithms	A well-defined list of mathematical instructions which describe generalised processes.
Aqueous nutrient solution	Mineral nutrient solutions used to cultivate plants without the use of soil.
Aqueous phase	Chemical dissolved in water.
Aqueous solubility	Amount of a chemical dissolved in water, at a given temperature.
Assessment criteria	Criteria used to evaluate contaminant concentrations, derived using a generic or site-specific set of factors for the characteristics and behaviour of contaminants, pathways and receptors, which are designed to be protective of human health in a range of defined conditions.
Attenuation factor	Ratio of chemical concentration between two media, assuming that the concentration decreases from the source media to the receptor media. For example, the attenuation factor from the soil gas to the indoor air is used to assess vapour intrusion.

Average daily exposure	The average daily amount of a contaminant per kg bodyweight, which a critical human receptor might take in over the duration of exposure.
Averaging time	Time period over which aggregated exposure is averaged to derive a daily exposure that can be compared to a relevant Health Criteria Value. In deriving Soil Guideline Values, averaging time is equal to the exposure duration.
Background sources	Sources of human exposure to a chemical other than the soil itself, either directly or indirectly. For example, ambient air, diet, and drinking water.
Backward mode	Use of a computer model to calculate the soil concentration that would result in a prescribed level of human exposure using assumptions about exposure characteristics.
Bioaccessibility	The degree to which a chemical is released from soil into solution (and thereby becomes available for absorption) when that soil is ingested and undergoes digestion.
Bioavailability	The degree to which a substance is absorbed and becomes available to the target tissue (that is, without first being metabolised).
Building ventilation	The exchange of indoor and outdoor air through circulation within the building, either naturally through cracks in doors and windows or mechanically by air conditioning or fans.
Cation exchange capacity	A measure of the number of sites on soil surfaces that can retain positively charged ions (cations) by electrostatic forces.
Chemical gradient	The graduated difference in concentration of a chemical per unit distance within a media or between media (for example, within a soil solution or between soil and air).
Chemical intake/uptake rate	The daily amount of a soil contaminant expressed as an intake or an uptake from exposure to chemicals in soil, food, water and air.
Chemical lipophilicity	A chemicals affinity for, tendency to combine with, or preference to dissolve in lipids (fats)
Conceptual model	A representation of the characteristics of a site in diagrammatic or written form that shows the possible relationships between contaminants, pathways and receptors.
Critical adverse effect	The adverse effect judged to be the most important for setting a **Health Criteria Value**. This is usually the most sensitive adverse effect (that is, the lowest effect level) or sometimes a more serious effect, not necessarily having the lowest effect level.
Critical receptor	The individuals or subgroup of the population most likely to be exposed and/or susceptible to the presence of soil contamination.

Darcy’s Law	Physical law that describes the proportional relationship between the instantaneous discharge rate through a porous medium, the viscosity of the fluid and the pressure drop over a given distance. It is used to quantify the flow of a fluid through a porous media.
Dermis	One of the layers of mammalian skin which consists of connective tissue, hair follicles, glands and blood vessels. It is located below the outer skin (epidermis).
Detailed quantitative risk assessment	The purpose of detailed quantitative risk assessment is to establish and use more detailed site-specific information and criteria to decide whether there are unacceptable risks. It may be used as the sole method for quantitative risk assessment of risks, or it may be used to refine earlier assessments using generic assessment criteria.
Deterministic model	One in which the variables are given fixed values, so that the system is at any time entirely defined by the initial/boundary conditions chosen. A given set of input variables produces a fixed output.
Dermal absorption fraction	An empirical measure of the proportion of chemical compound in soil that is absorbed through the skin by a typical soiling event.
Diffusion	Random movement of molecules due to their inherent kinetic energy.
Diffusion coefficient	Proportionality coefficient from Fick’s first law of diffusion.
Dose-response relationship	Relationship between the dose of a chemical taken into an organism and the response (in the form of a measured biological, systemic or physiological effect) that is detected.
Dual porosity	In hydrogeology, it is the presence of two different porosity systems within a porous media that alter the flow of water or gas, often at different scales. For example, the flow of a fluid through a fractured sandstone system must account for flow within the sandstone and along its fractures. It is also known as double porosity.
Dynamic effect	Pressure driven air flow into a building as a result of differences across a structure induced by wind speed and direction.
Emission flux	Rate at which particles of dust or vapour are released from a surface.
Empirical model	A model based only on experimental observation that is used to establish plausible relationships between parameters.
Epidermis	Outer skin layer which forms a waterproof protective layer.
Epidemiological studies	The study of the incidence, prevalence and distribution of diseases (or injuries) in human populations in order to ascertain the determinants or causes of those diseases.

