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CLEA Software (Version 1.03 beta) Handbook

Science Report – SC050021/SR4
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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.

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The CLEA Guidance incorporates the following


2) Science Report SC050021/SR3: Updated technical background to the CLEA model.


4) CLEA Software version 1.03 beta (2008)

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. Neither does it cover risks to the environment or the pollution of water.

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Regulators are under no obligation to use the CLEA Guidance.
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- **Delivering information, advice, tools and techniques**, by making appropriate products available to our policy and operations staff.


Steve Killeen

Head of Science
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1 Introduction

1.1 Background to the CLEA software and handbook

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).

The report on the technical background to the CLEA model has been updated to incorporate many of the changes to exposure assessments that were introduced in *Soil Guideline Values: The Way Forward* but includes other changes as well (Environment Agency, 2008c). Assumptions in the CLEA model (Environment Agency, 2008c) apply to the derivation of *Soil Guideline Values* (SGV), but offer a useful starting point for assessors developing their own *site-specific assessment criteria*.

The CLEA software (Environment Agency, 2008d) has been updated to reflect the changes to the CLEA model and other changes as well as user feedback on the CLEA UK software (Environment Agency, 2005a). The CLEA software replaces the CLEA UK software published in 2005. This report updates and replaces the CLEA UK handbook (Environment Agency, 2005b) published in 2005 to reflect the changes to the CLEA software.

The software and this accompanying handbook contain further information on using the CLEA model outside the scope of the CLEA report (Environment Agency, 2008d).

1.2 Updates to and advice on using the software

1.2.1 Using the software

The CLEA software is based on the CLEA model. 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 potentially living, working, and/or playing on contaminated sites over long time periods (Environment Agency, 2008c). The software allows you to derive *assessment criteria* and to enter your own chemical, soil, building or land use datasets. Such criteria can assist you to assess the risks posed to human health from chronic exposure to soil contamination in relation to land use. They can be derived using generic or site-specific assumptions on the characteristics and behaviour of contaminants, pathways and receptors.

You can use the CLEA software to do the following:

- Derive generic assessment criteria by using standard assumptions about the characteristics and behaviour of contaminants, pathways and receptors; these assumptions are usually conservative within a defined range of conditions. The software contains general datasets that describe these standard land-use scenarios and the facility for you to add additional ones such as a new land-use scenario or further building or soil types.
- Derive site-specific assessment criteria by combining standard assumptions with further site-specific information collected in order to refine the risk assessment. Using the advanced user datasheets, you can amend existing default values for more than one hundred parameters to tailor the assessment to observed site conditions; for example, by using site-specific information on consumption of home-grown produce.

- Compare directly the estimated average daily exposure (ADE) with the relevant health criteria value (HCV) from representative site concentrations in soil, air and plants using 'ratio mode'. You can use ratio mode with standard or site-specific assumptions.

It is important to note that although you can derive generic assessment criteria using broadly the same assumptions as those used to produce Soil Guideline Values (SGV), these values are not considered to be SGV which are assessment criteria published by the Environment Agency which are subject to review by other Government departments and agencies. For information on how SGVs are derived, refer to Environment Agency (2008c).

1.2.2 Updates to the software

The CLEA software has changed significantly since 2005 (Environment Agency, 2005), although many of the features will be familiar to experienced CLEA users. However, it is strongly recommended that you read through this handbook at least once before using the software to calculate assessment criteria.

The CLEA software is now a deterministic model. This means that in any calculation each parameter (such as body weight and amount of homegrown produce) is represented by a single value. Many of these values are assigned on the basis of average or conservative (the most health protective) measurements and by expert judgement (Environment Agency, 2008c).

There are two distinct flowcharts within the software that you can follow, to derive assessment criteria:

1. Generic assessment criteria (basic); this is called basic because by following this process you will only use the library datasets. Whether or not the criteria generated using customised datasets are truly generic assessment criteria will depend on the assumptions behind the conceptual model used to design the scenario and the parameter choices made.

2. Site-specific assessment criteria (advanced); this is called advanced because by following this process you will not only define the land-use scenario by using library datasets but can also change individual parameters to reflect site-specific data.

Some of the functionality and user interface of the software has changed following recommendations and comments by users of the CLEA UK software.

The main changes to the functionality of the software are:

- the time taken to calculate assessment criteria has been greatly reduced;
- assessments can use any of the library datasets that the user has added (chemical, land use, building or soil type), any start and end age class, soil organic matter and exposure pathways;
- the majority of data used within any assessment can be modified;
the library can be copied and pasted to other worksheets or MS Office applications.

The main changes to the user interface of the software are as follows:
- the process flowchart for calculating assessment criteria is interactive;
- user help text has been added within the databases;
- values can be entered into the databases in numeric or scientific format;
- the output report highlights those default or generic parameters that have been changed in the derivation of the assessment criteria.

1.2.3 Using this handbook

This is the handbook for the CLEA software version 1.03 beta (Environment Agency, 2008d). It provides information on how to use the CLEA software to derive generic or site-specific assessment criteria and ADE/HCV ratios.

The remainder of this publication has been divided into four parts.

Section 2 provides a quick start guide, which takes you quickly through the main features of the software.

Section 3 is a detailed user guide with illustrated screenshots explaining how to operate all of the functions of the software.

Section 4 is a scientific and technical guide giving a brief summary of the information which underpins the software (with links to more detailed information contained within other guidance) and relating this to the ways in which the CLEA software can be used.

Appendix A provides a software familiarisation walk-through, which takes you through the steps required to add a chemical and to derive generic assessment criteria.

Key points are identified throughout this report using grey-shaded text boxes.

Terms that are included in the list of abbreviations or glossary are defined in bold the first time that they are used within each section.


1.3 Technical specification and installation

CLEA Software Version 1.03 beta is not a stand alone application and requires the use of Microsoft® Excel. The spreadsheet was developed using Microsoft® Excel 2003 SP1 and backward compatibility to earlier versions of Microsoft® Excel cannot be guaranteed. The system requirements for Microsoft® Excel 2003 are:

**Computer and processor**  
Personal computer with an Intel Pentium 233-MHz or faster processor (Pentium III recommended)

**Memory**  
128 megabytes (MB) of RAM or greater

**Hard disk**  
150 MB of available hard-disk space; optional installation files cache (recommended) requires an additional 200 MB of available hard-disk space

**Drive**  
CD-ROM or DVD drive

**Display**  
Super VGA (800 x 600) or higher-resolution monitor

**Operating system**  
Microsoft Windows 2000 with Service Pack 3 (SP3), Windows XP or later

Additional recommended requirements for CLEA Software Version 1.03 beta are:

**Computer and processor**  
-

**Memory**  
-

**Hard disk**  
10 MB of available hard-disk space (unzipped file size is 3MB)

**Drive**  
-

**Display**  
Super VGA (1280 x 768) or higher resolution is recommended

**Operating system**  
-

To run the software double click on the software Excel file.
2 Quick start guide

You can use the quick start guide to take you through the main features of the CLEA software. However, it is strongly recommended that you read Section 3 of this software handbook before using the software to calculate assessment criteria. You can also carry out the software familiarisation walk-through in Appendix A, which takes you through the steps required to add a chemical and to derive generic assessment criteria.

The CLEA software takes you through a flowchart, containing five steps, to calculate assessment criteria. The flowchart is the same whether you are calculating generic assessment criteria or site-specific assessment criteria, with the exception that Step 4 ‘Advanced Settings’ is only used when calculating site-specific assessment criteria. These steps can be accessed from the interactive CLEA Software Guide and are as follows:

Step 1: Report Details
Step 2: Basic Settings
Step 3: Select Chemicals
Step 4: Advanced Settings
Step 5: Find Results

Database Management is a feature that allows you to add new datasets to the software before you begin calculation of assessment criteria. There are four types of datasets that you can add: building, chemical, land use and soil. You can select these datasets when you are calculating either generic or site-specific assessment criteria. The datasets you add may be for a new generic land use or relate to a particular site which you intend to use more than once (otherwise you may wish to edit the individual parameters using Advanced Settings, see section 2.2).

You can use the CLEA software in generic assessment criteria (basic mode) or site-specific assessment criteria (advanced mode). Within both basic and advanced mode, the 'Interactive CLEA Software Guide' guides you through the process to set up and calculate the assessment criteria.

In both basic and advanced mode, you can select standard and user-defined datasets contained within the buildings, chemicals, land uses or soils databases. In advanced mode you can change more of the default parameters and can tailor the simulation to a wider range of site-specific conceptual models than in basic mode.

1. When selecting a conceptual model, you should take care to consider whether it is appropriate for the site. If it is not, you should add a new land use to the software (see Section 2.1) for use when calculating assessment criteria.

2. You cannot create a new pathway and use this in your assessments. If a pathway other than the ones described in the CLEA report (Environment Agency, 2008c) is important to the conceptual model for your site, then you need to either use an alternative modelling tool or calculate the results and integrate separately.

3. Care must be taken to consider whether the algorithms in the CLEA report (Environment Agency, 2008c) are valid for site conditions when you are developing a revised conceptual model.
Follow the flowchart for generic assessment criteria if you want to set up the software to:

- derive assessment criteria based on the standard conceptual models that underpin SGVs;
- derive generic assessment criteria using a combination of standard or user-added datasets within the CLEA software (for example, selection of a residential land use with a clay soil).

Follow the flowchart for site-specific assessment criteria if you want to set up the software to:

- derive site-specific assessment criteria based on temporary amendments to standard or user-defined library data;
- derive assessment criteria based on temporary amendments to homegrown produce data and/or receptor data, or date relevant to the air dispersion or vapour model.

In both modes you can select a generic land use which automatically determines default input values including receptor type, building type, soil type, age class, exposure and averaging periods, receptor characteristics, some site characteristics and exposure pathways (see Section 2.2).

The majority of input parameters are stored within the databases. You can add new building, chemical, land use and soil datasets permanently to the software databases (see Section 2.1).

2.1 Database management

There are four databases within which you can add a new dataset or edit an existing dataset. If amendments to the databases are required, you must undertake these prior to calculating assessment criteria in basic or advanced mode.

To access the databases, select the appropriate database within the Database Management section at the bottom of the 'Interactive CLEA Software Guide'. You only need to do this if you want to create new datasets or modify existing custom datasets.

The four databases are:

i. Buildings
ii. Chemicals
iii. Land uses
iv. Soils.

The databases contain only user-added datasets. Generic datasets used for the calculation of SGVs (for example, a residential with plant uptake land use) are hidden from view to prevent you from overwriting them. However you can view and temporarily change this data in advanced mode Step 4 (see Section 2.2). To add a new dataset you must first provide a name for the dataset, then enter the appropriate data in a new row under each parameter name listed at the top of the worksheet. By selecting each parameter data field, user help text (shown as a pop up box) will provide supporting information for each parameter. The information also provides guidance on when a parameter value is not relevant and therefore does not need to be provided. In these instances, 'NR' should be added to the data field.
Press the 'Back to Guide' button to exit the databases and return to the Interactive CLEA Software Guide.
The information entered can be permanently stored within the database by saving the software as you would normally for an Excel file. To save the software:

- with the same file name select, from the Microsoft toolbar, 'File' → 'Save';
- with a different file name select, from the Microsoft toolbar, 'File' → 'Save As' then insert the new file name and press the 'Save' button.

2.2 Running the simulation

The 'Interactive CLEA Software Guide' will take you through the process and is divided into five steps. You should follow the flowchart for either generic assessment criteria (basic mode) or site-specific assessment criteria (advanced mode). In both modes, you can derive assessment criteria or you can calculate the Average Daily Exposure (ADE) to Health Criteria Value (HCV) ratio (also known as ratio mode or the Hazard Quotient) for a given representative site soil concentration.

The 'Interactive CLEA Software Guide' divides the process for calculating assessment criteria into five steps:

- **Step 1: Report Details.**
  You can enter project or file details to personalise output reports with a clear reference. Details entered about the user, company and report title will be added to the output report. Entry of information is optional.

  Press the 'Back to Guide' button to return to the 'Interactive CLEA Software Guide'.

- **Step 2: Basic Settings.**
  If you want to calculate ADE/HCV ratios for a given representative site soil concentration, you should tick the box next to 'Ratio Mode' by clicking on it.

  You can select a generic land use that is used in the calculation of SGVs or a land use dataset that you have added to the database. By selecting a land use, default options will automatically be selected for receptor, building and soil type, start and end age class and soil organic matter and exposure pathways. You can make changes to these default selections.

  Don't forget to press the 'Apply Settings to Model' button so that the selections you have made are used when the assessment criteria are calculated. A warning will appear to remind you that if you have made changes within Step 4, these will be overwritten. By pressing the 'OK' button in the dialogue box, the settings will be applied to the model and a popup box will appear to confirm that settings have been updated successfully.

  Press the 'Back to Guide' button to return to the 'Interactive CLEA Software Guide'.

> Soil pH is no longer applied within the CLEA model, as a result you are not required to add a value for pH. This functionality will be reconsidered in the development of SGVs.
• **Step 3: Select Chemicals**
Select the chemicals, for which you want to carry out an assessment, from the drop down menu. You can add one chemical per row and up to thirty chemicals in total. If you are calculating an ADE/HCV ratio (ratio mode), you need to enter the representative site soil concentration into the ‘Soil’ site-measured media concentration for each contaminant selected.

Don’t forget to press the ‘Apply Chemicals to Model’ button so that changes made are used in the simulation. A warning will appear to remind you that if you have made changes within Step 4, these will be overwritten for all chemicals. By pressing the ‘OK’ button, the chemical data will be applied to the model and a text box will appear to confirm that chemical data has been loaded successfully.

Press the ‘Back to Guide’ button to return to the Interactive CLEA Software Guide’

• **Step 4: Advanced Settings**
This step should only be used by those with a thorough understanding of the CLEA model and the basis for the underlying algorithms. Within this step, you can make temporary changes to data to be used within the calculation. Changes to data within Step 4 cannot be permanently saved to the software databases; however, if you choose to save a version of the software it will save the data that you have changed within Step 4, until the default data is restored or edited.

Select the dataset that you want to change from ‘Chemical Data’, ‘Homegrown Produce Data’, ‘Land Use and Receptor Data’ or ‘Soil and Building Data’. Cells that are highlighted in yellow are the values that will be used in the calculation of assessment criteria, unless you make changes. To make a change, enter a new value into the appropriate cell. A cell is highlighted in pink when its value differs from the default data within the database.

You do not need to save the software for the changes made within Step 4 to be used in the calculation of the assessment criteria.

Press the ‘Back to Guide’ button to return to the Interactive CLEA Software Guide’.

• **Step 5: Find Results**
If you are deriving generic or site-specific assessment criteria, press the ‘Find AC’ button to calculate the assessment criteria. You may receive a warning box if you have selected ratio mode previously in Step 2. Any previously calculated assessment criteria will also be overwritten. The soil assessment criteria calculated are shown within the yellow cells. The ADE/HCV ratios are reported as an oral HCV, inhalation HCV and combined HCV.

If you are deriving ADE/HCV ratios from representative site soil concentrations, you do not need to press the ‘Find AC’ button as the results will already have been calculated when you enter Step 5.

The lowest of the soil saturation limits (solubility or vapour saturation limit) is reported in the ‘Soil saturation limit’ column. ‘NR’ is reported for those substances for which a soil saturation limit cannot be calculated, such as metals.

To assist in the interpretation of results, the CLEA software includes a check to highlight when saturated soil conditions have been exceeded during calculation...
of assessment criteria. The coloured cells within the 'Soil Assessment Criteria' column represent the following:

i. **Green** – the saturated soil concentration has not been exceeded in the calculation of the assessment criteria.

ii. **Amber** – the saturated soil concentration has been exceeded in the calculation, but it will not affect the significant exposure pathways.

iii. **Red** – the saturated soil concentration has been exceeded in the calculation and this will affect the interpretation of exposure.

The percentage contribution from each pathway to exposure is displayed in the far right columns. In ratio mode, the percentage contributions from each pathway are calculated using the data entered for site-measured soil concentrations in Step 3 "Select Chemicals".

Press the 'Print reports' button to:

- Print the results and/or settings.
- Save the results and/or settings by printing to Adobe Acrobat (if you have this facility installed, such as Adobe Distiller).
- Save the workbook, which will save the selections made in Steps 1 to 5 (including temporary amendments made within Step 4).
- Cancel to return to Step 5.

Press the 'Back to Guide' button to return to the 'Interactive CLEA Software Guide'.
3 Detailed user guide

3.1 Introduction and purpose

This section explains how to use all of the features of this software and is illustrated with screenshots to help guide you through these. It does not discuss the wider technical principles of the CLEA model, which are described in the CLEA report (Environment Agency, 2008c). Further details on how to use this software for site-specific assessments can be found in the scientific and technical guide (Section 4 of this handbook).

The screenshots that are shown throughout this handbook assume a screen resolution of 1024 by 768 and that the software workbook is maximised. You may see less of the worksheet area than is shown in the handbook and will need to use the scrollbar to scroll up/down or left/right to view all parts of the worksheet.

3.2 CLEA software structure

The CLEA software takes you through a flowchart, containing five steps, to calculate assessment criteria. The flowchart is the same whether you are calculating generic assessment criteria or site-specific assessment criteria, with the exception that you only have the option to complete Step 4 'Advanced Settings' when calculating site-specific assessment criteria. These steps can be accessed from the 'Interactive CLEA Software Guide' and are as follows:

Step 1: Report Details
Step 2: Basic Settings
Step 3: Select Chemicals
Step 4: Advanced Settings
Step 5: Find Results

Database Management is a feature that allows you to add new datasets to the software before you begin calculation of assessment criteria. These datasets may be for a new generic land use or relate to a particular site which you intend to use more than once (otherwise you may wish to edit the individual parameters using Advanced Settings). You can select these datasets when you are calculating generic or site-specific assessment criteria. There are four types of datasets that you can add: building, chemical, land use and soil.

You can use the CLEA software in generic assessment criteria (basic mode) or site-specific assessment criteria (advanced mode). Within both basic and advanced mode, the 'Interactive CLEA Software Guide' guides you through the process to set up and calculate the assessment criteria.

In basic and advanced mode, you can select datasets contained within the buildings, chemicals, land uses or soils database. However it is expected that only generic datasets will be selected within basic mode. In advanced mode, you have greater control of the default parameters and can tailor the simulation to a wide range of conceptual models and, in addition, you can amend more parameters than in basic mode.

Follow the flowchart for generic assessment criteria if you want to set up the software to:
- derive assessment criteria based on the standard conceptual models that underpin SGVs;
- derive generic assessment criteria using a combination of standard or user-added datasets within the CLEA software (for example, selection of a residential land use with a clay soil).

Follow the flowchart for site-specific assessment criteria if you want to set up the software to:

- derive site-specific assessment criteria based on temporary amendments to standard or user-defined library data;
- derive assessment criteria based on temporary amendments to homegrown produce data and/or receptor data.

In both modes, you can select a generic land use which automatically determines default input values including receptor type, building type, soil type, age class, exposure and averaging periods, receptor characteristics, some site characteristics and exposure pathways (see Section 2.2).

The majority of input parameters are stored within the databases. You can add new building, chemical, land use and soil datasets permanently to the software databases (see Section 2.1).

### 3.2.1 Deriving generic assessment criteria

The interactive guide flowchart for generic assessment criteria takes you through four steps to derive generic assessment criteria:

- **Step 1 – Report Details.** Allows you to enter project details and information relating to the user calculating the assessment criteria.

- **Step 2 – Basic Settings.** Sets out the overall conceptual model that will be used in calculating assessment criteria. Information you can select in Step 2 is the land use, receptor, building and soil type, start and end age class, soil organic matter (SOM) and relevant exposure pathways.

- **Step 3 – Select Chemicals.** Add or change the chemicals for which assessment criteria are to be derived.

- **Step 4 – Advanced Settings.** This step is not used in basic mode.

- **Step 5 – Results.** This step provides the soil assessment criteria, ADE/HCV ratios, the value of the solubility or vapour soil saturation limit (the lower of the two) and the calculated average percentage exposure contribution from each pathway.

### 3.2.2 Calculating site-specific assessment criteria

The interactive guide flowchart for site-specific assessment criteria takes you through five steps to derive site-specific assessment criteria:

- **Step 1 – Report Details.** Allows you to enter project details and information relating to the user calculating the assessment criteria.
• **Step 2 – Basic Settings.** Sets out the overall conceptual model that will be used in calculating assessment criteria. Information you can select in Step 2 is the land use, receptor, building and soil type, start and end age class, soil organic matter (SOM) and relevant exposure pathways.

• **Step 3 – Select Chemicals.** Add or change the chemicals for which assessment criteria are to be derived.

• **Step 4 – Advanced Settings.** This step allows you to make amendments to individual parameter values to be used in the calculation of assessment criteria, and allows you to change a wider range of parameters than those available within 'Database Management'.

• **Step 5 – Results.** This step provides the soil assessment criteria, ADE/HCV ratios, the value of the solubility or vapour soil saturation limit (the lower of the two) and the calculated average percentage exposure contribution from each pathway.

### 3.2.3 Calculating ADE/HCV ratios

The interactive guide takes you through the steps to derive assessment criteria as the ADE/HCV ratio (also known as ratio mode or the Hazard Quotient) for a given **representative site soil concentration**.

Using the ratio mode allows you to assess whether estimated **Average Daily Exposure** calculated using representative concentrations of contaminants at a specific site would exceed the relevant **Health Criteria Values.** This is also known as the "hazard index".

The interactive guide flowchart for generic or site-specific assessment takes you through the steps required to derive ADE/HCV ratios:

• **Step 1 – Report Details.** Allows you to enter project details and information relating to the user calculating the assessment criteria.

• **Step 2 – Basic Settings.** Allows you to select information for use in calculating assessment criteria. Information you can select in Step 2 is the land use, receptor, building and soil type, start and end age class, soil organic matter (SOM) and relevant exposure pathways. You must tick the box next to ‘Ratio Mode’ by clicking on it so that ADE/HCV ratios are calculated.

• **Step 3 – Select Chemicals.** Add or change the chemicals for which assessment criteria are to be derived. You must enter a representative site soil concentration to derive ADE/HCV ratios. You can also enter site-specific media concentrations to override those that are calculated within the software.

• **Step 4 – Advanced Settings.** This step is only used if you are following the flowchart for site-specific assessment and allows you to make temporary amendments to individual parameter values in the calculation and to amend a wider range of parameters than those available for change within 'Database Management'.

• **Step 5 – Results.** This step provides the assessment criteria for ADE/HCV ratios, the value of the solubility or vapour soil saturation limit (the lower of the two) and the calculated average percentage exposure contribution from each pathway.
3.2.4 Database Management

In ‘Database Management’ there are four databases within which you can add a new dataset or edit an existing user added dataset. If you add or make changes to a database, they will not be applied to the model until the datasets are selected in either Step 2 or Step 3. If amendments to the databases are required, you must make these prior to calculating assessment criteria in basic or advanced mode. The four databases are:

1. Buildings
2. Chemicals
3. Land uses

The databases contain only user-added datasets. Generic datasets used for the calculation of SGV s (for example, a residential with plant uptake land use) are hidden from view to prevent you from overwriting them. However you can view and temporarily change this data in advanced mode Step 4 (see Section 3.3).

Use of the ‘Interactive CLEA Software Guide’, shown in Figure 3.1, is described in Section 3.3.2.

Figure 3.1: Interactive CLEA Software Guide
3.3 Calculating assessment criteria

3.3.1 Introduction

You can use the CLEA software to calculate generic assessment criteria (basic mode) or site-specific assessment criteria (advanced mode). Within both basic and advanced modes, the 'Interactive CLEA Software Guide' guides you through the process to set up and calculate the assessment criteria.

In either mode, you can select datasets contained within the buildings, chemicals, land uses or soils database. In advanced mode, you have greater control of the default parameters and can tailor the simulation to a wide range of conceptual models and, in addition, you can amend more parameters than you can within basic mode.

Follow the flowchart for basic mode if you want to set up the software to:

- derive assessment criteria based on the conceptual models that underpin SGVs;
- derive assessment criteria using a combination of generic or user-added datasets contained within the CLEA software (for example, selection of a residential land use with a clay soil);
- derive assessment criteria using site-measured media concentrations.

Following the flowchart for advanced mode also allows you to:

- derive assessment criteria based on temporary amendments to the library data for soil, building, land use and chemicals;
- derive assessment criteria based on temporary amendments to other datasets including homegrown produce data and/or receptor data, data relevant to the air dispersion or vapour model.

Information on the difference between generic and site-specific assessment criteria is provided in Section 4.3.2.

3.3.2 Interactive CLEA Software Guide

Figure 3.2 highlights three areas within the 'Interactive CLEA Software Guide' that can be accessed interactively by the user.

The 'Interactive CLEA Software Guide' gives you the following options:

- calculate assessment criteria in basic mode;
- calculate assessment criteria in advanced mode;
- access the four databases within the database management area.
3.3.3 Calculating assessment criteria in basic or advanced mode

This section discusses steps in the software to calculate assessment criteria using either basic or advanced mode flowcharts. Note that Step 4 is not used in basic mode.

Step 1: Report Details

The first step in the flowchart is accessed by pressing the Step 1 ‘Report Details’ button. This will take you to the report details worksheet shown in Figure 3.3. You can record details about the assessment including the name of the user, report title and job number. Details entered about the user, company and report title will be added to the output report. Entry of information is optional.

You can press the ‘Clear All Details’ button to remove all information in the worksheet.

When you have completed Step 1, press the ‘Back to Guide’ button which will take you back to the ‘Interactive CLEA Software Guide’.
**Step 2: Basic Settings**

Pressing the Step 2 ‘Basic Settings’ button within the ‘Interactive CLEA Software Guide’ will take you to the basic settings worksheet shown in Figure 3.4.

**Ratio mode**

If you are deriving ADE/HCV ratios, you must be able to provide site soil concentrations (and if available, other site-measured media concentrations, see Step 3). You should select this mode by clicking the box next to ‘Ratio Mode’ to tick it. By selecting this mode, the software will derive ADE/HCV ratios and calculate percentage exposure contributions from each pathway based on the data entered for site-measured soil concentrations (see Step 5). Section 4.3.3 provides information on when background exposure is taken into account in the calculation of assessment criteria. When you select ‘Ratio Mode’ the software reminds you that you are entering ratio mode and that current assessment criteria will be deleted; this means that any soil assessment criteria results that may have been calculated in Step 5 ‘Find Results’ will be deleted in order for the software to switch to ratio mode. You have the option of selecting ‘No’, which will exit you from the procedure and enable you to save existing results prior to resuming the process for switching on ratio mode. If you press the ‘Yes’ button, the software will confirm that ratio mode is switched on.

To switch off ratio mode, click on the ticked box; a confirmation box appears to confirm that ratio mode is switched off. Press the ‘OK’ button to close the confirmation box.
Land use
Select the land use required for the simulation from the drop down menu. The land uses available for selection are:

- residential with homegrown produce
- residential without homegrown produce
- allotments
- commercial
- all user-added land use datasets added to the database (see Section 3.4).

![Figure 3.4: Step 2: Basic Settings worksheet](image)

When you select a land use this automatically determines the basic default input values for the conceptual model, including receptor, building and soil type, start and end age class and SOM and exposure pathways (you will specify these options within custom land use datasets added within Database Management).

### Notes:

1. Soil pH is no longer applied within the CLEA model and therefore you are not required to add a value for pH. This functionality will be re-considered in the development of Soil Guideline Values.

2. If you have already pressed the 'Apply Settings to Model' button in Step 2, you do not need to press this again if you only want to make changes to selecting or deselecting 'Ratio mode'.
You can change the information in Land Use Options as follows.

**Receptor**
Select the receptor required for the calculation of assessment criteria from the drop down menu. The receptors available for selection are:

- female (residential)
- female (allotment)
- female (commercial)
- male (residential)
- male (allotment)
- male (commercial).

Further information on selection of the receptor is provided in Section 4.4.

**Building**
Select the building required for calculation of assessment criteria from the drop down menu. The buildings available for selection are:

- no building
- bungalow
- small terraced house
- medium/large terraced house
- semi-detached house
- detached house
- warehouse (pre-1970)
- warehouse (post-1970)
- office (pre-1970)
- office (post-1970)
- all building datasets added to the database (see Section 3.4).

**Soil type**
Select the soil required for the calculation of assessment criteria from the drop down menu. The soil types available for selection are:

- clay
- silty clay
- silty clay loam
- clay loam
- sandy clay loam
- silty loam
- sandy loam
- sand
- all soil datasets added to the database (see Section 3.4).

See Section 4.5.4 for further information on soil properties.

**Start and end age class**
Select the start and end age class (AC) required from the drop down menu. In selecting a start and end age class, you must ensure that the land use database contains the data for these age classes; alternatively, you can add the data for the additional age classes required in Step 4 ‘Advanced Settings’. You can only add data for additional age classes for the standard land uses residential, allotment and commercial within Step 4 ‘Advanced Settings’.
You must ensure that the youngest AC is selected as the Start AC. It is possible to carry out the assessment for a single AC, for example a Start AC of 1 and End AC of 1. The human lifetime is subdivided into age classes which are shown in Table 3.1.

### Table 3.1: Age classes used within the CLEA software

<table>
<thead>
<tr>
<th>Age Class (AC)</th>
<th>Age (years)</th>
<th>Exposure Duration (years)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0 - 1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>1 - 2</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>2 - 3</td>
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<td>5 - 6</td>
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</tr>
<tr>
<td>7</td>
<td>6 - 7</td>
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<tr>
<td>8</td>
<td>7 - 8</td>
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<td>10</td>
<td>9 - 10</td>
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</tr>
<tr>
<td>11</td>
<td>10 - 11</td>
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<td>12</td>
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<td>13</td>
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<td>17</td>
<td>16 - 65</td>
<td>49</td>
</tr>
<tr>
<td>18</td>
<td>65 - 75</td>
<td>10</td>
</tr>
</tbody>
</table>

Note: In selecting a critical receptor you should be aware of the exposure and physiological characteristics that is assumed for each receptor (see section 4.4.1 for further information).

Note: Data for the commercial receptor are available within the software for Age Class 17 only, data for the allotment receptor are available within the software for Age Classes 1 to 6 only. You should not select a commercial or allotment receptor for any other Age Class unless you add data for the additional Age Classes selected in step 4 'Advanced Settings'.

### Soil organic matter (SOM)

You can enter a percentage SOM value by clicking and typing the value in the yellow-shaded box. You can enter whole numbers or decimals. See Section 4.5.4 for further information on SOM.

### Exposure pathways

You can change the default exposure pathways to be included within the calculation of assessment criteria by clicking on the box provided to the right of the exposure pathway, to select (shown by a tick) or deselect (box will be blank) an exposure pathway. You cannot add new pathways to those listed.

Three routes of exposure are included: (i) oral, (ii) dermal and (iii) inhalation.
Oral exposure pathways available for selection are:
- direct soil and dust ingestion;
- consumption of homegrown produce;
- soil attached to homegrown produce.

Dermal exposure pathways available for selection are:
- indoor (dermal uptake from soil and dust);
- outdoor (dermal uptake from soil and dust).

Inhalation exposure pathways available for selection are:
- indoor dust;
- outdoor dust;
- indoor vapour;
- outdoor vapour.

See Section 4.6 for further information on exposure pathways.

Apply settings to model
When you have made the appropriate selections, you must press the ‘Apply Settings to Model’ button to ensure that your selections are used within the calculation. An information box warns you that all user changes in advanced settings will be lost and you have the choice to continue. If you press the ‘Yes’ button, any changes that you have made to parameter values within Step 4 ‘Advanced Settings’ will be overridden. If you press the ‘No’ button, changes you have made to the selections or values within Step 2 ‘Basic Settings’ will not be applied to the calculation of assessment criteria. If settings are applied to the software, an information box will confirm when all settings have been applied. Press the ‘OK’ button to close the information box.

Back to guide
When you have completed this step, press the ‘Back to Guide’ button which will take you back to the ‘Interactive CLEA Software Guide’.
‘Ghosted’ ticks (that is, ticks that appear in a light grey colour rather than a solid black tick) within the user interface are not readily interpreted by the model as a YES. Ghosted ticks are caused when information is copied into the database from an external source (that is not another copy of the software) and there are spaces present before or after the words ‘True’ or ‘False’. Ghosted ticks can be avoided by entering information directly into the software using the drop down menus.

Changes made within Step 2 will be stored when the software is saved. Therefore, in order to ensure that the correct default data is provided within Step 2, the user should select any land use within the drop down menu and then re-select the required land use before proceeding. This will ensure that default data for the scenario selected is reloaded.

When selecting a start and end age class, you must ensure that the land use database contains the data for these age classes; alternatively, you can add the data for the additional age classes required in Step 4 ‘Advanced Settings’. You can only add data for additional age classes for the generic land uses residential, allotment and commercial within Step 4 ‘Advanced Settings’.

For generic land uses; data for age classes 1 to 6 is available within the software for the residential and allotment land use and data for age class 17 is available within the software for the commercial land use.

The exposure pathway ‘direct dust ingestion’ is included within the direct soil ingestion pathway in the CLEA software and a combined soil and dust ingestion rate is used. There is a lack of supporting data to identify the fraction of dust derived from a soil source (see Sections 6.13 and 6.14 of the CLEA report).

You can go back to Step 2 at any time during the calculation of assessment criteria by clicking on the ‘Basic Settings’ button in the ‘Interactive CLEA Software Guide’. However, if you have made changes within Step 4 these will be overwritten if you apply changes made in Step 2 to the model.

If you want to make changes within Step 4 ‘Advanced Settings’, you should do this after completing Step 2 and 3. When selections made within Step 2 and 3 are applied to the simulation, this will override any changes made in Step 4.

Dermal contact is also called skin contact.

---

**Step 3: Select Chemicals**

You can use the software to calculate:

- ADE/HCV ratios from representative site soil concentrations;
- soil assessment criteria.

If you are calculating soil assessment criteria, you only need to select the relevant chemicals for your assessment within Step 3 ‘Select Chemicals’; you do not need to add any information to the ‘Site-Measured Media Concentration’ columns.

If you are calculating ADE/HCV ratios (that is, you have selected ‘Ratio Mode’ in Step 2 ‘Basic Settings’), you must also enter a representative concentration into the site-
measured media concentrations column for soil. You can also enter other measured site media concentrations.
Press the Step 3 button ‘Select Chemicals’ within the 'Interactive CLEA Software Guide'. This takes you to the select chemicals worksheet shown in Figure 3.5.

**Clear all chemicals**
You should press the 'Clear All Chemicals' button to empty the list of chemicals and media concentrations entered from previous calculations. This will also clear the results calculated from previous assessments within Step 5 ‘Results’.

**Chemicals**
Select the chemicals required for calculation of assessment criteria from the drop down menu under the column 'Chemical'. Up to 30 chemicals can be assessed at one time and, if required, these can be a mixture of organic and inorganic chemicals.

**Site-measured media concentrations**
If you are calculating assessment criteria as ADE/HCV ratios, you must input the representative site soil concentration under the ‘Soil’ column (that is, the grey-shaded box under ‘Site-Measured Media Concentrations’) to correspond with the appropriate chemical. You can also add additional site-measured media concentrations by entering media concentrations to be used in the simulation under the corresponding column. You do not have to complete the yellow-shaded columns, only those for which site-measured media concentrations are available. These will override the software calculations.

Site-measured media concentrations that can be added are:

- soil gas air concentrations;
- outdoor air concentrations;
- indoor air concentrations;
- soil-to-plant concentration factor for green vegetables;
- soil-to-plant concentration factor for root vegetables;
- soil-to-plant concentration factor for tuber vegetables;
- soil-to-plant concentration factor for herbaceous fruit;
- soil-to-plant concentration factor for shrub fruit;
- soil-to-plant concentration factor for tree fruit.
**Figure 3.5: Step 3: Select Chemicals worksheet**

**Apply chemicals to model**
When you have completed the chemicals worksheet, you must press the 'Apply Chemicals to Model' button. This will ensure that your chemical selections and any site-measured media concentrations entered are used in the calculation of assessment criteria. An information box warns you that all user changes in advanced settings will be lost and you have the choice to continue. If you press the 'Yes' button, data supplied and chemicals selected will be applied to the model for use in calculating assessment criteria. An information box will confirm when all chemical data has been loaded successfully. Press the 'OK' button to close the information box.

**Back to guide**
When you have completed this step, press the 'Back to Guide' button which will take you back to the 'Interactive CLEA Software Guide'.
If you add site-measured media concentration data, it is necessary to click outside of
the cell that you have added data to before you select 'Apply Chemicals to Model'. A
confirmation box will appear when data have been successfully loaded for the software
to use in the calculation of assessment criteria.

Within site-measured media concentrations, the air concentrations apply only to the
vapour pathway. It is not possible to enter dust data at this time for either the outdoor
or indoor pathway.

You can go back to Step 3 at any time during the calculation by clicking on the 'Select
Chemicals' button in the 'Interactive CLEA Software Guide'. However, if you have
made changes within Step 4 these will be overwritten when you apply chemicals to the
model in Step 3.

If you want to make changes within Step 4 'Advanced Settings', you should do this
after completing Step 2 and 3. When selections made within Step 2 and 3 are applied
to the simulation, this will override any changes made by the user in Step 4.

If the drop down box within Step 3 does not show all the chemicals that are within the
database, you will need to alter the screen resolution on your computer.

You should not add a zero into the site-measured media concentration columns in
order to switch off a pathway, as the software will interpret this as a value of zero to
calculate the assessment criteria.

---

**Step 4: Advanced Settings**

Step 4 is only accessed when following the advanced mode flowchart.

Press the Step 4 'Advanced Settings' button within the advanced mode flowchart of the
'Interactive CLEA Software Guide'. This takes you to the menu shown in Figure 3.6.

Within 'Advanced Settings' information is located within four worksheets, these are:

1. Chemical data
2. Homegrown produce data
3. Land use and receptor data
4. Soil and building data.

You can use advanced settings to make temporary changes to data used in the
calculation of assessment criteria. In addition, there are parameters that you can make
temporary changes to that are not included within the databases accessed from the
'Interactive CLEA Software Guide'. These parameters are as follows:

Within chemical data:
- soil bioaccessible fraction;
- airborne dust bioaccessible fraction.

Within homegrown produce data:
- consumption rate by age class;
- dry weight conversion factor;
- homegrown fraction (average and high end);
- soil loading factor;
- preparation factor.
Within land use and receptor data:
- body weight;
- body height;
- inhalation rate;
- maximum exposed skin fraction (indoor and outdoor).

Within soil and building data:
- ambient soil temperature;
- mean annual wind speed (10 m);
- air dispersion factor at height of 0.8 m and 1.6 m;
- fraction of site with hard or vegetative cover;
- depth to top of source (beneath building);
- depth to top of source (no building);
- thickness of contaminant layer.

You can access individual worksheets by pressing the appropriate button within the menu, see Figure 3.6. This will take you to a worksheet allowing parameters to be temporarily altered for use in calculating the assessment criteria. Cells highlighted in yellow are the values that will be used within the calculation of assessment criteria unless you make changes. To make a change, enter a new value into the appropriate cell. A cell is highlighted in pink when its value differs from the default data within the database. In addition, within the soil and building data, you can also select for the software to calculate a soil gas ingress rate (rather than use the generic value) and/or to calculate assessment criteria assuming a finite source (see Section 4.7 and 4.9 for limitation on its use and for further information).

You do not need to save the software for changes made within Step 4 to be used within the calculation of assessment criteria. Changes made to the parameters in advanced settings will be identified in the output reports (see Section 3.5). Changes to data within Step 4 cannot be permanently saved to the software databases; however, if you choose to save a version of the software it will save the data that you have changed within Step 4, until the default data is restored.

**STEP 4: ADVANCED SETTINGS**
Use Advanced Settings to make temporary changes to individual parameters

Figure 3.6: Step 4: Advanced Settings worksheet
Restore all defaults
You can press the 'Restore All Defaults' button to remove temporary changes to all the databases amended in Step 4 and to restore all default values from the original library databases.

Back to Guide
When you have completed this step, press the 'Back to Guide' button which will take you back to the 'Interactive CLEA Software Guide'.

Chemical Data
Press the 'Chemical Data' button within Step 4 'Advanced Settings'. This takes you to the advanced settings chemical data worksheet, the first part of which is shown in Figure 3.7.

The data for each chemical is set out across the row. To access all the data you can move and scroll through the worksheet using the arrow keys or using the scroll bar. Any cell that is highlighted with a pale yellow background can be edited.

The chemical data in advanced settings allows you to temporarily change the following data (the use of each parameter within the CLEA software is provided in the sections referenced after each parameter):

i. chemical type  (Section 4.5.5)
ii. oral and inhalation HCV (Section 4.3.3)
iii. select comparison of HCV with exposure routes (Section 4.3.3)
iv. combine oral and inhalation assessment criteria (Section 4.3.3)
v. physical-chemical properties (Section 4.5.2)
vi. dermal absorption fraction (Section 4.6.5)
vii. plant correction factors (Section 4.6.3)
viii. plant concentration factors (Section 4.6.3)
ix. Soil-to-dust transport factor (Section 4.6.5, 4.6.6)
x. bioaccessible fraction. (Section 4.6.2, 4.6.6, 4.10)

Where data is not relevant, for example plant correction factors are not required for organic chemicals, the text 'NR' should be inserted into the appropriate field.

You cannot add temporary chemical datasets in Step 4. Chemical datasets can only be added within Database Management of the 'Interactive CLEA Software Guide' (see Section 3.4).

You can save temporary changes within Step 4 by saving an instance of the software.

If you are following the flow chart for calculating generic assessment criteria you should ensure that you do not make changes in Step 4 'Advanced Settings' of the site-specific assessment criteria flow chart as these changes will be used in Step 5 of the flow chart for calculating generic assessment criteria.
Figure 3.7: Step 4: Advanced Settings Chemical Data

Homegrown produce data
Press the ‘Homegrown Produce Data’ button within Step 4 ‘Advanced Settings’. This takes you to the advanced settings homegrown produce data worksheet, the first part of which is shown in Figure 3.8.