Exposure	Contact between a chemical and the external surfaces of the human body. Quantitatively, it is the amount of a chemical that is available for intake by a target receptor/population. Exposure may be quantified as the dose or the concentration of the chemical in the medium (for example, air, water, food) integrated over the duration of exposure, expressed in terms of mass of substance per kg of soil, cubic metre of air, or litre of water.
Exposure assessment	The process of estimating or measuring the magnitude, frequency, and duration of exposure to an agent, along with the number and characteristics of the population exposed. Ideally, it describes the sources, pathways, routes, and uncertainties in the risk assessment.
Exposure characteristics	Physiological and behavioural characteristics such as body weight, body height, consumption rates, and activity patterns that influence the amount of exposure to soil contaminants for the critical receptor.
Exposure duration	The specified period of exposure in years over which the chemical intake/uptake rate for a critical receptor is accumulated
Exposure frequency	The number of days per year in which a daily exposure event is considered to occur.
Exposure pathway	Route through the environment by which a receptor plausibly comes into contact with a chemical in or derived from soil.
Exposure scenario	A specific conceptual model that sets out a discrete set of circumstances where exposure may occur including the source, the pathways, the exposed population, and the time frame of exposure.
Fick's law	A law relating the rate of diffusion of a substance in a given direction to the gradient of its concentration.
Forward mode	Use of a computer model to calculate human exposure from a prescribed soil concentration using assumptions about exposure characteristics.
Free-phase	Chemical present in soil or water in its natural physical form under ambient conditions, for example, solid, liquid or gas.
Fugacity	A measure of the preference of a substance to one phase (that is, solid, liquid or gas) over another, at a specific temperature and pressure.
Gaussian distribution	A mathematical solution for the observed dispersion of particles in three dimensions from a source.
Generic assessment criteria	Criteria derived using largely generic assumptions about the characteristics and behaviour of sources, pathways and receptors. These assumptions will be conservative in a defined range of conditions.

Generic quantitative risk assessment	The purpose of generic quantitative risk assessment is to establish whether generic assessment criteria and assumptions are appropriate for assessing the risks, and, if so, to apply them to establish whether there are actual or potential unacceptable risks.
Geometric mean	The n^{th} root of the product of all the numbers of a dataset.
Health Criteria Value	A generic term used in this report to describe a benchmark level of exposure to a chemical derived from available toxicity data for the purposes of safeguarding human health (for example, a **Tolerable Daily Intake**).
Index Dose	The term used in this report to refer to an estimate of the amount of a soil contaminant (expressed as a daily intake) that can be experienced over a lifetime with minimal cancer risk.
Intake	Amount of a chemical entering the human body at the point of entry (that is, mouth, nose or skin) by ingestion, inhalation, or skin contact.
Lipophilic tendency	Literally 'fat-loving', the term lipophilic is used to describe compounds with a high solubility in fat and low aqueous solubility. Such substances will have a high octanol-water partition coefficient (K_{ow}).
Mean daily intake	The average intake of a soil contaminant from other, non-soil, sources, expressed as an amount per day. The mean daily intake is estimated for each route of exposure and arises principally from exposure to the contaminant in food, water, and air.
Mechanistic model	A model that establishes a plausible relationship between parameters based on theoretical understanding of the processes and mechanisms that give rise to the system being investigated.
Mode of action	The collective key biochemical events that are initiated or altered by the chemical that result in observed adverse effects.
Monolayer saturation	Theoretical circumstance where a surface is exactly covered by a single layer of particles.
Particle Emission Factor (PEF)	The relationship between the concentration of a contaminant in soil and its concentration in air as a consequence of dust resuspension.
Partition coefficient	The experimental or calculated ratio of the concentrations of the same chemical species in two phases.
Pharmacokinetic models	A mathematical scheme used to describe physiological processes, such as chemical distributed within the body.
Phloem	A complex tissue in the vascular system of higher plants that consists mainly of sieve tubes and elongated cells usually with fibres and that functions in translocation and in support and storage.