Figure 3.8: Step 4: Advanced Settings Homegrown Produce Data
The data for each homegrown produce type is set out across the row. To access all the data you can move and scroll through the worksheet by clicking on any cell, using the arrow keys or using the scroll bar. Any cell that is highlighted with a pale yellow background can be edited.

The homegrown produce data in advanced settings allows you to temporarily change the following data (the use of each parameter within the CLEA software is provided in the sections referenced after each parameter):

i. consumption rates for each age class (Sections 4.6.3 and 4.6.4)
ii. dry weight conversion factor (Sections 4.6.3 and 4.6.4)
iii. homegrown fractions (Sections 4.6.3 and 4.6.4)
iv. soil loading factor (Section 4.6.4)
v. preparation factor (Section 4.6.4)
vi. gardener type: select average, high or none (Sections 4.6.3 and 4.6.4)

See also Section 4.4.3 on receptor behavioural characteristics for information relating to consumption rates of homegrown produce.

1. For the residential with homegrown produce land use the average homegrown fraction is used, that is the default gardener is ‘average’. For the allotment land use the high end homegrown fraction is used, that is the default gardener is ‘high’.

2. Selecting ‘None’ for gardener type assumes that within the land use scenario, no fruit and vegetables are grown for home consumption. If you select ‘None’, the software inputs zero for the intake associated with plant uptake and soil attached to vegetables (however, media concentrations are not switched off and will still be reported). For consistency, you should switch off the exposure pathways for consumption of homegrown produce and soil attached to homegrown produce in Step 2 ‘Basic Settings’, as this will switch off the media concentrations. The option to select ‘None’ is placed in Step 4 ‘Advanced Settings’ to enable you to switch off intake from these pathways if you need to do so at this later stage in the process.

3. Within ‘Homegrown Produce Data’ consumption rates for all age classes are shown, regardless of the start and end age class used in the calculation of assessment criteria. Where temporary amendments are required, you only need to make these to the age classes to be used in the assessment.

**Land use and receptor data**
Press the ‘Land Use and Receptor Data’ button within Step 4 ‘Advanced Settings’. This takes you to the advanced settings land use and receptor data worksheet, the first part of which is shown in Figure 3.9.
**ADVANCED SETTINGS**

- Restores all land use and receptor data to default values
- Takes you back to the 'Interactive CLEA Software Guide'

<table>
<thead>
<tr>
<th>LAND USE</th>
<th>AGE CLASS</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>EF (oral and gust ingestion)</td>
<td>day⁻¹</td>
<td>180</td>
<td>365</td>
<td>365</td>
<td>355</td>
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<td>180</td>
<td>365</td>
<td>365</td>
<td>365</td>
<td>365</td>
<td>365</td>
<td>365</td>
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<tr>
<td>EF (skin contact, indoor)</td>
<td>day⁻¹</td>
<td>180</td>
<td>365</td>
<td>365</td>
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<td>365</td>
<td>365</td>
<td>365</td>
<td>365</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>EF (inhalation of dusts and vapours, indoor)</td>
<td>day⁻¹</td>
<td>365</td>
<td>365</td>
<td>365</td>
<td>365</td>
<td>365</td>
<td>365</td>
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<td>0</td>
</tr>
<tr>
<td>EF (inhalation of dusts and vapours, outdoor)</td>
<td>day⁻¹</td>
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<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Occupancy Period (indoor)</td>
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<td>23</td>
<td>23</td>
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<td>23</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Occupancy Period (outdoor)</td>
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<td>1</td>
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<td>1</td>
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</tbody>
</table>

| Soil to skin adherence factor (indoor) | cm³/g⁻¹ day⁻¹ | 0.0E+00 | 0.0E+00 | 0.0E+00 | 0.0E+00 | 0.0E+00 | 0.0E+00 | 0.0E+00 | 0.0E+00 | 0.0E+00 | 0.0E+00 |
| Soil to skin adherence factor (outdoor) | cm³/g⁻¹ day⁻¹ | 1.0E+01 | 1.0E+01 | 1.0E+01 | 1.0E+01 | 1.0E+01 | 1.0E+01 | 1.0E+01 | 0.0E+00 | 0.0E+00 | 0.0E+00 |
| Soil and dust ingestion rate | g/day⁻¹ | 1.0E+01 | 1.0E+01 | 1.0E+01 | 1.0E+01 | 1.0E+01 | 1.0E+01 | 1.0E+01 | 0.0E+00 | 0.0E+00 | 0.0E+00 |

**Figure 3.9: Step 4: Advanced Settings Land Use and Receptor Data**

The data for land use and receptor is set out across the row. To access all the data you can move and scroll through the worksheet by using the arrow keys or using the scroll bar. Any cell that is highlighted with a pale yellow background can be edited.

The land use and receptor data in advanced settings allows you to temporarily change the following data (the use of each parameter within the CLEA software is provided in the sections referenced after each parameter):

**Land use data:**
1. exposure frequencies (Sections 4.6.2 to 4.6.8)
2. occupancy periods (Sections 4.6.6 to 4.6.8)
3. soil-to-skin adherence factors (Section 4.6.5)
4. soil and dust ingestion rate (Section 4.6.2)

**Receptor data:**
1. body weight (Table 4.2)
2. body height (Table 4.2)
3. inhalation rate (Sections 4.6.6 to 4.6.8)
4. maximum exposed skin fraction (Section 4.6.5)

See also Section 4.4.3 for further information on receptor behavioural characteristics (that is, exposure frequencies, occupancy periods, soil-to-skin adherence factors and soil and dust ingestion rates) and receptor physiological characteristics (that is body weight, body height, inhalation rate and maximum exposed skin fractions).
Soil and building data
Press the 'Soil and Building Data' button within Step 4 'Advanced Settings'. This takes you to the advanced settings soil and building data worksheet shown in Figure 3.10.

The data for the soil and building data is set out in columns. To access all the data you can move and scroll through the worksheet by clicking on any cell, using the arrow keys or scroll bar. Cells highlighted with a pale yellow background can be edited.

The soil and building data in advanced settings allows you to temporarily change the following data (the use of each parameter within the CLEA software is provided in the sections referenced after each parameter):

- Soil properties:
  i. air-filled and water-filled porosity
  ii. residual soil water content
  iii. saturated hydraulic conductivity
  iv. van Genuchten shape parameter (m)
  v. bulk density
  vi. threshold value of wind speed at 10 m
  vii. empirical function (F_1) for dust model
  viii. ambient soil temperature

You do not need to enter a value for soil total porosity, as the software automatically calculates this value from the air-filled and water-filled porosity. See also Section 4.5.4 for further information on soil properties.

![Advanced Settings](image)

**ADVANCED SETTINGS**

<table>
<thead>
<tr>
<th>Soil Properties</th>
<th>Sandy loam</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity, total</td>
<td>0.52 cm³/cm³</td>
</tr>
<tr>
<td>Porosity, air-filled</td>
<td>0.20 cm³/cm³</td>
</tr>
<tr>
<td>Porosity, water-filled</td>
<td>0.75 cm³/cm³</td>
</tr>
<tr>
<td>Residual soil water content</td>
<td>0.12 cm³/cm³</td>
</tr>
<tr>
<td>Saturated hydraulic conductivity (cm/s)</td>
<td>3.2E-03</td>
</tr>
<tr>
<td>Van Genuchten shape parameter (m)</td>
<td>2.2687</td>
</tr>
<tr>
<td>Bulk density (g/cm³)</td>
<td>1.21</td>
</tr>
<tr>
<td>Threshold value of wind speed at 10m (m/s)</td>
<td>7.20</td>
</tr>
<tr>
<td>Empirical function (F_1) for dust model</td>
<td>1.22</td>
</tr>
<tr>
<td>Ambient soil temperature (°C)</td>
<td>20.3</td>
</tr>
</tbody>
</table>

**Building Properties**

<table>
<thead>
<tr>
<th>Building</th>
<th>No building</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume (m³)</td>
<td>0.00844004</td>
</tr>
<tr>
<td>Height (m)</td>
<td>0.6</td>
</tr>
<tr>
<td>Porous area (m²)</td>
<td>0.00284004</td>
</tr>
<tr>
<td>Dust loading factor</td>
<td>0.00284004</td>
</tr>
</tbody>
</table>

**Air Dispersion Model**

- Mean annual wind speed (10 m) (m/s) |
- Air dispersion factor at height of 6.0 m (m³ s⁻¹ g⁻¹) |
- Air dispersion factor at height of 1.0 m (m³ s⁻¹ g⁻¹) |
- Fraction of the with hanging vegetative cover |

**Vapour Model**

- Use default soil gas ingress rate |
- Default soil gas ingress rate (cm³ s⁻¹) |
- Depth to top of source (dense building) (cm) |
- Depth to top of source (r-e building) (cm) |
- Use limited source thickness |
- Trichloroethylene (TCE) contamination level (cm) |

Select for assessment criteria to be calculated assuming a finite source (see Section 4.8)
Deselect for software to calculate a soil gas ingress rate (see Section 4.7)

Figure 3.10: Step 4: Advanced Settings Soil and Building Data
Air dispersion model:
   i. mean annual wind speed (10 m) (Section 4.6.6)
   ii. air dispersion factor at height of 0.8 m (Section 4.6.6 and 4.6.8)
   iii. air dispersion factor at height of 1.6 m (Section 4.6.6 and 4.6.8)
   iv. fraction of site with hard or vegetative cover (Section 4.6.6)

Building properties:
   i. building footprint (Section 4.6.7)
   ii. living space air exchange rate (Section 4.6.7)
   iii. living space height (above ground) (Section 4.6.7)
   iv. living space height (below ground) (Section 4.6.7)
   v. pressure difference (soil to enclosed space) (Section 4.7.2)
   vi. foundation thickness (Section 4.6.7)
   vii. floor crack area (Section 4.6.7)
   viii. dust loading factor (Section 4.6.6)

Vapour model:
   i. use default soil gas ingress rate (switch on/off) (Section 4.7)
   ii. default soil gas ingress rate (Section 4.6.7)
   iii. depth to top of source (beneath building) (Section 4.6.7, 4.7.2, 4.8)
   iv. depth to top of source (no building) (Section 4.6.8 and 4.8)
   v. use limited source thickness (switch on/off) (Section 4.8)
   vi. thickness of contaminant layer (Section 4.6.7)

You can select a calculated soil gas ingress rate (see Section 4.7) by unticking the ticked box to the right of 'use default soil gas ingress rate' by clicking on it. You can select to calculate assessment criteria using the finite source vapour model (see Section 4.9 for limitations on its use and for further information) by ticking the check box next to 'Use limited source thickness'. Note: If you use the finite source option, you must specify a thickness for the contaminated layer.

⚠️ Advanced settings cannot be used to add a new chemical, soil, land use or building dataset to the database.

Step 5: Find Results

Press the Step 5 'Find Results' button within the 'Interactive CLEA Software Guide'. This takes you to the results worksheet, the first part of which is shown in Figure 3.11.

If you have selected ratio mode, by entering site-measured soil concentrations in Step 3 'Select Chemicals', ADE/HCV ratios will already be populated in the column 'Ratio of ADE to relevant Health Criteria Value'. If you want to calculate soil assessment criteria, Step 5 allows you to calculate these for each chemical that you have selected in Step 3 'Select Chemicals'.

Find AC

**Deriving soil assessment criteria**
To calculate soil assessment criteria, press the 'Find AC' button. An information box warns you that current assessment criteria and soil concentration values will be lost and you have the choice to continue. If you press the 'No' button, soil assessment criteria will not be calculated and you can choose to save a version of the software. If you press the 'Yes' button, the following data is calculated:

- ratio of ADE to HCV at the soil concentration of the assessment criteria;
- soil assessment criteria;
- soil saturation limit;
- exposure pathway contributions.

A text box appears to confirm that assessment criterion calculations have completed, press the 'OK' button to close this box.

The results data for each chemical is set out in rows. To access all the data, move and scroll through the worksheet by clicking on any cell, using the arrow keys or scroll bar.
To aid interpretation of the results, the software includes a check to highlight when saturated soil conditions have been exceeded during calculation of assessment criteria. The coloured cells within the 'Soil Assessment Criteria' column represent the following:

i. Green – the saturated soil concentration has not been exceeded in the calculation of the assessment criteria.

ii. Amber – the saturated soil concentration has been exceeded in the calculation, but it will not affect the significant exposure pathways.

iii. Red – the saturated soil concentration has been exceeded in the calculation and this will affect the interpretation of exposure.

The 'Soil Saturation Limit' column reports the lowest of the soil saturation limits (solubility or vapour saturation limit). 'NR' is reported for those substances for which a soil saturation limit cannot be calculated. Where a saturation limit has been reported, the output reports specify whether the lowest value reported is solubility or vapour based by including either (sol) or (vap) after the reported value.

Percentage exposure contributions from each pathway are reported. In ratio mode the percentage contributions from each pathway are calculated using the data entered for site-measured soil concentrations in Step 3.

**Deriving ADE/HCV ratios**

If you have entered representative site soil concentrations in Step 3 'Select Chemicals', ADE/HCV ratios and exposure pathway contributions are automatically calculated and will be available when you enter Step 5 'Results'. You should not press the 'Find AC' button as this would override information entered for site-measured soil concentrations within Step 3 'Select Chemicals'. If you do press the 'Find AC' button, a text box appears explaining that soil assessment criterion cannot be calculated in ratio mode and that ratio mode can be switched off under 'Basic Settings'.

---

1. Soil assessment criteria are calculated for the individual oral and inhalation HCV and a combined route of exposure. Section 2.3.2 of the CLEA report gives further information.

2. If you are using site-measured media concentrations, these are used to override predicted values but in doing so the link is broken to changes in soil concentration (that is, as soil concentration changes these values will remain fixed). Therefore, you should normally only calculate ADE/HCV ratios when using site-measured media concentrations. If you choose to calculate soil assessment criteria using site-measured media concentrations you should interpret the soil assessment criteria cautiously.

3. There may be cases when you can generate soil assessment criterion using site-measured media concentrations, however this must be assessed on a case-by-case basis and requires expert judgement.

---

**Print Report**

If you press the 'Print Reports' button, this will provide you with four options

i. Print Results

ii. Print Settings

iii. Save Workbook as

iv. Cancel.
Print Results
Pressing the ‘Print Results’ button will open a preview of the simulation results. Use the ‘Next’ and ‘Previous’ buttons at the top left of the screen to move between the pages.

To print or save the report, press the ‘Print’ button at the top of the page. You can also save the report by printing to PDF if you have Adobe Acrobat/Distiller or similar.

Press the ‘Close’ button at the top right of the screen to go back to Step 5 ‘Results’. Section 3.5.1 provides further information on the ‘Print Results’ report.

Print Settings
Press the ‘Print Settings’ button to see the results of the settings used for calculating the assessment criteria. If the user has changed default parameter values within Step 4 ‘Advanced Settings’, these values will be shown in bold with a shaded background.

To print or save the report, press the ‘Print’ button at the top of the page. You can also save reports by printing to PDF if you have Adobe Acrobat/Distiller or similar.

Press the ‘Close’ button at the top right of the screen to go back to Step 5 ‘Results’. Section 3.5.2 provides further information on the ‘Print Settings’ report.

Save Workbook as
Press the ‘Save Workbook as’ button to save the workbook and simulation. You can select the location and file name to save the workbook. Selections made in Steps 1 to 5 will be saved, including temporary amendments made within Step 4.

Cancel
Press the ‘Cancel’ button to take you back to Step 5 ‘Results’.

Back to Guide
When you have completed this step, press the ‘Back to Guide’ button which will take you back to the ‘Interactive CLEA Software Guide’.

If you have made changes to the parameter values within Step 4 ‘Advanced Settings’ these values are shown in the output reports in bold with a shaded background cell.

3.4 Database management

3.4.1 Introduction
The databases store the default library datasets that the CLEA software uses for predicting exposure and calculating assessment criteria. The information is grouped into datasets that you can select in the ‘Database Management’ area of the ‘Interactive CLEA Software Guide’, see Figure 3.2. There are four databases:

i. Buildings
ii. Chemicals
iii. Land Uses
iv. Soils.
3.4.2 Accessing and sharing datasets

You can access the datasets by pressing the buttons 'Buildings', 'Chemicals', 'Land Uses' or 'Soils' for the required database in the 'Interactive CLEA Software Guide'.

Information for each dataset is set out in rows. To access all the data, you can move and scroll through the worksheet by using the arrow keys or the scroll bars.

You can have more than one database open at any time. When you have accessed a database, a tab will appear at the bottom of the spreadsheet indicating the database that you currently have open. Press the 'Guide' tab to go back to the 'Interactive CLEA Software Guide' and select the next database that you want to open. You can toggle between the databases that you have opened using the tabs at the bottom of the spreadsheet. If you press the 'Back to Guide' button, this will return you to the 'Interactive CLEA Software Guide' and will close the database.

You can share information from within a database by highlighting and copying the data and pasting it into a new worksheet. This can be distributed to other users who can copy and paste data directly into their version of the software.

3.4.3 Adding, editing and saving datasets

In the databases you can:

- view the information for each parameter within a user-added dataset;
- add a new dataset, such as a soil or building type;
- edit an existing user-added dataset;
- delete an existing user-added dataset.

The databases only show datasets that you have added. The CLEA software contains default generic datasets that are available for selection whilst running the software in basic or advanced mode. These default generic datasets are used in the derivation of SGVs and are hidden within 'Database Management' to prevent you from overwriting them. You can make temporary changes to parameter values within these default generic datasets in Step 4, see Section 3.3.3. The names of the default generic datasets that are hidden within each database are provided in Section 3.4.4 to 3.4.7.

If you add datasets to the database, these will be available for selection whilst running the software in basic or advanced mode.

Adding and editing a dataset

To add a new dataset, you must first provide a name for the new dataset in a new row. The name should be different from a hidden generic dataset or an existing user-added dataset so that you can identify the correct dataset in basic or advanced mode. It is recommended that you fill in the data from left to right. Enter the appropriate data under each parameter name listed at the top of the worksheet. The units required for data entry are provided under each parameter name. If you click on a parameter data field, user help text (shown as a pop-up box) will provide supporting information for each parameter. The information also provides guidance on when a parameter value is not relevant and therefore does not need to be provided. In these instances you should add 'NR' to the data field.
You can edit any value by clicking in the field to be changed and typing in the new value. Be careful to comply with any formatting restrictions. Parameter values can be entered in text, numeric or scientific format.

- Changes should not be made to the database during completion of the steps within the interactive CLEA guide as these will not be applied correctly to the calculated assessment criteria. Changes made to the database must be re-applied in Step 2 and/or Step 3 depending on which data has been amended.

- Subscripts can not be incorporated into standard Excel validation comments (pop-up box). An underscore has been added to the help text to indicate a subscript.

- If you prepare data for the databases in a separate Excel workbook to copy into the databases, you should use "paste special" and "values" when copying data into the database in order to not overwrite the advice and settings in the data input cell.

- Ghosted ticks appearing within the user interface are not readily interpreted by the model as a YES. Ghosted ticks are caused when information is copied into the database from an external source (that is not another copy of the software) and there are spaces present before or after the words ‘True’ or ‘False’. Ghosted ticks can be avoided by entering information directly into the software using the dropdown menus.

- You must input all the required information into the databases. Ensure that you scroll from the start to the end of each worksheet when entering new data. Failure to input required data will, for example, default to entering a value of zero if the value for the empirical function for dust model is not entered or no default data may be entered and the calculation will fail.

Saving a dataset

The new datasets can be permanently stored within the database by saving the software as you would normally for an Excel file. To save the software:

- with the same file name select, from the Microsoft toolbar, ‘File’ → ‘Save’

- with a different file name select, from the Microsoft toolbar, ‘File’ → ‘Save As’ then insert the new file name and select ‘Save’.

- You should not use the same name more than once for any dataset.

- New datasets will not be recognised if they have not been given a name (see Figure 3.12 to Figure 3.15).

- You can enter values into the databases in text, numeric, scientific format or by selecting from a fixed list.

- If you require a new dataset to calculate assessment criteria, you must enter this information into the database before proceeding within basic or advanced mode.
3.4.4 Buildings database

Press the 'Buildings' button within the 'Interactive CLEA Software Guide' to go to the buildings database worksheet, the first screen of which is shown in Figure 3.12.

Information for each dataset is set out in rows. To access all the data, move and scroll through the worksheet by clicking on any cell, using the arrow keys or the scroll bar.

![Database Management Buildings Database](image)

**Figure 3.12: Database Management Buildings Database**

Default generic datasets that are available for selection in basic and advanced mode, but are hidden within the buildings database to prevent you from overwriting them, are:

- no building
- bungalow
- small terraced house
- medium/large terraced house
- semi-detached house
- detached house
- warehouse (pre-1970)
- warehouse (post-1970)
- office (pre-1970)
- office (post-1970)

The data that is required for a new building dataset is as follows (the use of each parameter in the software is provided in the sections referenced after each parameter):

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>i. building footprint</td>
<td>Section 4.6.7</td>
</tr>
<tr>
<td>ii. living space air exchange rate</td>
<td>Section 4.6.7</td>
</tr>
<tr>
<td>iii. living space height (above ground)</td>
<td>Section 4.6.7</td>
</tr>
<tr>
<td>iv. living space height (below ground)</td>
<td>Section 4.6.7</td>
</tr>
<tr>
<td>v. pressure difference (soil to enclosed space)</td>
<td>Section 4.7.2</td>
</tr>
<tr>
<td>vi. foundation thickness</td>
<td>Section 4.6.7</td>
</tr>
<tr>
<td>vii. floor crack area</td>
<td>Section 4.6.7</td>
</tr>
<tr>
<td>viii. dust loading factor</td>
<td>Section 4.6.6</td>
</tr>
<tr>
<td>ix. default soil gas ingress rate</td>
<td>Section 4.6.7</td>
</tr>
</tbody>
</table>
3.4.5 Chemicals database

Press the 'Chemicals' button within the 'Interactive CLEA Software Guide' to go to the chemicals database worksheet, the first screen of which is shown in Figure 3.13.

Information for each dataset is set out in rows. To access all the data, move and scroll through the worksheet by clicking on any cell, using the arrow keys or the scroll bar.

Figure 3.13: Database Management Chemicals Database

The data that is required for a new chemical dataset is as follows (the use of each parameter in the software is provided in the sections referenced after each parameter):

i. chemical type
ii. oral and inhalation HCV, type
iii. oral and inhalation HCV, value
iv. comparing HCV with exposure
v. combine oral and inhalation acceptance criteria
vi. physical-chemical properties
vii. dermal absorption fraction
viii. plant correction factors
ix. plant concentration factors
x. apply soil-to-dust transport factor (select yes or no)

The bioaccessible fraction for soil and airborne dust is automatically input as one when you enter a new chemical. The bioaccessible fraction can be amended during Step 4 'Advanced Settings' only.

See Section 4.5.5 for further information on chemical properties.

The following parameters have some form of restricted values (either text or numeric) on the data that can be entered into the cells:

- chemical type (organic or inorganic);
- oral HCV type (ID or TDI);
- oral HCV compare with oral exposure (Yes, No or NR);
- oral HCV compare with dermal exposure (Yes, No or NR);
- oral HCV compare with inhalation exposure (Yes, No or NR);
- inhalation HCV type (ID or TDI);
- inhalation HCV compare with oral exposure (Yes, No or NR);
- inhalation HCV compare with dermal exposure (Yes, No or NR);
- inhalation HCV compare with inhalation exposure (Yes, No or NR);
- combine oral and inhalation AC (Yes or No);
- water solubility, maximum (enter a value greater than or equal to zero);
- dermal absorption fraction (enter a value greater than or equal to zero);
- soil-to-plant concentration factor values (enter a value greater than or equal to zero);
- soil-to-plant concentration factor type (model, numeric dw or number fw);
- soil-to-dust transport factor (enter a value greater than zero).

You can enter a Tolerable Daily Intake (TDI) or an Index Dose (ID) for the oral pathway and a TDI or ID for the inhalation pathway. You can, for example, select an ID for the inhalation pathway and a TDI for the oral pathway. If a substance has both a TDI and an ID for the inhalation pathway for example, and you are unsure which is more critical, you can enter a chemical as two different entries into the chemical database and carry out an analysis on both.

Mandatory fields will change depending on your choice of organic or inorganic chemical; the user help text boxes will provide guidance on whether data is required.

When entering numeric soil-to-plant concentration factors, you should take care to select correctly fresh weight or dry weight.

3.4.6 Land uses database

Press the 'Land Uses' button within the 'Interactive CLEA Software Guide' to go to the land use database worksheet, the first screen of which is shown in Figure 3.14.

Information for each dataset is set out in rows. To access all the data, you can move and scroll through the worksheet by using the arrow keys or the scroll bar.
If you are adding a new land use that relies on selection of a user-added soil or building dataset, you must add the new building and/or soil to the database first so that it can be selected as the default for the new land use.

Default generic datasets that are available for selection in basic and advanced mode but are hidden within the land uses database to prevent you from overwriting them, are:

- residential with homegrown produce
- residential without homegrown produce
- allotments
- commercial.

The data that is required for a new land use dataset is as follows (the use of each parameter in the software is provided in the sections referenced after each parameter):

- i. exposure frequencies (Sections 4.6.2 to 4.6.8)
- ii. occupancy periods (Sections 4.6.6 to 4.6.8)
- iii. soil-to-skin adherence factors (Section 4.6.5)
- iv. soil and dust ingestion rate (Section 4.6.2)
- v. fraction of the site with hard or vegetative cover (Section 4.6.6)
- vi. air dispersion factor at 0.8 m and 1.6 m (Section 4.6.6 to 4.6.8)
- vii. start and end age class (Section 3.3.3)
- viii. default building (Section 3.3.3)
- ix. default receptor (Section 3.3.3)
- x. default soil (Section 3.3.3)
- xi. default gardener type (Sections 4.6.3 and 4.6.4)
- xii. use finite source model (select true or false) (Section 4.9)
- xiii. use fixed value for soil gas ingress (select true/false) (Section 4.6.7)
- xiv. select default exposure pathways (switch true/false) (Section 4.6)

See Section 4.4.3 for further information on receptor behavioural characteristics (that is exposure frequency, occupancy periods, soil-to-skin adherence factors and soil and dust ingestion rate), Section 4.5.4 for further information on soil properties.
You must select to turn on (true) or off (false) each exposure pathway when you enter a new land use. If you leave these fields blank, the software assumes that these pathways are switched off.

In the land uses database, the options of switching on (TRUE) or off (FALSE) are selected by means of a drop down box. Click in the relevant cell and the drop down box will appear. If you cause an error within the cells by trying to delete the information or entering anything other than TRUE or FALSE, an error message will appear. You need to select 'Cancel' on this error message and enter the correct information. However for users of EXCEL 97, if you encounter this problem, data will be inserted erroneously into other cells within the land use worksheet; you must close the software without saving and re-open the software. This problem will only occur on the first initialisation of the worksheet and has been corrected within other versions of EXCEL.

3.4.7 Soils database

Press the 'Soils' button within the 'Interactive CLEA Software Guide'. This takes you to the soils database worksheet, the first screen of which is shown in Figure 3.15.

Information for each dataset is set out in rows. To access all the data, move and scroll through the worksheet by clicking on any cell, using the arrow keys or scroll bar.

![Soils database diagram](image)

**Figure 3.15: Database Management Soils Database**

Default generic datasets that are available for selection in basic and advanced mode, but are hidden within the soils database to prevent you from overwriting them, are:

- clay
- silty clay
- silty clay loam
• clay loam
• sandy clay loam
• silty loam
• sandy loam
• sand.

The data that is required for a new soil dataset is as follows (the use of each parameter within the CLEA software is provided in the sections referenced after each parameter):

i. air-filled and water-filled porosity (Sections 4.6.3, 4.6.7, 4.6.8)
ii. residual soil water content (Sections 4.6.3 and 4.7)
iii. saturated hydraulic conductivity (Sections 4.7)
iv. van Genuchten shape parameter ($m$) (Sections 4.7)
v. bulk density (Section 4.6.3 and 4.6.8)
vi. threshold value of wind speed at 10 m (Section 4.6.6)
vii. empirical function ($F_n$) for dust model (Section 4.6.6)

See Section 4.5.4 for further detail on soil properties.

3.5 CLEA software output reports

There are two output reports that can be generated within the CLEA software, ‘Print Results’ and ‘Print Settings’. The ‘Print Results’ report contains chemical-specific information and the ‘Print Settings’ report contains non-chemical specific information. Each page of the report is replicated below with explanation of the details within it.

3.5.1 ‘Print Results’ report

![Figure 3.16: 'Print Results' information page](image)

Figure 3.17: ‘Print Results’ results page

Figure 3.17 shows the results provided in the ‘Print Results’ report. Calculated soil assessment criteria are shown within the ‘Assessment Criterion’ columns. When ADE/HCV ratios are calculated from representative site soil concentrations, the value ‘0.00E +00’ is displayed in the ‘Assessment Criterion’ column.

ADE/HCV ratios are reported within the ‘Ratio of ADE to HCV’ columns.

‘Not relevant’ may be shown as ‘NR’ within the ‘Assessment Criteria’ or ‘Ratio of ADE to HCV’ columns. This may occur for several reasons:

- ‘NR’ is shown in the ‘oral’ or ‘inhalation’ column when data in the chemical database shows that there is no HCV for that exposure route.

- ‘NR’ is shown in the combined column when information in the chemical database has requested that the oral and dermal assessment criteria are not combined or when no HCV is available for either the oral or inhalation exposure route.

The ‘Soil Saturation Limit’ column reports the lowest of the soil saturation limits (solubility or vapour saturation limit). ‘NR’ is reported for those substances for which a soil saturation limit cannot be calculated. Where a saturation limit has been reported, the output reports specify whether the lowest value reported is solubility or vapour-based by including either (sol) or (vap) after the reported value.

The ‘50% rule?’ reports as yes or no (for both the oral and inhalation pathway) according to whether the 50 per cent rule has been implemented during the calculation of assessment criteria (see Section 4.3.3 for explanation of this rule).
Figure 3.18: ‘Print Results’ soil distribution and media concentrations

Figure 3.18 shows the soil distribution and media concentrations that are provided in the ‘Print Results’ report.

Soil distributions are reported to one significant figure so that a value of zero (0.0) in the vapour column, for example, does not necessarily mean that the contaminant has not partitioned to the vapour phase. Media concentrations should be consulted alongside the soil distribution values.

Media concentrations are reported according to the combined assessment criteria. However if assessment criteria are not combined, the lowest of the calculated assessment criteria is used to calculate and report the media concentrations.

If you have selected ratio mode, by entering site-measured soil concentrations in Step 3 ‘Select Chemicals’ the data entered will be displayed within the relevant media concentrations column with a shaded background cell (note, however, that the shaded background will not be applied to the soil concentration as the goal seek also uses the same cell).
Figure 3.19: ‘Print Results’ ADE and distribution by pathway

Figure 3.19 shows the ADE and distribution by pathway provided in the ‘Print Results’ report. ADE and distribution by pathway is reported for each pathway. Reporting takes into account the pathways selected for calculation of assessment criteria.
Figure 3.20: ‘Print Results’ HCV, fate and transport data and bioaccessible fraction

Figure 3.20 shows the HCV, fate and transport data and physical-chemical data and bioaccessible fractions that are provided in the ‘Print Results’ report. This data reflects the data that is provided in the chemicals data report. However, if the user has changed default parameter values within Step 4 ‘Advanced Settings’, these values are shown in bold with a shaded background cell.

The word ‘model’ is shown in the cell when the soil-to-plant concentration factor has been calculated by the software. If you have input a value for the soil-to-plant
concentration factor, 'dw' or 'fw' is shown with the value to distinguish whether you have identified this as a dry or fresh weight value.

3.5.2 'Print Settings' report

<table>
<thead>
<tr>
<th>Land Use</th>
<th>Residential with homegrown produce</th>
</tr>
</thead>
<tbody>
<tr>
<td>Building</td>
<td>Small terraced house</td>
</tr>
<tr>
<td>Receptor</td>
<td>Female (6y)</td>
</tr>
<tr>
<td>Soil</td>
<td>Sandy loam</td>
</tr>
<tr>
<td>Exposure Pathways</td>
<td></td>
</tr>
<tr>
<td>Direct soil and dust ingestion</td>
<td>Yes</td>
</tr>
<tr>
<td>Consumption of homegrown produce</td>
<td>Yes</td>
</tr>
<tr>
<td>Induced ingestion of attached soil</td>
<td>Yes</td>
</tr>
<tr>
<td>Oral contact with indoor dust</td>
<td>Yes</td>
</tr>
<tr>
<td>Oral contact with soil</td>
<td>Yes</td>
</tr>
<tr>
<td>Inhalation of indoor dust</td>
<td>Yes</td>
</tr>
<tr>
<td>Inhalation of soil dust</td>
<td>Yes</td>
</tr>
<tr>
<td>Inhalation of outdoor dust</td>
<td>Yes</td>
</tr>
<tr>
<td>Inhalation of outdoor vapour</td>
<td>Yes</td>
</tr>
</tbody>
</table>

**Figure 3.21: 'Print Settings' basic settings**

Figure 3.21 shows the basic settings information provided in the 'Print Settings' report and used in the calculation of assessment criteria. This page reports information entered in Step 1 'Basic Settings'. **Exposure duration** is calculated by the software from the choices you have made for the start and end age class.

<table>
<thead>
<tr>
<th>Land Use</th>
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<tr>
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<td>180</td>
</tr>
<tr>
<td>Consumption of produce</td>
<td>180</td>
</tr>
<tr>
<td>Oral contact with indoor dust</td>
<td>180</td>
</tr>
<tr>
<td>Oral contact with soil</td>
<td>23</td>
</tr>
<tr>
<td>Inhalation of indoor dust</td>
<td>0</td>
</tr>
<tr>
<td>Inhalation of soil dust</td>
<td>0</td>
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</table>

**Figure 3.22: 'Print Settings' land use information**

Figure 3.22 shows the land use information provided in the 'Print Settings' report. The data is taken from the land use database according to the land use selected in Step 2 'Basic Settings'. However, if you change default parameter values within Step 4 'Advanced Settings' or enter data for additional age classes, these values are shown with a shaded background cell.
Data is included for all the age classes for which data is provided within the land use database, regardless of the age classes selected in Step 2 ‘Basic Settings’.

### Table

<table>
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<th>Receptor</th>
<th>Female (m)</th>
<th>Male</th>
<th>Exposed skin factor</th>
<th>Max exposed skin factor</th>
<th>Consumption rates in F/W kg⁻¹ and day⁻¹</th>
<th>Skin area</th>
<th>RISK</th>
<th>RISK</th>
<th>RISK</th>
<th>RISK</th>
<th>RISK</th>
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<td>(cm²)</td>
<td>(cm²)</td>
<td>(cm²)</td>
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<td>1.81</td>
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</tbody>
</table>

**Figure 3.23: ‘Print Settings’ receptor information**

Figure 3.23 shows the receptor information provided in the ‘Print Settings’ report. If the user has made changes to the data within Step 4 ‘Advanced Settings’ for body weight, body height, inhalation rate, maximum exposed skin factor or consumption rates, these values are shown with a shaded background cell.

Total skin area is a calculated value (calculated from body weight and body height, see Equation 4.4 of the CLEA report); changes to the component data for calculation of the total skin area do not initiate a change to the background cell for total skin area.
Figure 3.24: ‘Print Settings’ building and soil information

Figure 3.24 shows the building and soil information that is shown in the ‘Print Settings’ report. The buildings and soils data is taken from the buildings and soils database according to the building and soil type selected in Step 2 ‘Basic Settings’. However, if you change default parameter values within Step 4 ‘Advanced Settings’, these values are shown with a shaded background cell.

‘Soil Organic Matter content’ is taken from the data entered in Step 2 ‘Basic Settings’, ‘Fraction of organic carbon’ is a calculated value (calculated from ‘Soil Organic Matter’).

Parameter values for effective total fluid saturation, intrinsic soil permeability, relative soil air permeability and effective air permeability are calculated. Changes to the component data for these calculations do not initiate a change to the background cell for these parameter values.
Figure 3.25: ‘Print Settings’ vapour, air dispersion and plant model information

Figure 3.25 shows the soil-vapour model, soil-plant model and air dispersion model data that is shown in the ‘Print Settings’ report.

If you change the soil-vapour model data within Step 4 ‘Advanced Settings’, the value is shown with a shaded background cell.

If you have selected not to use the default gas ingress rate within Step 4 ‘Advanced Settings’, the ‘Default soil gas ingress rate?’ will be shown as ‘No’ (and will not have a shaded background); this indicates that the soil gas ingress rate shown in the report is a calculated value. If the ‘Soil gas ingress rate’ is shown with a shaded background, then the default soil gas ingress rate has been changed by the user within Step 4 ‘Advanced Settings’.

The ‘Building ventilation rate’ is a calculated value; changes to the component data for calculation of the building ventilation rate do not change the background cell.

If you change the air-dispersion model data or the soil-plant model data within Step 4 ‘Advanced Settings’, the value is shown with a shaded background cell.

Within the print setting reports, data is included for all the age classes for which data is provided within the land use database, regardless of the age classes selected in step 2 ‘Basic Settings’.
4 Scientific and technical guide

4.1 Purpose of the scientific and technical guide

The purpose of the scientific and technical guide is to provide further advice on the scientific and technical information that underpins the CLEA model, and to show you how it can be used for the software. In addition, the CLEA report (Environment Agency 2008) describes how SGVs are derived; however, this handbook provides further scientific and technical information for site-specific assessment. It provides references to other technical guidance in which a particular topic is covered in more detail. The guide does not replace any of these pieces of technical guidance, but acts as a signpost to them. Where referenced, it is recommended that you refer to these more detailed documents for a fuller explanation of specific topics.

4.2 Use of the scientific and technical guide

It is not intended that you read the guide from start to finish, but to consult the guide when there is a particular topic that interests you. The guide is not structured to mirror the screenshot manual, because this is not the most intuitive way to explain the scientific and technical principles. However, in each section there is reference to the appropriate input screens/databases of the software.

In order to avoid repetition, definitions included in the glossary are not reproduced in the text of the guide. Instead, terms that are included in the glossary are defined in bold the first time that they are used in each section.

4.3 General principles

4.3.1 Introduction to the CLEA software

The introduction to the handbook describes the purpose of the CLEA software (version 1.03 beta) and its key differences to its predecessor (CLEA UK software). This section of the scientific and technical guide focuses on the principles underpinning the CLEA model (Environment Agency, 2008d) upon which the software was developed.

The CLEA software is a tool that estimates human exposure to a chemical from a soil source, either by direct contact (such as soil ingestion) or following transport from the soil into another media (such as homegrown produce or indoor air). It does this by using information about:
• building characteristics (see Section 4.5 of the CLEA report);
• chemical properties (see Section 4.2 of the CLEA report);
• land use characteristics (see Section 3 of the CLEA report);
• soil properties (see Section 4.3 of the CLEA report);
• human characteristics (see Section 4.4 of the CLEA report);
• media concentrations (see Section 5 of the CLEA report).

The underlying approach to this process of estimating exposure (referred to as 
Average Daily Exposure or ADE) is provided in Section 2.1.2 and Equation 2.1 of the 
CLEA report. The ADE is compared with to relevant toxicological values that are 
protective of human health. These are known as Health Criteria Values (HCV) and 
are described briefly in Section 4.3.3.

The ADE formulas within the software are consistent with Equation 2.1 of the CLEA 
report; however, additional code has been added. This additional code enables the 
ADE to be calculated for each age class individually by weighting the results to total 
exposure duration, which are then summed. This is a coding convenience and does 
don not affect the calculated results.

The CLEA software is a deterministic model (see Section 2.4.2 of the CLEA report). 
This means that in any calculation each parameter (such as body weight and amount 
of homegrown produce) is represented by a single value.

The CLEA software can be used to:

• derive assessment criteria for human health;
• derive ADE/HCV ratio (ratio mode).

4.3.2 Derivation of assessment criteria

Introduction

Assessment criteria are concentrations of contaminants in soil to which actual 
representative site soil concentrations may be compared to determine whether they 
are likely to represent a human health risk. There are two broad categories of criteria: 
generic assessment criteria and site-specific assessment criteria.

Deriving assessment criteria

Assessment criteria are derived at a soil concentration where the ADE equals the HCV. 
Further information can be found in Section 2.3.2 of the CLEA report. In order to derive 
assessment criteria, the CLEA software derives both the oral and dermal, and the 
inhalation assessment criteria (linked to the HCV) simultaneously until the soil chemical 
concentration is at a level where Equation 2.4 in the CLEA report holds.

Generic and site-specific assessment criteria

Generic assessment criteria (GAC) are derived using largely generic assumptions 
about the characteristics and behaviour of contaminants, pathways and receptors and 
apply to a range of different sites. GAC are protective of health across a wide range of 
circumstances and reasonable range of possible activities. They do not take into
account circumstances relevant to a specific site. **Soil Guideline Values** (SGVs) are generic assessment criteria derived by the Environment Agency using the CLEA model (Environment Agency, 2008c).

Where circumstances relevant to a specific site (such as information on the characteristics and behaviour of contaminants, pathways and receptors) are taken into account by replacing generic assumptions within the software, the assessment criteria derived are referred to as site-specific assessment criteria (SSAC).

You can derive GAC and SSAC using the CLEA software. Table 2.1 of the CLEA report illustrates how detailed assessment may be used to replace generic assumptions used in the derivation of generic assessment criteria including SGVs.

**ADE/HCV ratio**

In both generic and site-specific assessment mode, the software can derive an ADE/HCV ratio (known as ratio mode or hazard quotient). This process is similar to the derivation of assessment criteria, except that instead of establishing a soil concentration of a contaminant at which the ADE/HCV is equal to one, the ADE/HCV ratio for the representative site soil concentration of that contaminant is reported.