Pica	Persistent eating of non-nutritive substances (such as soil, paint chippings). It may occur as one of many symptoms that are part of a more widespread psychiatric disorder (such as autism), or as a relatively isolated psychopathological behaviour; only the latter is classified separately by the International Classification of Diseases.
Pollutant linkage	The particular combination of a contaminant, pathway and receptor.
Porosity	Fraction of void space within a porous media such as a rock or soil.
Quantitative Structure Activity Relationships	Estimation methods developed and used to predict certain effects or properties of chemical substances that are primarily based on the structure of the substance. They have been developed on the basis of experimental data on model substances.
Residual phase contamination	See free-phase contamination.
Route-to-route extrapolation	The prediction of the total amount of a substance administered by one route of exposure that would produce the same toxic endpoint or response to that obtained for a given amount of that substance administered by another route.
Sensitivity analysis	Study of the variation in output of a mathematical model with respect to changes in input values. Often the analysis attempts to identify those variables with the greatest influence on outputs and the areas of greatest uncertainty/variability.
Site occupancy	Amount of time each day that the critical receptor spends either indoors or outdoors according to the activity pattern for the land use scenario.
Site-specific assessment criteria	Values for concentrations of contaminants that have been derived using detailed site-specific information on the characteristics and behaviour of contaminants, pathways and receptors, and that correspond to relevant criteria in relation to harm or pollution for deciding whether there is an unacceptable risk.
Soil gas	The gaseous elements and compounds in the small spaces between particles of soil.
Soil Guideline Values	Non-statutory and scientifically based generic assessment criteria for assessing the risk to human health from chronic exposures to chemicals in soil.
Soil-to-plant concentration factor	Empirical ratio of the amount of chemical in edible plant fractions to the amount in the soil in which the plant is grown.
Soil vapour	The gaseous elements and compounds from a soil source found within the small spaces within and between the fabric and structure of buildings.
Sorbed phase	Chemical in soil that is sorbed reversibly to the surfaces of soil particles and organic matter.
Stack effect	Pressure driven flow into a structure as a result of the temperature difference between indoor air and outdoor air.

Stochastic model	One that takes into consideration the presence of some randomness in one or more of its input parameters or variables. It predicts the probabilities of occurrences of exposures in a population. Random model input variables are represented as probability density distributions from which values are selected randomly and substituted into the equations of the model to produce an output.
Systemic circulation	The part of the blood system that transports blood from the heart to and from the rest of the body, except for the lungs which have their own circulatory system (the pulmonary circulation). In toxicology, the term is usually used to describe the main blood circulatory system that is reached by a chemical (or the proportion of a chemical dose) after being absorbed and successfully bypassing first-pass metabolism.
Systemic dose	The amount of a chemical that reaches the main blood circulation system unchanged following absorption and successfully bypassing first-pass metabolism.
Systemic effect	An effect of a chemical that is either of a generalised nature or that occurs at a site distant from the site of entry of the chemical.
Threshold friction velocity	An empirical measure of the wind speed needed to erode particles from a surface.
Tolerable Daily Intake	Originally defined as an estimate of the amount of a soil contaminant, expressed on a body weight basis, that can be ingested daily over a lifetime without appreciable health risk, the term has been expanded to apply to exposure via inhalation and dermal contact.
Tolerable Daily Soil Intake	The portion of the **Tolerable Daily Intake** of a contaminant that is allocated to exposure from soil, once background exposure from other sources (the **mean daily intake**) has been accounted for.
Toxicity	The inherent property of a substance to cause injury or an **adverse effect** in a living organism.
Transpiration rate	Rate at which plants take up water through their roots from soil. Water is usually lost through evaporation from leaf surfaces.
Uncertainty	A lack of knowledge about specific factors in a risk or exposure assessment including parameter uncertainty, model uncertainty and scenario uncertainty.
Uptake	The amount of a contaminant that enters the body having been absorbed through the skin, the gastrointestinal system and/or the pulmonary system (lungs).
Vapour intrusion	Generic term used to describe the migration of volatile chemicals in soil gas from the subsurface into overlying buildings.
Variability	A type of uncertainty, referring to natural or inherent differences in a sampled population. For example, the changing soil concentration across a site or the heights of people of the same age in the UK.

Xylem	A complex tissue in the vascular system of higher plants that functions chiefly in the conduction of water and dissolved minerals but also in the support of food storage, and typically constitutes the woody element.

Appendix 1

Equations for calculating the volumetric flow rate of soil gas into buildings

Indoor Vapour Intrusion

Equation A1: Area of enclosed space below ground

$$A_b = (A_{foot} + (4H_{cellat}\sqrt{A_{foot}})) \quad \times \quad 10000\ cm^2\ m^{-2}$$

Where A_b is the area of enclosed space below ground, cm^2
A_{foot} is the building footprint in contact with contaminated soil, m^2
H_{cellar} is the height of living space below ground, m

Note that the area of enclosed space below ground is equal to the floor area where the living space height below ground is zero. Where the height of living space below ground level is greater than zero, the area below ground includes the area of floors and walls (USEPA, 2003). The building dimensions are assumed to be square.