### 4.3.3 Toxicological values

A full discussion of the collation and interpretation of toxicological data, and the derivation of HCV, can be found in the TOX guidance report (Environment Agency, 2008b). HCV describe a level of exposure to a chemical derived from toxicity and/or epidemiology data for the purposes of safeguarding human health. Most HCV are expressed as an intake dose, that is, an amount of chemical per kilogram body weight per day (for example, mg kg\(^{-1}\) bw day\(^{-1}\)).

HCV differ according to whether they relate to adverse effects that are expected to demonstrate a threshold or effects for which no threshold is assumed (principally, non-threshold **genotoxic carcinogenesis**), see section 2.2.1 of the TOX guidance report for discussion of threshold and non-threshold toxicity. When dealing with threshold effects, a certain amount of intake of a chemical can be tolerated without appreciable health risks, and a **Tolerable Daily Intake (TDI)** is derived. For non-threshold carcinogens, for which there is at least a theoretical risk at any level of exposure, an **Index Dose (ID)** associated with minimal health risk is derived, with the additional requirement to keep any exposure as low as reasonably practicable (the **ALARP principle**).

The TDI and ID differ in a number of aspects, but one of the most important is how they are used in setting SGV. When using a TDI, background exposure (calculated as the **Mean Daily Intake**, MDI, for the UK population) to the contaminant from non-soil **background sources** (predominantly, ambient air, drinking-water, and food **products**) is accounted for to determine the proportion of the TDI that may be allocated to exposure from soil.

Within the CLEA model (Environment Agency, 2008c) the portion of the TDI that remains once background has been accounted for is termed the **Tolerable Daily Soil Intake**, TDSI, so that the soil ADE = TDSI at the SGV. Section 2.3.1 of the CLEA report explains how the TDSI is calculated.

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, 2008b; Defra, 2008b). In the
derivation of SGV, this minimum proportion is set (Defra, 2008b) at 50 per cent (called the 50 per cent rule). This minimum proportion from soil sources applies to comparisons with individual and multiple routes of exposure. When setting assessment criteria the CLEA software automatically limits the non-soil background exposure to be no greater than that from soil, ensuring that soil always contributes a minimum of half of the total exposure when combining pathways.

The 50 per cent rule is implemented within the CLEA software as follows:

- In calculating the soil assessment criteria, the objective is to find the combination of soil ADE plus background ADE that equals the TDI. In the CLEA software, this is achieved by limiting the background ADE to be no larger than the soil ADE (to ensure that a minimum of 50% of the TDI is allocated to exposure from land). This enables the goal to seek to run smoothly for both the individual and combined AC.

- If only a single HCV is known and it is a TDI, then background exposure from all routes are compared with it.

- If an oral and an inhalation HCV is known and they are both a TDI, the oral background ADE is compared only with the oral TDI and the inhalation background ADE is compared only with the inhalation TDI.

- It is the aggregated exposure across all age classes included in the assessment that is compared when deciding whether the 50 per cent is applied and varying proportions of background may occur for individual age ranges.

- The background exposure is not accounted for when the HCV is an ID.

- In calculating ADE/HCV ratios (in ratio mode), the soil ADE is fixed by the user-entered site data. The background aggregated ADE, up to a maximum of 50 per cent of the TDI, is combined with the soil ADE in calculating the ratio.

Sections 2.3.1 and 2.3.2 of the CLEA report provide further information on how background exposure is taken into account.

The HCV is usually based on the critical adverse effect identified from the available toxicological dataset. Guidance on the selection of an appropriate HCV is provided within the TOX guidance report (Environment Agency, 2008b).

The MDI provided within the TOX reports is for an adult but individual MDIs for each age class are calculated within the software. Although children generally eat and drink less than adults, they consume proportionally more for their body weight. Equally, although inhalation rate is related to body weight, children have higher inhalation rates per kilogram body weight than adults. The correction factors for the adaptation of the MDI are provided in Table 3.4 of the TOX guidance report.

If there is local information relevant to background exposure, for instance on air quality, you can change the data within the MDI field of the chemicals database or you can incorporate this information by creating a new chemical dataset (see Section 3.4.5).

A chemical may have a different HCV for each of the routes of entry into the body (that is, oral and inhalation – the CLEA model does not require a dermal HCV since it is usually not possible to derive one). Within the software, the user is able to select which...
route of exposure (oral, inhalation and dermal) each HCV should be compared with. Assessment criteria aim to ensure that the total risk from exposure via all three routes of entry into the body is no greater than the risk due to exposure at the HCV for any single route of entry. Section 2.3.2 of the CLEA report and Section 3.5.4 of the TOX guidance report consider exposure via multiple routes.

Decisions on how to compare exposure to HCVs is a difficult part of risk assessment, especially where HCVs are not available for each route of entry (see Section 2.3.2 of the CLEA report and Section 3.5.4 of the TOX guidance report).

Under normal circumstances you should combine oral and inhalation assessment criteria when deriving assessment criteria.

4.3.4 Land use

Standard land use

In line with the UK policy of “suitable for use”, assessment criteria are derived for specific land uses. There are three standard land uses for which conceptual exposure models are described in the CLEA report:

i. residential land use

ii. allotment land use

iii. commercial land use

(Section 3.2 of CLEA report)

(Section 3.3 of CLEA report)

(Section 3.4 of CLEA report)

Section 3.4.6 provides a list of the parameter values that describe each of the standard land uses, including the relevant exposure pathways and a defined critical receptor.

You should check whether the conceptual model for your site reasonably matches a standard land use. If it does not, you should create a new land use dataset in the land use database (see Section 3.4.6).

Non-standard land use

In both basic and advanced mode you can derive assessment criteria for non-standard land uses, which are defined as those for which the conceptual exposure model differs from those described in Section 3 of the CLEA report. You will need to develop an appropriate conceptual exposure model for a non-standard land use and enter the new land use dataset into the land use database (see Section 3.4.6).

You may want to make small adjustments to data for a standard land use, including receptor characteristics (such as maximum exposed skin fraction). You can do this by making temporary changes to the data in advanced mode Step 4 (see Section 3.3.3).

When defining a new land use, you can add or remove existing default pathways in the CLEA software; however, you cannot create a new pathway and use this in your assessment. If an additional pathway is important to the conceptual model for your site and is not included within the CLEA software, you can calculate the results and integrate separately or you can use an alternative modelling tool.
The standard commercial land use described in the CLEA software assumes a typical commercial or light industrial property; it does not apply to heavy industrial workers and facilities, nor to work that is predominantly undertaken outside such as construction work or landscape maintenance. Soil and soil-derived dust ingestion rates, proportion of time spent inside and outside, number of hours on site and proportion of time spent in active and passive respiration are defined for the patterns of an office or warehouse worker undertaking relatively light work indoors with standard hour days and short outside breaks. If you wish to develop assessment criteria for such a scenario, you need to define a conceptual model and enter it into the land use database as a new land use.

4.4 Receptors

4.4.1 Critical Receptors

Introduction

Receptors of different ages exposed to the same level of contamination in the soil have a different ADE because of differences in physiology and behaviour. The critical receptor represents the individual or subgroup of the population most likely to be exposed and/or susceptible to the presence of soil contamination.

The male and female receptors defined in the software are slightly different, due to physiological differences such as body weight and height. Also for some age ranges, the behavioural characteristics may differ slightly. The default critical receptor is usually female because body weight is typically lower than for a comparable male receptor, resulting in a higher dose from the same chemical concentration in soil.

Age class is a concept described in the CLEA report (Section 2.1.2) to accommodate the fact that some exposure characteristics, such as bodyweight, change significantly with age in a general single category such as "child", and that this may have an impact on an exposure assessment. The CLEA software divides a lifetime into eighteen age classes to account for variations in exposure characteristics with age. The first sixteen age classes correspond to the first sixteen years of life, the seventeenth interval is typical of an adult working life (age 16-65), and the eighteenth represents retirement (age 65-75). The age classes have been chosen to represent those stages in life where the most significant differences in exposure characteristics are likely to occur. The age classes used within the CLEA software are provided in Table 3.1.

The choice of critical receptor differs according to land use. The critical receptors for standard land uses are shown in Table 4.1. For non-standard land uses, you need to select one or more receptors, based on the sensitivity of different receptors for the land use.

<table>
<thead>
<tr>
<th>Standard land use</th>
<th>Critical receptor</th>
<th>Age class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Residential</td>
<td>0 to 6-year old female child</td>
<td>1 to 6</td>
</tr>
<tr>
<td>Allotments</td>
<td>0 to 6-year old female child</td>
<td>1 to 6</td>
</tr>
<tr>
<td>Commercial</td>
<td>16 to 65-year old female working adult</td>
<td>17</td>
</tr>
</tbody>
</table>

Selection of critical receptor in the CLEA software

In the CLEA software, selection of the critical receptor is performed in Step 2 ‘Basic Settings’ (see Section 3.3.3).

In both basic and advanced mode, the database corresponding to the default critical receptor is automatically selected when you select the land use, as is the start and end age classes appropriate to the critical receptors.

When adding a new land use to the database, you need to select the default critical receptor from one of the existing receptors in the software. These are:

- female (res) (available for age classes 1 - 18)
- male (res) (available for age classes 1 - 18)
- female (allot) (available for age classes 1 - 6 only)
- male (allot) (available for age classes 1 - 6 only)
- female (com) (available for age class 17 only)
- male (com) (available for age class 17 only).

The exposure characteristics of the commercial and residential receptors differ for the exposed skin area due to the differences in assumed clothing worn (see Section 4.4.3 of this report and Section 4.4.2 of the CLEA report).

The physiological characteristics of residential and allotment receptors differ for the inhalation rate. Inhalation rate for the allotment receptor is based on short-term exposure, and for the residential receptor is based on long-term exposure (see Section 4.4.3 of this report and Section 4.4.3 of the CLEA report).

Data for commercial receptors are only available within the software for age class 17 and data for allotment receptors are only available within the software for age classes 1 to 6. You should therefore not select a commercial or allotment receptor for any other age class unless you add the data for the additional age classes in Step 4 ‘Advanced Settings’.

4.4.2 Exposure duration and averaging time

Exposure duration (ED) refers to the length of time in years that a critical receptor is assumed to be exposed for the purposes of modelling. Averaging time (AT) refers to the number of days over which the exposure is aggregated and averaged to produce an intake/uptake dose in μg kg\(^{-1}\) bodyweight day\(^{-1}\). UK policy is that AT should be the same as the relevant ED for both threshold and non-threshold substances (although ED is expressed in years and AT is expressed in days). Section 2.1.2 of the CLEA report provides further information. Selection of start and end age classes automatically sets the exposure duration and the averaging time (discussed in Section 4.4.2).

In the CLEA software, ED and AT are calculated automatically for the choices entered for starting and ending age classes.
Data for commercial receptors is only available within the software for age class 17. You should therefore not select a commercial receptor for any other age class.

Children are not the critical receptor for long-term risks for the commercial land use scenario, as they are not typical regular users of the land. However, where short-term risks may be an issue (for instance for cyanide), you should consider this age group. If children are regularly present in a commercial setting (for instance, if there is a crèche on the premises), this is not consistent with the commercial standard land use and you should treat it as a non-standard land use (see Section 4.3.4).

It may not always be clear who the critical receptor for a non-standard land use is, without further assessment for a number of different receptors. For instance, children have higher soil ingestion rates and lower body weights but may use the site on a less frequent basis than older children or adults. To consider more than one receptor, you will need to run the software more than once using a different receptor each time.

Female body weights for age class 18 (age 65 to 75) are slightly higher than those for age class 17 (age 16 to 65); see Table 4.8 of the CLEA report. The exposure patterns for this group in a residential setting are also slightly different from those of other adults. There may be non-standard land uses such as sheltered housing where this age group is the critical receptor.

The critical receptor may differ for non-standard land uses according to the contaminant and the key applicable pathways.

Age class 2 (age 1 to 2) is likely to be the most critical receptor for the soil ingestion pathway in the residential and allotment scenarios. Soil ingestion rate is highest for age classes 1 to 6, body weight is the lowest except for age class 1, and Exposure Frequency (EF) is 365 days per year (EF is 180 days per year for age class 1).

4.4.3 Characterising receptors

Introduction

There are two types of exposure characteristics considered in the CLEA software. The first type is physiological characteristics, which do not vary with land use (only with the choice of critical receptor). The second type is behavioural characteristics, which will vary with land use.

Physiological characteristics

The physiological characteristics are referred to in the CLEA software as 'receptor data'. These data and their use within the CLEA software are detailed in Table 4.2.

When creating a new land use, the receptor data can only be temporarily altered in Step 4 'Advanced Settings'; that is, they cannot be stored permanently as part of a new receptor dataset. The physiological characteristics data are based on authoritative UK data and therefore changes to the data must be based on sound justification.
Table 4.2: Physiological characteristics

<table>
<thead>
<tr>
<th>Physiological characteristic</th>
<th>Description of use within the CLEA software</th>
</tr>
</thead>
</table>
| Body weight (Section 4.4.1 of the CLEA report) | • Used in the calculation of ADE because dose is required in units per kg body weight per day to compare with the HCV, which are in units per kg body weight per day.  
• Used in the calculation of total skin area, inhalation rates and vegetable consumption rates. |
| Body height (Section 4.4.1 of the CLEA report) | • Used in the calculation of the total body skin surface area.  
• Used qualitatively for comparison and selection of data used to predict outdoor exposure to volatile contaminants. |
| Maximum exposed skin fraction (Section 4.4.2 of the CLEA report) | • Used to calculate the total skin area exposed to potential contact with contaminated soils and indoor dust. |
| Inhalation rate (Section 4.4.3 of the CLEA report) | • Used to estimate exposure to soil contamination from the inhalation of dust and vapours. |

**Behavioural characteristics**

Behavioural characteristic data are contained within the land uses database (see Section 3.4.6). These data and their use within the software are detailed in Table 4.3.

When creating a new land use, behavioural characteristics can be stored permanently as part of a new land use dataset, except for consumption rate of homegrown produce which can only be temporarily amended in Step 4 ‘Advanced Settings’. See Table 4.3 for the behavioural characteristics that can be amended in the CLEA software.

It is important to note that behavioural characteristics for the standard land uses (see Section 4.3.4) can only be temporarily changed in Step 4 ‘Advanced Settings’.

Table 4.3: Behavioural characteristics

<table>
<thead>
<tr>
<th>Land use characteristics</th>
<th>Description of use within the CLEA software</th>
</tr>
</thead>
</table>
| Exposure frequency (Section 2.1.2 and Section 3 of the CLEA report) | • Represents the number of days per year in which a daily exposure event is considered to occur.  
• An exposure frequency is assigned to each exposure pathway. |
| Occupancy period, indoors and outdoors (Section 3 of the CLEA report) | • Provides information on indoor and outdoor site occupancy, in hours per day, in which an exposure event is considered to occur. Cannot exceed 24 hours for any age class.  
• Used to estimate exposure to soil contamination from the inhalation of dusts and vapours. |
<p>| Soil-skin adherence factor, indoors and outdoors | • Provides information on the amount of soil adhered to, or in... |</p>
<table>
<thead>
<tr>
<th>Land use characteristics</th>
<th>Description of use within the CLEA software</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Section 8.1.1 of the CLEA report)</td>
<td>intimate contact with the skin, over the contact period for a single event.</td>
</tr>
<tr>
<td></td>
<td>• Used to estimate exposure to soil contamination from dermal absorption.</td>
</tr>
<tr>
<td>Soil and dust ingestion rate (Section 6.1 of the CLEA report)</td>
<td>• Provides information on the amount of soil and indoor dust ingested on a daily basis.</td>
</tr>
<tr>
<td></td>
<td>• Used to estimate exposure to soil contamination from ingestion of soil and indoor dust (outdoors and indoors).</td>
</tr>
<tr>
<td>Consumption rate of homegrown produce (Section 4.4.5 of the CLEA report)</td>
<td>• Provides information on the amount of homegrown fruit and vegetables consumed per day.</td>
</tr>
<tr>
<td></td>
<td>• Used to estimate exposure to soil contamination from consumption of contaminated homegrown produce.</td>
</tr>
</tbody>
</table>

> When creating a non-standard land use, you will need to ensure that the conceptual model is consistent between exposure pathways. For instance, the CLEA model does not automatically check that the number of days of dermal contact does not exceed the numbers of days on which inhalation occurs.

> Within the CLEA model, consumption rates (g fw kg⁻¹ bw day⁻¹) for homegrown produce are based on annualised data and therefore a hypothetical exposure frequency of 365 days per year should always be assumed (except age class 1, when it is assumed to be 180 days per year to account for the period prior to weaning).

### 4.5 Fate and transport of chemicals in soil

#### 4.5.1 Introduction

The term ‘fate and transport’ is a commonly used 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 present in the soil gas phase;
- transport of a chemical from one place to another, such as 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.

A brief discussion of these aspects can be found in Sections 4.5.2 and 4.5.3 of this handbook, with references to other parts of the guide where appropriate. For further information, refer to Sections 4.1 and 5 of the CLEA report.
4.5.2 Behaviour of chemicals in soil – general principles

The behaviour of a chemical in soil depends on the properties of the chemical and soil.

Properties vary from chemical to chemical depending on the structure. Examples include how easily it dissolves in water, enters the vapour phase from solution, adsorbs to soil organic matter and travels through the soil. These properties (often termed physical-chemical properties) should be provided on a chemical-specific basis in the chemicals database of the CLEA software. They are discussed in more detail in Section 4.2 of the CLEA report.

Properties vary from soil to soil; examples include the proportion of air spaces, the proportion of these which are filled with water, the dry soil bulk density and the amount of organic matter. These properties are provided on a soil-specific basis in the soils database of the CLEA software. They are discussed in more detail in Section 4.3 of the CLEA report.

The soil and chemical properties determine the partitioning of the chemical between the solid phase of the soil, the water phase (dissolved in the pore water solution) or the soil gas phase (in air spaces in the soil).

There are limits to the amount of chemical that can dissolve in the soil water (saturated water concentration) or exist as soil gas (saturated vapour concentration). These limits vary depending on the soil and chemical properties and are discussed in more detail in Section 5.3 of the CLEA report. When these limits are exceeded, free product may occur. If the ambient temperature is at or above the melting point of the chemical, this chemical phase may also be referred to as a non-aqueous phase liquid (NAPL). Section 3.3.3 provides information on how to identify whether solubility limits have been exceeded in the calculation of assessment criteria. Further detail on chemical partitioning is provided in Section 5 of the CLEA report.

- Within the CLEA model, chemical partitioning between environmental media and different phases including air, water, soil and lipids is assumed to reach chemical equilibrium. Partitioning does not take into account the presence of free phase contaminants. The distribution between the different environmental media is shown in the ‘Print Results’ report of the CLEA model.

- Partitioning calculations are based on chemical and soil properties and assume that chemical concentrations and soil properties are homogenous across the site and throughout the soil profile. In reality this is not the case, and free phase contamination may occur locally at levels that on average are below the theoretical saturation limit. Similarly, contamination may be found in soil at levels much higher than the theoretical saturation limit where free phase is not present.

- The CLEA model uses the Air-water partition coefficient to predict chemical partitioning in soil systems. The degree of conservatism when using this approach to predict the soil gas concentration in the subsurface will vary considerably according to site conditions and the types of volatile chemicals 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 (see Section 10.1.1 of the CLEA report for further information).
4.5.3 Relationship between chemical concentrations in soil and those in other environmental media – general principles

The relationship between chemical concentrations in soil and those which enter environmental media (for example, plants, groundwater or air) depend on the physical-chemical properties of the chemical (see Section 4.2 of the CLEA report) and the soil properties (see Section 4.3 of the CLEA report). The partitioning of the chemical in the soil has an effect on the eventual destination of the chemical. For example, if most of a chemical is adsorbed to the solid phase of the soil, less will be present in the soil solution and/or vapour phase. This has the implication that, for example, less chemical can be taken up into plant roots and/or enter a building. In addition, physical-chemical properties such as the diffusion coefficients in air and water will determine how quickly the chemical can travel through the soil compartment. Soil properties can also affect how easily the contaminant travels through a particular compartment, for example, diffusion of the contaminant through the vapour phase if there is limited connectivity of the air spaces.

Other considerations which influence contaminant concentrations in the media relate to the media themselves or their immediate surroundings. For example, the concentration of a chemical in ambient air is influenced by the site conditions such as the extent of hard cover on site affecting the potential for dust resuspension (see Section 4.6.6 on indoor and outdoor dust inhalation and Section 4.6.8 on outdoor vapour inhalation) and contaminant concentrations in indoor air will be influenced by the properties of the building (see Section 4.6.7 on indoor vapour inhalation). These factors are by their nature specific to the media involved and associated exposure pathways.

- Approaches to calculating concentrations in other media from soil concentrations are usually indications of concentrations rather than accurate quantitative predictions. During further detailed quantitative risk assessment (DQRA) reliable measurements of, say, vapour in buildings are likely to reduce the uncertainty of the assessment. Such measurements can be entered directly into the CLEA model (see Section 3.3.3).
- Soil pH is no longer applied within the CLEA model and thus you are not required to add a value for pH. This functionality will be reconsidered in the development of SGVs.

4.5.4 Soil properties

The CLEA software contains standard generic soil types defined by properties detailed in Table 4.4 of the CLEA report. The default soil type used in the CLEA software is sandy loam soil and this is used for the derivation of SGVs.

You may want to use Figure 4.1 or Table 4.4 in the CLEA report to decide which broad category a soil falls into based, for example, on trial pit logs or particle size determination. Alternatively, you can enter a new soil dataset in the database (see Section 3.4.7) or adjust the properties of an existing soil in Step 4 ‘Advanced Settings’ (see Section 3.3.3). You can select any added soil dataset or standard generic soil type in Step 2 ‘Basic Settings’ of both basic and advanced mode (see Section 3.3.3).

The soil properties and their description are provided in Table 4.3 of the CLEA report. Default values for the generic soil types are provided in Table 4.4 of the report. Only one value may be entered into the database to represent each of the properties, though there may be considerable variation between samples of the same material from the same site. You should take care to select representative values and may find it useful to conduct a sensitivity analysis to guide this selection.
The one soil property set outside the soil database is percentage soil organic matter (SOM). This value can be changed in both modes within Step 2 (see Section 3.3.3).

Soil organic matter (SOM) is used within the CLEA software to estimate the soil organic carbon fraction. The organic carbon fraction is used to estimate the partitioning of organic chemical between soil, water and air phases. The greater the amount of organic matter in the soil, the more the contaminant will be adsorbed to it, so that less is available in soil solution for uptake into plants or in the vapour phase where it can migrate into the ambient air or air in buildings.

Section 5 of the CLEA report describes how chemical properties are used to determine the partitioning of the chemical in the soil environment.

1. The software automatically calculates total porosity from water-filled and air-filled porosity.

2. Many of the soil matrix properties (for example, porosity and density) are related to each other. You should be careful not to alter one property for which you have site-specific data, without considering the implications for the other soil properties.

3. The CLEA software does not determine the form of readily ionisable compounds such as chlorinated phenols based on the pH. You need to consider the implications on a substance-specific basis when undertaking a risk assessment.

4. Some laboratories report soil organic matter (SOM) in the form of either % total organic carbon (% TOC), total organic carbon (mg kg⁻¹) or fraction organic carbon (fTOC). These are different from SOM because not all organic matter is organic carbon. Only % SOM can be entered directly into the CLEA software. The software automatically calculates fTOC, the conversion used is:

   \[ f_{\text{TOC}} = \text{SOM}/100 \times 0.58 \]

5. % TOC can be converted into SOM by dividing by 0.58.

### 4.5.5 Chemical properties

You can add data for a new chemical in the chemical database (see Section 3.4.5) or temporarily adjust the chemical properties of any chemical in Step 4 'Advanced Settings' (see Section 3.3.3). In addition to appropriate HCV, a number of physical-chemical properties are required to describe the behaviour of the chemical in soil, as discussed in Section 4.5.2 and 4.5.3.

You can select any chemical in Step 3 'Select Chemicals' (see Section 3.3.3).

Not all chemical property data is required for each chemical. Data requirements depend on the chemical type (organic or inorganic). Data required for inorganic and organic chemicals and the description of each parameter is provided in Table 4.2 of the CLEA report. Many of the reference properties of a chemical should be adjusted to 10°C, the annual average soil temperature in the UK. Methods for the most common adjustments are presented in Environment Agency (in press), which also has guidance on the selection of parameters for the derivation of SGVs for a number of organic chemicals including petroleum hydrocarbons, chlorinated solvents, and pesticides.

Section 5 of the CLEA report describes how chemical properties are used to determine the partitioning of the chemical in the soil environment.
The assumption in the CLEA software is that the bioaccessible fraction is one (that is, during ingestion and digestion all the chemical enters into solution in the gut and during inhalation all the chemical enters into solution in the lung). You can find information on the use of bioaccessibility in land contamination assessments on the Environment Agency’s website at www.environment-agency.gov.uk.

You are no longer required to enter data for chemical boiling point, critical temperature, enthalpy of vaporisation at normal boiling point or Henry’s Law constant in units of atm m³ mol⁻¹. You can calculate the air-water partition coefficient ($K_{ow}$), in units of cm³ cm⁻³, at ambient soil temperature, 283K, and enter this value directly into the CLEA software chemical database. Environment Agency (in press) provides methods for calculating $K_{ow}$ at ambient soil temperature. ($K_{ow}$ was formerly referred to as HLC dimensionless within the CLEA model).

When calculating the air-water partition coefficient at ambient soil temperature, for all substances the boiling point is lower than the critical temperature.

The CLEA software uses chemical data reported in the International System of Units (SI). Values from the literature can be corrected to SI units using conversion factors presented in NIST (1995).

4.6 Exposure Pathways

4.6.1 Introduction

The CLEA software includes the ten exposure pathways listed Table 4.4.

Table 4.4: Exposure pathways in the CLEA software

<table>
<thead>
<tr>
<th>Routes of entry</th>
<th>Exposure pathways</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral</td>
<td>Direct soil ingestion</td>
</tr>
<tr>
<td></td>
<td>Direct dust ingestion</td>
</tr>
<tr>
<td></td>
<td>Consumption of homegrown produce</td>
</tr>
<tr>
<td></td>
<td>Consumption of soil attached to homegrown produce</td>
</tr>
<tr>
<td>Dermal</td>
<td>Indoor dermal uptake</td>
</tr>
<tr>
<td></td>
<td>Outdoor dermal uptake</td>
</tr>
<tr>
<td>Inhalation</td>
<td>Indoor dust inhalation</td>
</tr>
<tr>
<td></td>
<td>Outdoor dust inhalation</td>
</tr>
<tr>
<td></td>
<td>Indoor vapour inhalation</td>
</tr>
<tr>
<td></td>
<td>Outdoor vapour inhalation</td>
</tr>
</tbody>
</table>

The exposure pathway, direct dust ingestion, is included within the direct soil ingestion pathway within the CLEA software and a combined soil and dust ingestion rate is used. There is a lack of supporting data to identify the fraction of dust derived from soil.

The default exposure pathways that are applicable to each of the standard land uses within the CLEA model are dependent on each land use conceptual exposure model. The conceptual exposure model for each of the standard land uses (residential, allotment and commercial) is discussed in Section 3 of the CLEA report.
The approach to the modelling of each exposure pathway is discussed in detail in Sections 6 to 10 of the CLEA report. You can find the calculated average percentage exposure contribution from each pathway to the ADE in the results report of the CLEA software (see Section 3.5).

There are additional exposure pathways that are NOT included in the CLEA model or software and cannot be added. A list of some such pathways is provided below:

- inhalation of vapours (indoors and outdoors) volatilised from shallow groundwater;
- dermal contact with shallow groundwater;
- ingestion of shallow groundwater;
- inhalation of vapours when bathing/showing either directly with groundwater obtained from an on-site source or following permeation of plastic pipes;
- dermal contact when using water obtained from an on-site source or following permeation of plastic pipes;
- ingestion of drinking water from an on-site source or following permeation of plastic pipes;
- consumption of crops irrigated with an on-site source or following permeation of plastic pipes;
- dermal contact with water from a sprinkler;
- consumption of homegrown foodstuffs other than fruit and vegetables (for example poultry, meat, eggs, shellfish, fish);
- ingestion of water and/or sediment while swimming in a contaminated source;
- dermal contact with water or sediment while swimming in a contaminated source.

Site-specific information may indicate that some of these non-standard pathways are present for a standard or user-added land use. Their presence may make the site use more sensitive than the generic conceptual model. If qualitative assessment suggests that the contribution from one of these pathways is significant, an alternative tool should be used instead of or in addition to the CLEA software.

4.6.2 Direct soil and dust ingestion

The approach to modelling direct ingestion of soil and dust is described in Section 6 of the CLEA report. This pathway often represents the most significant route of exposure for non-volatile chemicals.

Parameters and location within the software

Parameters in the soil and dust ingestion pathway that can be changed in the software:

- Exposure frequency of soil and dust ingestion varies with age class and land use and represents the number of days a year in which daily exposure occurs. Generic values used in the software are provided in Tables 3.1, 3.6 and 3.9 of
the CLEA report for residential, allotment and commercial land uses. The data is contained within the ‘Land Uses’ database of the CLEA software.

- **Soil and dust ingestion rate.** Currently, there is insufficient knowledge to separate ingestion of soil and soil-derived dust. The combined rate is a single point value each for children and adults for all the standard land uses. Generic values used in the CLEA software are provided in Section 6.1.4 of the CLEA report. The data is contained within the ‘Land Uses’ database.

- **Soil bioaccessible fraction (oral bioaccessibility factor)** is the fraction of a chemical that is released into solution from the soil during digestion, making it available for absorption. The software assumes the bioaccessible fraction to be one; that is, during ingestion and digestion all the chemical enters into solution in the gut. The data is contained within the ‘Chemicals’ database of the CLEA software. See Section 4.10 for further information.

**How parameter values can be changed in the software**

You can change parameter values for exposure frequency and ingestion rates by:

i. entering a new land use in the ‘Land Use’ database for use in either basic or advanced mode;

ii. making temporary amendments to ‘Land Use and Receptor Data’ in advanced mode, Step 4.

You can change the parameter values for soil bioaccessible fraction by:

i. making temporary amendments to ‘Chemical Data’ in advanced mode, Step 4.

---

1. **SGVs** are derived assuming that absorption from soil is the same as the absorption from the medium (for example, water and food) used in the critical study to derive the HCV.

2. The phenomenon of **pica** or geophagia (the persistent and purposeful consumption of soil, often in relatively large quantities) has not been incorporated within the soil ingestion rates in the CLEA report. Such a (long-term) psychopathological condition should not normally be accounted for in generic assessment criteria (see Section 6.1.4 of the CLEA report). There are many types of psychopathological behaviour that can affect adults and children, and where it is considered that protective measures are necessary, it may be appropriate to consider pica when selecting a soil ingestion rate.

3. The pathway direct ingestion of soil-derived dust is not identified as a separate pathway within the CLEA software. By selecting the direct soil ingestion pathway, the direct dust ingestion is automatically included.

4. It is not recommended that you change the soil ingestion rates for standard land uses, as the data is not available to support replacement values in the CLEA report. However for some non-standard land uses you may wish to select alternative values, for example, for an adult receptor engaging in an activity where you think the soil ingestion rate might be higher than those in a residential or commercial setting.
4.6.3 Consumption of homegrown produce

Introduction

The consumption of fruit and vegetables that have taken up contamination is often a significant pathway for mobile and semi-volatile chemicals. The approach to modelling consumption of homegrown produce is described in the CLEA report Section 7.

The key parameters in the consumption of homegrown produce are the soil-to-plant concentration factor and the behavioural characteristics of the critical receptor.

Parameters and location within the software

Chemical concentrations in the edible portions of fruit and vegetables are predicted from the relationship between the soil and plant; this is known as the soil-to-plant concentration factor. The approach to estimating the soil-to-plant concentration factor is described in the CLEA report (Section 7.2) and varies according to whether the type of contaminant in question is inorganic or organic.

Inorganic chemicals:
The parameters used in estimating the soil-to-plant concentration factors for inorganic chemicals that can be changed within the CLEA software are:

- **Soil-plant availability correction** varies according to the chemical and accounts for a number of variable factors found in plant uptake pot experiments including the total plant density (including roots), depth of pot soil, duration of the experiment and an empirical calibration parameter. It is used to estimate the soil-to-root concentration factor and subsequently the soil-to-plant concentration factor, of inorganic chemicals, representative of edible plant parts of fruit and vegetables. Generic values used within the software are provided in Table 7.2 of the CLEA report. The data is contained within the 'Chemicals' database of the software.

- **Water-filled soil porosity** is dependent on the soil type and is used to estimate the soil-to-root concentration factor and subsequently the soil-to-plant concentration factor, of inorganic chemicals, representative of edible plant parts of fruit and vegetables. Water-filled porosity is the amount of soil pore space occupied by water based on a suction head at 50 cm H₂O. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the 'Soils' database of the CLEA software.

- **Dry soil bulk density** varies according to soil type and is used to estimate the soil-to-root concentration factor and subsequently the soil-to-plant concentration factor, of inorganic chemicals, representative of edible plant parts of fruit and vegetables. It is a measure of the apparent density of field soil. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the 'Soils' database of the CLEA software.

- **Sorbed soil-water partition coefficient (Kₘₐₜ) varies according to the chemical selected and is used to estimate the soil-to-root concentration factor and subsequently the soil-to-plant concentration factor, of inorganic chemicals, representative of edible plant parts of fruit and vegetables. It is a measure of the relationship between the concentration of sorbed chemical and that in aqueous solution. Information on chemical-specific soil-water partition coefficients is
provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the CLEA software.

- **Root-shoot/root-root/root-tuber/root-fruit correction factor.** These values vary according to the chemical and are used to correct the soil-to-root concentration factor to derive a soil-to-plant concentration factor representative of edible plant parts of fruit and vegetables. They represent the fraction of a chemical in the root system that reaches edible plant parts, including root store, tubers, fruits and shoots. Information on chemical-specific correction factors is provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the CLEA software.

- **Dry weight conversion factor** varies according to the homegrown produce type (that is, green vegetables, root vegetables, tuber vegetables, herbaceous fruit, shrub fruit or tree fruit). They are used to correct dry weight (dw) soil-to-plant concentration factors to fresh weight (fw) to enable comparison with consumption data. The data is contained within the ‘Homegrown Produce Data’ in advanced mode Step 4 of the CLEA software.

Further information on the approach for inorganic chemicals is provided in Section 7.2.1 of the CLEA report.

**Organic chemicals:**

- **Soil-to-plant concentration factors** vary according to the homegrown produce type (that is, green vegetables, root vegetables, tuber vegetables and tree fruit) and are used to estimate the chemical concentrations in the edible portions of fruit and vegetables. Literature values can be used, where these are available, or they can be calculated generically for each produce group within the CLEA software. Information on chemical-specific soil-to-plant concentration ratios is provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the CLEA software. Section 7.2.2 of the CLEA report provides information on the current default models used to calculate the soil-to-plant concentration factors for each produce group.

Site-measured fruit and vegetable chemical concentrations entered in Step 3 ‘Select Chemicals’ must be entered as fresh weight (fw) plant concentration to compare with the fresh weight consumption data. The calculation from dry weight to fresh weight and the dry weight conversion factors are provided in Equation 7.1 and Table 7.1, respectively, of the CLEA report.

The parameters used to estimate the soil-to-plant concentration factors for organic chemicals that can be changed within the CLEA software are:

- **Octanol-water partition coefficient (K_{ow})** varies according to the chemical and is used to calculate the soil-to-plant concentration factors for green, root and tuber vegetables and tree fruit. It is used as a measure of the chemical lipophilicity. Information on chemical-specific soil-water partition coefficients is provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the CLEA software.

- **Dry soil bulk density** varies according to soil type and is used to calculate the soil-to-plant concentration factor for green vegetables. It is a measure of the apparent density of field soil. Generic values used within the CLEA software
are provided in Table 4.4 of the CLEA report. The data is contained within the 'Soils' database of the CLEA software.

- **SOM (soil organic matter)** varies according to soil type and is used to calculate the soil-to-plant concentration factor for green vegetables and the sorbed soil-water partition coefficient (K_d) which is used to calculate the soil-to-plant concentration factor for root vegetables. It is a measure of the amount of organic material in soil, including humus. SOM is used by the CLEA model to estimate the organic carbon fraction (see Section 4.5.4). The default value used in the derivation of SGVs is SOM content of 2.5 per cent. The SOM value used within the software is 2.5 per cent; this can be temporarily changed, see below.

- **Water-filled soil porosity** is dependent on the soil type and is used to estimate the soil-to-plant concentration factor for green vegetables. Water-filled porosity is the amount of soil pore space occupied by water based on a suction head at 50 cm H_2O. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the ‘Soils’ database of the CLEA software.

- **Organic carbon-water partition coefficient (K_{oc})** varies according to the chemical selected and is used to calculate the soil-to-plant concentration factors for green vegetables and the sorbed soil-water partition coefficient (K_d) which is used to calculate the soil-to-plant concentration factor for root vegetables. It is a measure of how easily the chemical adsorbs to soil organic matter compared to water. Information on chemical-specific soil-water partition coefficients is provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the CLEA software.

- **Diffusion coefficient in water** varies according to the chemical type and is used to calculate the soil-to-plant concentration factor for tuber vegetables. It is a measure of the diffusion of a molecule in an aqueous medium and should be determined at the soil temperature where possible. Chemical-specific diffusion coefficients are provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the CLEA software.

**Behavioural characteristics:**

The receptor behavioural characteristics in the consumption of homegrown produce pathway, which can be changed in the CLEA software, are:

- **Exposure frequency of consumption of homegrown produce** varies with age class and represents the number of days a year in which daily exposure occurs. Generic values used within the CLEA software are provided in Tables 3.1 and 3.6 of the CLEA report for residential and allotment land uses respectively. The data is contained within the ‘Land Uses’ database of the CLEA software.

Exposure frequency of consumption of homegrown produce is assumed to be 365 days per year for all vegetables for all age classes except age class 1 when it is assumed to be 180 to account for the period prior to weaning. This does not mean that it is assumed that homegrown produce may be eaten all year round. Instead, the total amount of homegrown produce is calculated on a yearly basis using data from dietary surveys. This total yearly consumption is divided by 365 (180 in age class 1) to provide a daily consumption rate for each age class.

- **Consumption rates for fruit and vegetables** are an important characteristic for estimating exposure to soil contamination from consumption of contaminated
homegrown produce. The amount of fruit and vegetables consumed varies for each age class because of preference and habit and is calculated on a yearly basis using data from dietary surveys. The total yearly consumption (of both homegrown and shop bought) is divided by 365 (180 in age class 1) to provide a daily consumption rate for each age class. Further information is provided in Section 4.4.4 of the CLEA report. Generic values used within the CLEA software are provided in Table 4.17 of the CLEA report and are given for six categories of homegrown produce (green, root and tuber vegetaties and herbaceous, shrub and tree fruit). The data is contained within the 'Homegrown Produce Data' in advanced mode Step 4 of the CLEA software.

- **Homegrown fractions for each produce group** represent the proportion of fruit and vegetables consumed that is assumed to be grown and eaten from the potentially contaminated garden or allotment. Generic values used within the CLEA software are provided for the six categories of homegrown produce in Table 4.19 of the CLEA report. Fractions are provided for **gardener types**, both average and high end scenarios, such as allotment holders who can be assumed to consume a higher fraction of homegrown produce from the allotment than the average family consumption of homegrown garden produce. Further information is provided in Section 4.4.5 of the CLEA report. The data and selection of gardener type is contained within the 'Homegrown Produce Data' in advanced mode Step 4 of the CLEA software.

**How parameter values can be changed in the software**

You can change parameter values for **exposure frequency** by:

i. entering a new land use in the 'Land Uses' database;

ii. making temporary amendments to 'Land Use Data' in advanced mode, Step 4.

You can change parameter values for **water-filled soil porosity**, **residual soil water content** and **dry soil bulk density** by:

i. entering a new soil type in the 'Soils' database;

ii. making temporary amendments to 'Soil and Building Data' in advanced mode, Step 4.

You can change parameter values for **consumption rates**, **homegrown fractions** or **dry weight conversion factors** for each produce type by:

i. making temporary amendments to 'Homegrown Produce Data' in advanced mode, Step 4.
Currently, the plant uptake pathway is only considered within the conceptual exposure model for residential with plant uptake and allotments. You will need to decide whether non-standard land uses such as boarding schools and barracks may grow a proportion of their own vegetables when constructing an appropriate conceptual model and switch the pathway on or off accordingly.

The CLEA model does not take into account 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 Tolerable Daily Soil Intake, TDSI, (Environment Agency, 2008c).

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.

Within the software, the estimated generic soil-to-root concentration factor is adopted for each inorganic chemical across all the crops of interest. The range of uncertainty in the soil-to-root concentration factor for a particular plant is not significantly different from the total range of uncertainty across all plants (Thorne et al., 2005).

Site-measured fruit and vegetable chemical concentrations entered in Step 3 ‘Select Chemicals’ must be entered as fresh weight (fw). The calculation from dry weight to fresh weight and the dry weight conversion factors are provided in Equation 7.1 and Table 7.1, respectively, of the CLEA report.

The CLEA software does not model chemical uptake by herbaceous or shrub fruits for organic chemicals as no suitable model has been identified. You should therefore exercise caution when dealing with sites where these fruits constitute a much higher than average proportion of the total fruit and vegetables consumed.

You can change parameter values for octanol-water partition coefficient \( (K_{OW}) \), organic carbon-water partition coefficient \( (K_{OC}) \), diffusion coefficient in water, soil-plant availability correction, root-shoot/root-root/root-tuber/root-fruit correction factor and soil-to-plant concentration factors by:

i. entering a new chemical in the ‘Chemicals’ database;

ii. making temporary amendments to ‘Chemical Data’ in advanced mode, Step 4.

iii. entering site-measured soil-to-plant concentration factors from site-specific studies on appropriate vegetables, in Step 3 of both basic and advanced mode of the CLEA software. These values will override any values contained within the ‘Chemicals’ database or changed within Step 4.