Equation A2: Floor-wall seam perimeter

$$X_{crack} = 4\sqrt{A_{foot}} \quad \times \quad 100\ cm\,m^{-1}$$

Where X_{crack} is the floor-wall seam perimeter, cm
A_{foot} is the building footprint, m^2

Note that the perimeter is four times the length of the building. The building dimensions are assumed to be square (USEPA, 2003).

Equation A3: Effective crack radius

$$r_{crack} = \frac{A_{crack}}{X_{crack}}$$

Where r_{crack} is the effective crack radius, cm
X_{crack} is the floor-wall seam perimeter, cm
A_{crack} is the floor crack area, cm^2

This relationship holds while the ratio of A_{crack} / A_b is between zero and one (where A_b is the area of the enclosed floor and walls below ground, cm^2). Reference is Equation 10 of Appendix 1 of CLEA Briefing Note 2.

Equation A4: Effective total fluid saturation

$$S_{te} = \frac{(\theta_w - \theta_r)}{(\theta_t - \theta_r)}$$

Where S_{te} is the effective total fluid saturation, unitless
θ_w is the water-filled soil porosity, cm^3 cm^{-3}
θ_r is the residual soil water content, cm^3 cm^{-3}
θ_t is the total soil porosity, cm^3 cm^{-3}

Equation A5: Relative soil air permeability

$$k_{rg} = (1 - S_{te})^{0.5}(1 - S_{te}^{\ 1/M})^{2M}$$

Where k_{rg} is the relative air permeability, unitless
S_{te} is the effective total fluid saturation, unitless
M is the van Genuchten shape parameter, unitless

Equation A6: Soil intrinsic permeability

$$k_i = \frac{K_s\,\mu_w}{\rho_w\,g}$$

Where k_i is the soil intrinsic permeability, cm^2
K_s is the soil saturated hydraulic conductivity, cm s^{-1}
μ_w is the dynamic viscosity of water, g cm^{-1} s^{-1} [= 0.01307]
ρ_w is the density of water, g cm^{-3} [= 0.999]
g is the acceleration due to gravity, cm s^{-2} [= 980]

Equation A7: Effective air permeability

$$k_v = k_i k_{rg}$$

Where k_v is the effective air permeability, cm^2
k_i is the soil intrinsic permeability, cm^2
k_{rg} is the relative air permeability, unitless

Equation A8: Effective air viscosity

$$\mu_a = 0.00018\sqrt{\left(\frac{T_{amb}}{T_{ref}}\right)}$$

Where μ_a is the air viscosity at ambient temperature, g cm^{-1} s^{-1}
T_{amb} is the soil temperature, K
T_{ref} is the viscosity reference temperature, K [298.15]

Equation A9: Soil gas volumetric flow rate into the building

$$Q_{soil} = \frac{2\pi\, \Delta P\, k_v X_{crack} \times \; 10 gcm^{-1} s^{-2}\; Pa^{-1}}{\mu_a \ln\left(\frac{2Z_{crack}}{r_{crack}}\right)}$$

Where Q_{soil} is the volumetric flow rate of soil gas entering the building, cm^3 s^{-1}
π [= 3.14159]
ΔP is the pressure difference between soil air and the enclosed living space, Pa
k_v is the effective air permeability, cm^2
X_{crack} is the floor-wall seam perimeter, cm
μ_a is the air viscosity at ambient temperature, g cm^{-1} s^{-1}
Z_{crack} is the depth below ground to bottom of floor, cm
r_{crack} is the effective crack radius, cm

Equation A10: Where the Peclet number approaches infinity

$$Where \quad \exp\left(\frac{Q_s L_{crack}}{D_{crack} A_{crack}}\right) \to \infty \qquad \alpha = \frac{\left(\frac{D_{eff} A_B}{Q_b L_T}\right)}{\left(\frac{D_{eff} A_B}{Q_s L_T}\right) + 1}$$

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

We are The Environment Agency. It's our job to look after your environment and make it **a better place** – for you, and for future generations.

Your environment is the air you breathe, the water you drink and the ground you walk on. Working with business, Government and society as a whole, we are making your environment cleaner and healthier.

The Environment Agency. Out there, making your environment a better place.

Published by:

Environment Agency
Rio House
Waterside Drive, Aztec West
Almondsbury, Bristol BS32 4UD
Tel: 0870 8506506
Email: enquiries@environment-agency.gov.uk
www.environment-agency.gov.uk