You can change parameter values for soil organic matter (SOM) by:

i. making temporary amendments within Step 2 of both basic and advanced mode of the CLEA software.

4.6.4 Consumption of soil attached to homegrown produce

The approach to modelling inadvertent ingestion of entrained soil on homegrown produce is described in Section 6.2 of the CLEA report.
Parameters and location within the software

The parameters in the consumption of soil attached to homegrown produce pathway that can be changed in the CLEA software are:

- **Exposure frequency of consumption of homegrown produce** varies with age class and represents the number of days a year in which daily exposure occurs. Generic values used within the CLEA software are provided in Tables 3.1 and 3.6 of the CLEA report for residential and allotment land uses respectively. The data is contained within the ‘Land Uses’ database of the CLEA software.

- **Consumption rates for fruit and vegetables** varies for each age class because of preference and habit and is estimated from dietary surveys. Further information is provided in Section 4.4.4 of the CLEA report. Generic values used within the CLEA software are provided in Table 4.17 of the CLEA report and are given for six categories of homegrown produce (green, root and tuber vegetables and herbaceous, shrub and tree fruit). The data is contained within the ‘Homegrown Produce Data’ in advanced mode Step 4 of the CLEA software.

- **Homegrown fractions for each produce group** represent the proportion of fruit and vegetables consumed that is assumed to be from the garden or allotment. Generic values used within the software are provided for the six categories of homegrown produce in Table 4.19 of the CLEA report. Fractions are provided for gardener types, both average and high end scenarios, such as allotment holders who can be assumed to consume a higher fraction of homegrown produce from the allotment than the average family consumption of homegrown garden produce. Further information is provided in Section 4.4.5 of the CLEA report. The data and selection of gardener type is contained in the ‘Homegrown Produce Data’ in advanced mode Step 4 of the CLEA software.

- **Dry weight conversion factor** varies according to the homegrown produce type (that is, green vegetables, root vegetables, tuber vegetables, herbaceous fruit, shrub fruit or tree fruit). They are used to correct dry weight (dw) plant concentration factors to fresh weight (fw) ones to enable comparison with consumption data. The data is contained within the ‘Homegrown Produce Data’ in advanced mode Step 4 of the CLEA software.

- **Soil loading factor** varies according to vegetable type and refers to the amount of soil likely to be entrained on homegrown produce. Generic values used within the CLEA software are provided for the six categories of homegrown produce in Table 6.3 of the CLEA report. The data is contained within the ‘Homegrown Produce Data’ in advanced mode Step 4 of the CLEA software.

- **Preparation factors** vary according to vegetable type and take into account the influence of food preparation on soil loading prior to consumption. Generic values used within the CLEA software are provided for the six categories of homegrown produce in Table 6.3 of the CLEA report. The data is contained in the ‘Homegrown Produce Data’ in advanced mode Step 4 of the software.

- **Soil bioaccessible fraction (oral bioaccessibility factor)** is the fraction of a chemical that is released into solution from the soil during digestion, making it available for absorption. The assumption in the CLEA software is that the bioaccessible fraction is one; that is, during ingestion and digestion all the chemical enters into solution in the gut. The data is contained within the ‘Chemicals’ database of the CLEA software. See Section 4.10 for further information.
How parameter values can be changed in the software

You can change parameter values for exposure frequency by:

i. entering a new land use in the ‘Land Uses’ database;

ii. making temporary amendments to ‘Land Use Data’ in advanced mode, Step 4.

You can change parameter values for consumption rates, dry weight conversion factors and homegrown fractions of each produce type, soil loading factor and preparation factor by:

i. making temporary amendments to ‘Homegrown Produce Data’ in advanced mode, Step 4.

You can change the parameter value for soil bioaccessible fraction by:

i. making temporary amendments to ‘Chemical Data’ in advanced mode, Step 4.

4.6.5 Dermal uptake from soil and dust (indoors and outdoors)

The approach to modelling skin uptake from soil and dust is described in Section 8 of the CLEA report. This pathway may be an important exposure pathway for persistent and highly lipophilic chemicals in soil.

Parameters and location within the software

The parameters in the dermal uptake from soil and dust pathway that can be changed in the CLEA software are:

- Exposure frequency of dermal contact with soil and dust indoors and outdoors varies with age class and land use and represents the number of days per year in which daily exposure occurs. Generic values used within the CLEA software are provided in Tables 3.1, 3.6 and 3.9 of the CLEA report for residential, allotment and commercial land uses respectively. The data is contained within the ‘Land Uses’ database of the CLEA software.

- Soil-to-skin adherence factor varies according to the land use, the age of the receptor and whether exposure is indoors or outdoors and represents the amount of soil that adheres to the skin from which contamination can be dermally absorbed. Generic values used within the CLEA software are provided in Table 8.1 of the CLEA report. The data is contained within the ‘Land Uses’ database of the CLEA software.

- Dermal absorption fractions vary according to the chemical selected and are a measure of the proportion of contaminant in soil that is absorbed through the skin by a typical soiling event. Values for a limited number of chemicals are provided in Table 8.2 of the CLEA report. In the absence of literature values, the CLEA model uses a generic value of 0.1 for organic chemicals and zero for inorganic chemicals. Further information on chemical-specific dermal absorption fractions is provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the CLEA software.

- Maximum exposed skin fraction represents the fraction of total skin area that is exposed to potential contact with contaminated soil and dust; it is used to calculate the total skin area exposed to potential contact with contaminated soils and indoor dust. It varies according to age class and assumed coverage.
of typical clothing. Generic values used within the CLEA software are provided in Table 4.7 and 4.8 of the CLEA report for each land use. The data is contained within the 'Land Use and Receptor Data' in advanced mode Step 4 of the CLEA software.

- Soil-to-indoor dust transport factors vary according to the chemical selected and are an empirical measure of the tendency of an organic or inorganic compound to transfer into indoor dust from soil. It is used in the CLEA software to estimate the indoor dust concentration of inorganic and organic compounds from the soil concentration. Section 4.3.2 of the CLEA report provides further information. In the absence of literature values, the CLEA model uses a generic value of 0.7. Further information on chemical-specific transport factors are provided in individual SGV reports. The data is contained within the 'Chemicals' database of the CLEA software.

**How parameter values can be changed in the software**

You can change parameter values for exposure frequency and the soil-to-skin adherence factor by:

i. entering a new land use in the 'Land Uses' database;

ii. making temporary amendments to 'Land Use Data' in advanced mode, Step 4.

You can change parameter values for dermal absorption fraction or the soil-to-indoor dust transport factor by:

i. entering a new chemical in the 'Chemicals' database;

ii. making temporary amendments to 'Chemical Data' in advanced mode, Step 4.

You can change parameter values for the maximum exposed skin fraction by:

i. making temporary amendments to 'Land Use and Receptor Data' in advanced mode, Step 4.

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1. The maximum soil-to-skin adherence factor that is used within the software for a standard land use is 1 mg cm². The original studies referred to in Section 8.1.1 of the CLEA report indicate that for some activities, such as playing in mud, the adherence factor might exceed 1 mg cm². Within the CLEA software and in deriving SGVs, the number of daily soil contact events is assumed to be one. You should bear this in mind when defining the conceptual exposure model for a new land use.

2. The concentration of contaminant in indoor dust is assumed to be lower than in outdoor dust. Not all household dust is assumed to be soil-derived. In the generic CLEA land uses, tracking back into the building (and therefore the indoor exposure pathways) is only included when the building is located on the contaminated site.

3. There is no data relating to the exposed skin area within the CLEA software because it is calculated from the total body skin area and the maximum exposed skin fraction (see section 4.4.2 of the CLEA report). In addition, there is no data relating to total body skin area within the CLEA software because it is calculated from mean body height and weight for each age class (see Section 4.4.2 of the CLEA report). The mean body heights and weights used are provided in Table 4.8 of the CLEA report.
4.6.6 Indoor and outdoor dust inhalation

The approach to modelling inhalation of indoor and outdoor dust is described in Section 9 of the CLEA report. This pathway may be an important pathway for metal and persistent highly lipophilic chemicals.

Parameters and location within the software

The parameters in the inhalation of dust pathway that can be changed in the CLEA software and are relevant to both indoor and outdoor dust inhalation are:

- **Exposure frequency of inhalation of dust indoors and outdoors** varies with land use and represents the number of days per year in which exposure to dust indoors and outdoors is considered to occur. Generic values used within the CLEA software are provided in Tables 3.1, 3.6 and 3.9, of the CLEA report, for residential, allotment and commercial land uses respectively. The data is contained within the 'Land Uses' database of the CLEA software.

- **Occupancy period (indoors and outdoors)** accounts for the number of hours indoors and outdoors per day in which an exposure event is considered to occur and varies according to land use. Generic values used within the CLEA software are provided in Tables 3.2, 3.7 and Box 3.6 of the CLEA report, for residential, allotment and commercial land uses respectively. The data is contained within the 'Land Uses' database of the CLEA software.

- **Air dispersion factor at height of 0.8 and 1.6 m** 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. It is used to calculate the particle emission factor which represents an estimate of the relationship between the concentration of a contaminant in soil and the concentration of contaminant in air as a result of dust resuspension. A height of 0.8 m is representative of receptors aged zero to six and a height of 1.6 m is representative of older children and adults. Generic values are given in Section 9.2.1 and Table 9.1 of the CLEA report. The data is contained within the 'Land Uses' database of the CLEA software.

- **Fraction of the site with hard or vegetative cover** represents the fraction of the site with outdoor surface cover, such as grass and other vegetation and hard standing. This parameter is used to calculate the particle emission factor, which represents an estimate of the relationship between the concentration of a contaminant in soil and its concentration in air as a result of dust resuspension. Generic values used within the software are provided in Section 3.2.6, 3.3.6 and 3.4.6 of the CLEA report for residential, allotment and commercial land uses respectively. The data is contained within the 'Land Uses' database of the CLEA software.

- **Mean annual wind speed at height of 10 m** is used to calculate the particle emission factor (which represents an estimate of the relationship between the concentration of a contaminant in soil and its concentration in air as a result of dust resuspension) and the empirical function for the dust model. The generic value used within the CLEA software is provided in Equation 9.2 of the CLEA report. The data is contained within the 'Soil and Building Data' in advanced mode Step 4 of the CLEA software.

- **Threshold value of wind speed at 10 m** represents the threshold friction velocity (a measure of how much wind is needed to generate dust) at a given
site from an erodible surface) corrected for presence of non-erodible elements such as clumps of grass or stones. The threshold value of wind speed at 10 m is used to calculate the particle emission factor (which represents an estimate of the relationship between the concentration of a contaminant in soil and its concentration in air as a result of dust resuspension) and the empirical function for the dust model. The generic value used within the software is provided in Equation 9.2 of the CLEA report. The data is contained within the 'Soils' database of the CLEA software.

- **Empirical function for dust model** is an empirical constant derived using the threshold value of wind speed at 10 m and mean annual wind speed at height of 10 m by means of Equation 9.4 in the CLEA report. The empirical constant is used to calculate the particle emission factor, which represents an estimate of the relationship between the concentration of a contaminant in soil and its concentration in air as a result of dust resuspension. The generic value used within the CLEA software is provided in Equation 9.2 of the CLEA report. The data is contained within the 'Soils' database of the CLEA software.

- **Daily inhalation rate** is the volume of air inhaled per day during respiration and depends on a number of factors including age, gender, fitness level and the type of activity, since physical exertion increases our requirement for air. The inhalation rate is used to estimate exposure to soil contamination from the inhalation of dust and vapours. Generic values used within the software are provided in Table 4.14 of the CLEA report for residential and commercial land use and Table 4.15 for allotment land use. The data is contained within the 'Land Use and Receptor Data' in advance mode Step 4 of the software. Residential and commercial inhalation rates are based on USEPA recommendations for long-term exposure studies and the allotment inhalation rate on USEPA recommendations for short-term exposure studies. The values have been adjusted for body weight using authoritative UK data and therefore changes to the data must be based on a sound justification. To calculate inhalation rates for short-term site occupancy (i.e. a small proportion of the day) requires an estimate of the type of activities that would be undertaken for each hour of site occupation (for example, light intensity for three hours and high intensity for one hour). Inhalation rates provided within the CLEA report, can be used to calculate an average short-term exposure ventilation rate (m³ hour⁻¹) for each hour of site occupancy. By averaging over 24 hours, a daily inhalation rate of air at the site can be calculated (m³ day⁻¹).

- **Airborne dust bioaccessible fraction (inhalation bioaccessibility factor)** is the fraction of a chemical that is released from inhaled respirable dust following inhalation and enters into solution in the lung, making it available for absorption. The assumption in the CLEA software is that the bioaccessible fraction is one; that is, during inhalation all the chemical enters into solution in the lung. The data is contained within the 'Chemicals' database of the CLEA software.

Additional parameters that can be changed in the CLEA software and are relevant only to indoor dust inhalation are:

- **Soil-to-indoor dust transport factors** vary according to the chemical selected and are an empirical measure of the tendency of an inorganic or organic compound to transfer to indoor dust from soil. Section 4.3.2 of the CLEA report provides

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1. 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 not transferred to the lung (Paustenbach, 2000). Although not transferred to the lung, these particles are likely to be entrained in mucus and ingested.
further information. In the absence of literature values, the CLEA model uses a generic value of 0.7. Further information on chemical-specific transport factors are provided in individual SGV reports. The data is contained within the 'Chemicals' database of the CLEA software.

- Dust loading factor (indoors) accounts for the higher dust concentration in indoor air resulting from resuspension of dust through man-made surface disturbances and depends on the building type and use. Generic values used within the CLEA software are provided in Section 9.3 of the CLEA report. Section 9.1 of the CLEA report provides further information. The data is contained within the 'Buildings' database of the CLEA software.

**How parameter values can be changed in the software**

You can change parameter values for exposure frequency and occupancy periods by:

i. entering a new land use in the 'Land Uses' database;

ii. making temporary amendments to 'Land Use and Receptor Data' in advanced mode, Step 4.

You can change parameter values for air dispersion factors by:

i. entering a new land use in the 'Land Uses' database;

ii. making temporary changes to 'Soil and Building Data' in advanced mode, Step 4.

You can change values for fraction of the site with hard or vegetative cover by:

i. entering a new land use in the 'Land Uses' database;

ii. making temporary changes to 'Soil and Building Data' in advanced mode, Step 4.

You can change parameter values for mean annual wind speed at height of 10 m by:

i. making temporary changes to 'Soil and Building Data' in advanced mode, Step 4.

You can change parameter values for threshold value of wind speed at 10 m and empirical function for dust model by:

i. entering a new soil in the 'Soils' database;

ii. making temporary changes to 'Soil and Building Data' in advanced mode, Step 4.

You can change parameter values for inhalation rate by:

i. making temporary changes to 'Land Use and Receptor Data' in advanced mode, Step 4.

You can change parameter values for soil-to-indoor dust transport factors and airborne dust bioaccessible fraction by:

i. making temporary changes to 'Chemical Data' in advanced mode, Step 4.

You can change parameter values for dust loading factor (indoors) by:
i. entering a new building in the ‘Buildings’ database;

ii. making temporary changes to ‘Soil and Building Data’ in advanced mode, Step 4.

The fraction of the site with hard or vegetative cover equals zero for bare soil and does not include the fraction of the site that is covered by the building.

Only wind erosion is considered in the calculation of the PM10 emission flux for generic assessments.

4.6.7 Indoor vapour inhalation

Investigation of the indoor vapour inhalation pathway remains a difficult and highly uncertain scientific area. 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 particular land use scenarios.

The approach to generic modelling of indoor vapour inhalation is described in Section 10 of the CLEA report. However, it is strongly recommended that in any risk evaluation involving vapour intrusion, assessors take account of the limitations to generic modelling identified in the CLEA report and use additional lines of evidence.

The approach to site-specific modelling of this pathway using the CLEA software is provided in the CIRIA report (CIRIA, in preparation) which also provides technical guidance on investigating and assessing this pathway.

The vapour intrusion of soil gas from the subsurface into overlying buildings remains a highly uncertain scientific area.

The CLEA model uses the air-water partition coefficient to predict the soil gas concentration at source. The conservatism of this approach varies considerably according to site conditions. The CLEA report estimates that the approach, as a general rule of thumb, will estimate gas concentrations from dissolved and sorbed phase contamination by petroleum hydrocarbons at least a factor of ten higher than they are likely to be measured on site (see Section 10.1.1 of the CLEA report for further information).

The CLEA model may over or under-predict vapour intrusion. Vapour intrusion may under-predict when the contamination is at shallow depths in the unsaturated zone and it may over-predict when the chemical is highly degradable and the site conditions support biodegradation.

Adective transport of soil gas in the unsaturated zone is not considered within the CLEA model. Parameters used to calculate the effect of advective flow are likely to be highly site-specific and difficult to apply generically; in addition, 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 overall effect (see Section 10.1.2 of the CLEA report for further information).
Parameters and location within the software

The parameters in the inhalation of indoor vapour exposure pathway that can be changed in the CLEA software are the building, soil and chemical properties and physiological and behavioural characteristics of the critical receptor as follows:

- **Exposure frequency of inhalation of vapours indoors** varies with land use and represents the number of days a year in which daily exposure occurs. Generic values used within the CLEA software are provided in Tables 3.1 and 3.9, of the CLEA report, for residential and commercial land uses respectively. The data is contained within the ‘Land Uses’ database of the CLEA software.

- **Air-filled and water-filled soil porosity** are dependent on the soil type and are used to calculate the steady-state attenuation coefficient between soil and indoor air. Water-filled porosity is the amount of soil pore space occupied by water based on a suction head at 50 cm H$_2$O. 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. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the ‘Soils’ database of the CLEA software.

- **Diffusion coefficients in air and water** vary according to the chemical selected and are used to calculate the steady-state attenuation coefficient between soil and indoor air. They are a measure of the diffusion of a molecule in a gas or aqueous medium and should be determined at the soil temperature where possible. Chemical-specific diffusion coefficients are provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the software.

- **Air-water partition coefficient** varies according to the chemical selected and is used to calculate the steady-state attenuation coefficient between soil and indoor air. It is a measure of the preference of a chemical for the vapour phase compared to the dissolved water phase. Chemical-specific air-water partition coefficients are provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the CLEA software.

- **Living space heights (above/below ground)** vary according to the building type and are used to calculate the steady-state attenuation coefficient between soil and indoor air. Generic values used within the CLEA software are provided in Table 4.21 of the CLEA report. The data is contained within the ‘Buildings’ database of the CLEA software.

- **Building footprint** varies according to building type and is the area of building footprint directly in contact with contaminated soil. It is used to calculate the steady-state attenuation coefficient between soil and indoor air. Generic values used within the CLEA software are provided in Table 4.21 of the CLEA report. The data is contained within the ‘Buildings’ database of the CLEA software.

- **Living space air exchange rate** varies according to building type and is the rate at which the indoor air mixes with outdoor air through gaps in windows, doors and walls. It is used to calculate the steady-state attenuation coefficient between soil and indoor air. Generic values used within the CLEA software are provided in Table 4.21 of the CLEA report. The data is contained within the ‘Buildings’ database of the CLEA software.

- **Depth to top of source (beneath building)** represents the depth from the soil surface to the top of the contamination source beneath the building. It is used to calculate the soil gas ingress rate when the user selects not to use the generic rates. Generic values used in the software are provided in Section 3.2.6 and 3.4.6 of the CLEA report for residential and commercial land uses.
respectively. The data is contained within the 'Soil and Building Data' in advanced mode Step 4 of the software. Section 4.8 provides further information.

- **Default soil gas ingress rate** varies according to building and soil type and is the rate at which soil gas enters the building through the floor cracks. It is used to calculate the steady-state attenuation coefficient between soil and indoor air. Generic values used within the software are provided in Section 10.3 of the CLEA report for residential and commercial properties. Equations for calculating the volumetric flow rate of soil gas into buildings are provided in Appendix 1 of the CLEA report and further information is provided in Section 4.7 of this report. The data is contained within the 'Buildings' database of the CLEA software.

- **Foundation thickness** varies according to building type and is used to calculate the steady-state attenuation coefficient between soil and indoor air. Generic values used within the software are provided in Table 4.21 of the CLEA report. The data is contained within the 'Buildings' database of the CLEA software.

- **Floor crack area** varies according to building type and is the area of openings within the floor, such as cracks or gaps between the wall and floor, through which soil gas ingress into the building can occur. It is used to calculate the steady-state attenuation coefficient between soil and indoor air. Generic values used within the CLEA software are provided in Table 4.21 of the CLEA report. The data is contained within the 'Buildings' database of the CLEA software.

- **Daily inhalation rate** is the volume of air inhaled per day during respiration and depends on a number of factors including age, gender, fitness level and the type of activity, since physical exertion increases our requirement for air. The inhalation rate is used to estimate exposure to soil contamination from the inhalation of dust and vapours. Generic values used within the software are provided in Table 4.14 of the CLEA report for residential and commercial land use and Table 4.15 for allotment land use. The data is contained within the 'Land Use and Receptor Data' in advanced mode Step 4 of the software. Residential and commercial inhalation rates are based on USEPA recommendations for long-term exposure studies and the allotment inhalation rate on USEPA recommendations for short-term exposure studies. The values have been adjusted for body weight using authoritative UK data and therefore changes to the data must be based on a sound justification. To calculate inhalation rates for short-term site occupancy (i.e. a small proportion of the day) requires an estimate of the type of activities that would be undertaken for each hour of site occupation (for example, light intensity for three hours and high intensity for one hour). Inhalation rates provided within the CLEA report, can be used to calculate an average short-term exposure ventilation rate (m³ hour⁻¹) for each hour of site occupancy. By averaging over 24 hours, a daily inhalation rate of air at the site can be calculated (m³ day⁻¹).

- **Occupancy period (indoors)** accounts for the number of hours on site per day in which an exposure event is considered to occur and varies according to land use. Generic values used within the CLEA software are provided in Tables 3.2 and Box 3.6, in the CLEA report, for residential and commercial land uses respectively. The data is contained within the 'Land Uses' database of the CLEA software.

**How parameter values can be changed in the software**

You can change parameter values for air-filled and water-filled soil porosity by:

i. entering a new soil type in the 'Soils' database;
ii. making temporary changes to 'Soil and Building Data' in advanced mode Step 4.

You can change parameter values for diffusion coefficient in air and water and air-water partition coefficient by:

i. entering a new chemical in the 'Chemicals' database;

ii. making temporary amendments to 'Chemical Data' in advanced mode Step 4.

You can change values for living space height (above/below ground), building footprint, living space air exchange rate, foundation thickness, and floor crack area by:

i. entering a new building type in the 'Buildings' database;

ii. making temporary changes to 'Soil and Building Data' in advanced mode Step 4.

You can change the parameter value for depth to top of source (beneath building) by:

i. making temporary changes to 'Soil and Building Data' in advanced mode, Step 4.

You can change parameter values for default soil gas ingress rate by:

i. entering a new building type in the 'Buildings' database;

ii. making temporary amendments to the generic rate provided in 'Soil and Building Data' in advanced mode Step 4;

iii. temporarily deselecting use of a default soil gas ingress rate in 'Soil and Building Data' in advanced mode Step 4. The soil gas ingress rate is then estimated according to the soil and building properties selected for calculation of the assessment criteria (see Section 4.7 for further information).
The CLEA model requires the air-water partition coefficient ($K_{aw}$). When measured values are not available, you can use Henry’s Law constant in units of Pa m$^3$ mol$^{-1}$ to calculate $K_{aw}$ at ambient temperature. Environment Agency (in press) provides further information.

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.

Chemical transport within the soil is only assumed to occur by diffusion; advection is only assumed when the zone of influence of the building is reached.

If you change the default soil gas ingress rate, to ensure data consistency, you should ensure that soil and building data used to derive this revised rate is also used in the calculation of assessment criteria (you can do this by entering new data in the soil and building database or making temporary changes in Step 4 ‘Advanced Settings’).

A number of building parameters are interdependent. For instance, pressure difference is estimated from stack height which is related to the height of the building. You should check that values for individual inputs are plausible for the building considered.

The floor crack area is a required parameter for the modelling approach within the CLEA software and incorporates cracks in the foundations as well as the actual floor-wall seam crack itself. If there is no potential floor-wall seam crack in the planned construction, an appropriate value to represent the cracks in the foundations is required.

The depth to top of source (beneath building) is used to calculate the source-building separation used in the calculation of the soil gas ingress rate.

You can change parameter values for inhalation rate by:

i. making temporary amendments to ‘Land Use and Receptor Data’ in advanced mode, Step 4.

You can change parameter values for exposure frequency and occupancy periods by:

i. entering a new land use in the ‘Land Uses’ database;
ii. making temporary amendments to ‘Land Use and Receptor Data’ in advanced mode, Step 4.

In addition, you can enter site-measured indoor air concentrations and/or site-measured soil gas concentrations, from site-specific studies in Step 3 of both basic and advanced mode of the CLEA software. These values will override any values calculated by the CLEA software.

**Using the finite source model**

The assumption in the calculation of generic assessment criteria is that the amount of contaminant present in the soil over the period of exposure does not reduce (even though the mass of chemical lost, through the transport of vapours from the soil into the building and ambient air, increases with time). However, if you follow the flow chart for site-specific assessment criteria, you can choose to calculate the criteria assuming that the amount of contaminant present in the soil over the period of exposure does reduce over time, see Section 4.9 for limitations on its use and for further information.
selection can be made in Step 4 ‘Soil and Building Data’ by ticking the check box next to ‘Use limited source thickness’.

The CLEA software calculates indoor vapour concentrations, assuming a finite source, according to the equations set out in Sections 4.9.1.

4.6.8 Outdoor vapour inhalation

The approach to modelling ambient vapour inhalation is described in Section 10 of the CLEA report. It is often the critical outdoor 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 some land use scenarios.

Parameters and location within the software

The parameters in the inhalation of outdoor vapour exposure pathway that can be changed in the CLEA software are as follows:

- **Exposure frequency of inhalation of vapours outdoors** varies with land use and represents the number of days per year in which exposure to vapour outdoors is considered to occur. Generic values used within the CLEA software are provided in Tables 3.1, 3.6 and 3.9 of the CLEA report for residential, allotment and commercial land uses respectively. The data is contained within the ‘Land Uses’ database of the CLEA software.

- **Air-filled and water-filled soil porosity** are dependent on the soil type and are used to calculate the steady-state attenuation coefficient between soil and ambient air. Water-filled porosity is the amount of soil pore space occupied by water based on a suction head at 50 cm H2O. 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. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the ‘Soils’ database of the CLEA software.

- **Diffusion coefficients in air and water** vary according to the chemical selected and are used to calculate the steady-state attenuation coefficient between soil and ambient air. They are a measure of the diffusion of a molecule in a gas or aqueous medium and should be determined at the soil temperature where possible. Chemical-specific diffusion coefficients are provided in individual SGV reports. The data is contained in the ‘Chemicals’ database of the CLEA software.

- **Air-water partition coefficient** varies according to the chemical selected and is used to calculate the steady-state attenuation coefficient between soil and ambient air and the volatilisation factor from surface soil to ambient air. It is a measure of the preference of a chemical for the vapour phase compared to the dissolved aqueous phase. Chemical-specific air-water partition coefficients are provided in individual SGV reports. The data is contained within the ‘Chemicals’ database of the CLEA software.

- **Bulk density** varies according to soil type and is used to calculate the volatilisation factor from surface soil to ambient air. It is a measure of the apparent density of field soil. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the ‘Soils’ database of the CLEA software.
- **Air dispersion factor at height of 0.8 m and 1.6 m** 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. It is used to calculate the volatilisation factor from surface soil to ambient air. A height of 0.8 m is representative of receptors aged zero to six years and a height of 1.6 m is representative of receptors aged greater than six years. Generic values are provided in Table 9.1 of the CLEA report. The data is contained within the 'Land Uses' database of the CLEA software.

- **Daily inhalation rate** is the volume of air inhaled per day during respiration and depends on a number of factors including age, gender, fitness level and type of activity, since physical exertion increases our requirement for air. The inhalation rate is used to estimate exposure to soil contamination from the inhalation of dust and vapours. Generic values used within the software are provided in Table 4.14 of the CLEA report for residential and commercial land use and Table 4.15 for allotment land use. The data is contained within the 'Land Use and Receptor Data' in advanced mode Step 4 of the software. Residential and commercial inhalation rates are based on USEPA recommendations for long-term exposure studies and the allotment inhalation rate on USEPA recommendations for short-term exposure studies. The values have been adjusted for body weight using authoritative UK data and therefore changes to the data must be based on a sound justification. To calculate inhalation rates from short-term studies requires an estimate of the type of activities that would be undertaken for each hour of site occupation (for example, light intensity for three hours and high intensity for one hour). Inhalation rates from short-term studies, such as those provided within the CLEA report, can be used to calculate an average short-term exposure ventilation rate (m³ hour⁻¹) for each hour of site occupancy. By assuming an hourly rate for 24 hours, a daily inhalation rate can be calculated (m³ day⁻¹).

- **Occupancy period (outdoors)** accounts for the number of hours on site per day in which an exposure event is considered to occur and varies according to land use. Generic values used within the CLEA software are provided in Tables 3.2, 3.7 and Box 3.6 of the CLEA report for residential, allotment and commercial land uses respectively. The data is contained within the 'Land Uses' database of the CLEA software.

- **Depth to top of source (no building)** represents the depth from the soil surface to the top of the contamination source. The generic value in the software is given in Section 10.2 of the CLEA report. Where this value is changed to be greater than the generic value of 10 cm, the subsurface volatilisation factor (VF) is calculated using the equation in Section 4.8. The data is contained in the 'Soil and Building Data' in advanced mode Step 4 of the software.

**How parameter values can be changed in the software**

You can change parameter values for **air-filled and water-filled soil porosity** and **bulk density** by:

1. entering a new soil type in the 'Soils' database;
2. making temporary changes to 'Soil and Building Data' in advanced mode Step 4.

You can change parameter values for **diffusion coefficient in air and water** and **air-water partition coefficient** by:
i. entering a new chemical in the 'Chemicals' database;

ii. making temporary amendments to 'Chemical Data' in advanced mode Step 4.

You can change parameter values for air dispersion factors by:

i. entering a new land use in the 'Land Uses' database;

ii. making temporary changes to 'Soil and Building Data' in advanced mode, Step 4.

You can change parameter values for exposure frequency and occupancy periods by:

i. entering a new land use in the 'Land Use Database';

ii. making temporary amendments to 'Land Use and Receptor Data' in advanced mode, Step 4.

You can change parameter values for daily inhalation rate by:

i. making temporary amendments to 'Land Use and Receptor Data' in advanced mode, Step 4.

You can change the parameter value for depth to top of source (no building) by:

i. making temporary changes to 'Soil and Building Data' in advanced mode, Step 4.

The CLEA model requires the air-water partition coefficient (cm$^3$ cm$^{-3}$). This can be calculated from Henry's Law constant in units of Pa m$^3$ mol$^{-1}$ or by using solubility or vapour pressure data at the constant T (see Environment Agency, in press).

The CLEA software assumes that the contaminant source is uniformly distributed from the soil surface to a depth of at least one metre in open ground.

The CLEA software does not take into account chemical depletion by volatilisation or chemical/biological degradation.

Chemical transport within the soil is only assumed to occur by diffusion within unsaturated pore spaces and not as a result of water evaporation.

Using the finite source model

The assumption in the calculation of generic assessment criteria is that the amount of contaminant present in the soil over the period of exposure does not reduce (even though the mass of chemical lost, through the transport of vapours from the soil into the building and ambient air, increases with time). However, if you follow the flow chart for site-specific assessment criteria, you can choose to calculate the criteria assuming that the amount of contaminant present in the soil over the period of exposure does reduce over time, see Section 4.9 for limitations on its use and for further information. This selection can be made in Step 4 'Soil and Building Data' by ticking the check box next to 'Use limited source thickness'.

The CLEA software calculates outdoor vapour concentrations, assuming a finite source, according to the equations set out in Sections 4.9.2.
4.7 Changing the soil gas ingress rate

Soil gas ingress rate is the rate at which soil gas enters the building through the floor cracks and varies according to the building and soil properties. It is used to calculate the steady-state attenuation coefficient (alpha) between soil and indoor air.

You can choose to change the generic value for soil gas ingress rate within the CLEA software by:

i. entering a new default soil gas ingress rate into a new building type in the ‘Buildings’ database;

ii. making a temporary change to the generic rate in ‘Soil and Building Data’ in advanced mode Step 4 by temporarily adding a new soil gas ingress rate;

iii. deselecting use of the default soil gas ingress rate, within advanced mode Step 4 ‘Soil and Building Data’, so that the CLEA software calculates the soil gas ingress rate according to the soil and building properties selected for calculation of the assessment criteria.

4.7.1 Selecting a new default soil gas ingress rate

Within the CLEA software, the default soil gas ingress rate for a residential land use is 50 cm$^3$ s$^{-1}$ and is based on the properties of a detached house (see Table 4.21 of the CLEA report) and the properties of a sandy soil (see Table 4.4 of the CLEA report). For a commercial land use, the default soil gas ingress rate used in the CLEA software is 300 cm$^3$ s$^{-1}$ and is based on the properties of a post-1970 office (see Table 4.21 of the CLEA report) and the properties of a sandy soil (see Table 4.4 of the CLEA report). See Section 10.1.2 and 10.3 of the CLEA report for further information.

If appropriate, you can choose to input one of these generic values for use within a new building type or in making temporary changes to the generic value in advanced mode.

Alternatively, you can calculate a new soil gas ingress rate based on the calculations in Appendix 1 of the CLEA report.

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The sand soil type within Table 4.6 of the CLEA report represents the most conservative choice for modelling diffusion and advection transport processes; however, it is not used in calculations of SGVs as it is not very geographically widespread.

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4.7.2 Calculating a soil gas ingress rate

Within the CLEA software in advanced mode, Step 4 soil and building data, you can deselect use of the default soil gas ingress rate. By deselecting use of the generic rate the CLEA software will calculate a soil gas ingress rate based on the properties of the building and soil that have been selected for use in calculating assessment criteria.

The equations used within the CLEA software for calculating the soil gas ingress rate are provided in Appendix 1 of the CLEA report.

The parameters used in the calculation of soil gas ingress rate that can be changed in the CLEA software are as follows:
• **Building footprint** varies according to building type and is the area of building footprint directly in contact with contaminated soil. Generic values used within the CLEA software are provided in Table 4.21 of the CLEA report. The data is contained within the 'Buildings' database of the CLEA software.

• **Height of living space below ground** varies according to building type and is the height of a habitable basement or cellar. Within the CLEA software, generic values for all default building types are zero as it is assumed that there are no habitable cellars or basements. The data is contained within the 'Buildings' database of the CLEA software.

• **Floor crack area** varies according to building type and is the area of openings within the floor, such as cracks or gaps between the wall and floor, through which soil gas ingress into the building can occur. Generic values used within the CLEA software are provided in Table 4.21 of the CLEA report. The data is contained within the 'Buildings' database of the CLEA software.

• **Foundation thickness** may vary according to building type and is the thickness of the foundation slab. Generic values used within the CLEA software are provided in Table 4.21 of the CLEA report. The data is contained within the 'Buildings' database of the CLEA software.

• **Pressure difference** is the negative pressure difference between heated indoor air and colder outdoor air that drives advection of soil gas into buildings. It is used in the calculation of the soil gas ingress rate when the generic value is not being used. Generic values used for each building type within the CLEA software are provided in Table 4.21 of the CLEA report. The data is contained within the 'Buildings' database of the CLEA software.

• **Water-filled soil porosity** is dependent on the soil type. Water-filled porosity is the amount of soil pore space occupied by water based on a suction head at 50 cm H₂O. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the 'Soils' database of the CLEA software.

• **Residual soil water content** varies according to soil type. It is a measure of the soil moisture content under a suction head at 15,000 cm H₂O. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the 'Soils' database of the CLEA software.

• **van Genuchten shape parameter (m)** varies according to soil type and is an empirical parameter describing soil pore connectivity. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the 'Soils' database of the CLEA software.

• **Saturated hydraulic conductivity** varies according to soil type and is a 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. Generic values used within the CLEA software are provided in Table 4.4 of the CLEA report. The data is contained within the 'Soils' database of the CLEA software.

• **Depth to top of source (beneath building)** represents the depth from the soil surface to the top of the contamination source beneath the building. The generic value used within the CLEA software is provided in Section 10.3 of the CLEA report. The data is contained within the 'Soil and Building Data' in advanced mode Step 4 of the CLEA software. Section 4.6 provides further information.

• **Ambient soil temperature** has a generic value of 283K in the CLEA software. The data is contained within advanced mode Step 4 'Soil and Building Data'.

4.8 Changing the depth to top of source

4.8.1 Depth to top of source (beneath building)

The assumption in the development of Soil Guideline Values is that the depth from the soil surface to the top of the contamination source beneath the building is 65 cm. This is composed of the foundation slab thickness (CLEA uses a generic value of 15 cm for default building types) and a depth of 50 cm from beneath the building foundation to the top of the contamination source.

The foundation thickness is used within the software to calculate the source-building separation so that if you increase or decrease the foundation thickness to a value greater or less than 15 cm, you will reduce or increase the source-building separation unless you also change the depth to top of source beneath the building.

4.8.2 Depth to top of source (no building)

The assumption in the development of SGVs is that the soil contamination is uniformly distributed across the site from the surface to a depth of at least one metre and that the depth to the top of the source of outdoor air contamination is 10 cm. This is consistent with the conceptual model for the other direct contact exposure pathways including soil ingestion and dermal contact.

Within advanced mode Step 4 'Soil and Building Data', the generic value of 10 cm for depth to the top of the contaminant source (depth to top of source, no building) can be temporarily changed. Where the depth to top of source is changed to a value that is greater than 10 cm, the subsurface volatilisation factor (VF) is calculated with Equation 4.1 implemented within the CLEA software using the ASTM (2000) approach.

Equation 4.1

\[
VF = \frac{1}{\frac{Q/C_{\text{wind}} \times L_s}{10000 m^2 cm^{-2} \times 1000000 cm^3 m^{-3} \times \frac{1}{1000} kg g^{-1}} K_{sw} K_{aw}}
\]

Where:
- \( VF \) is the volatilisation factor from subsurface to ambient air, g cm\(^3\)
- \( Q/C_{\text{wind}} \) is the air dispersion factor, g m\(^2\) s\(^{-1}\) per kg m\(^3\)
- \( L_s \) is the depth to top of source (no building), cm
- \( D_{\text{eff}} \) is the effective diffusion coefficient for unsaturated soils, cm\(^2\) s\(^{-1}\)
- \( K_{sw} \) is the total soil-water partition coefficient, cm\(^3\) g\(^{-1}\)
- \( K_{aw} \) is the air-water partition coefficient, cm\(^3\) cm\(^{-3}\)

4.9 Using the finite source model

The assumption in the development of SGVs is that the amount of contaminant present in the soil over the period of exposure does not reduce (even though the mass of chemical lost, through the transport of vapours from the soil into the building and ambient air, increases with time). This is called the infinite source model and is consistent with the level of uncertainty associated with SGVs, where the source of contamination can only be described in generic terms.
A finite source model is also included in the CLEA software. It is intended to be used only as part of a detailed quantitative risk assessment and its results must be carefully interpreted to avoid problems such as the front loading effect. See text box.

The finite source model for vapour transport into indoor or ambient air assumes that as vapour is lost from soil the remaining chemical concentration in soil is steadily reduced. This is accounted for in one of two ways:

- Reducing the soil-to-air attenuation factor proportionately with time to account for the longer migration pathway for vapours as the chemical in the soil nearest the surface becomes depleted. The attenuation factor relates steady state gas concentrations at the source to the indoor air concentration and therefore is only accounted for in the indoor vapour intrusion pathway.

- Mass balance adjustment – assuming that the chemical is lost from soil evenly over the period of exposure until the source is used up. This can be applied to both the outdoor and indoor vapour pathways.

For indoor vapour intrusion, both approaches are used in the CLEA software with the mass balance approach applied only where the time to depletion of the source term is less than the exposure duration (that is, the source would all be consumed before the exposure period expires). In the case of a highly volatile substance such as benzene, this would occur for the standard residential land-use scenario at a contaminant layer thickness of less than 200 cm. For chemicals with much lower volatility, this indicative threshold would be reduced. For the outdoor vapour emission model, only the mass balance adjustment is incorporated.

An important drawback in the use of finite source models within CLEA is that the software itself estimates only the average daily exposure (ADE) over the period of exposure. Media concentrations are therefore reported only as time-averaged values and therefore the time-profile of chemical concentration, and exposure of users of the site, is lost. In extreme cases, this will mean that higher air concentrations early in the exposure period will be averaged with later zero air concentration values (since the source may be assumed to be all depleted). This may lead to the calculation of exposures or generation of assessment criteria that include disproportionate front loading of site exposure, an effect that is difficult to identify when using the software. It is likely to be a much more pronounced effect when the finite source model is using the mass balance adjustment method. This is because the mass balance adjustment method is only applied when the time to depletion of the source term is less than the exposure duration and therefore the air concentration will be averaged over time periods where potentially the source is depleted (that is; the air concentration would be zero).

It is not recommended that assessment criteria derived by using the mass balance adjustment method (which in the case of the indoor vapour pathway will occur when the time to source depletion is less than the exposure duration) are used directly in site risk assessments. However, they can be useful to evaluate the sensitivity of assessment criteria derived using the infinite source method. We consider that the finite source models and its supporting worksheet (“Vapour Calculations”) can best be used semi-quantitatively as a diagnostic tool and to assess the plausibility of a pollutant linkage when running in ratio mode.

You can select to use a finite source in advanced mode, Step 4 ‘Soil and Building Data’ by ticking the check box next to ‘Use limited source thickness’, see Figure 3.10. You must also specify a thickness for the contaminated layer.

The CLEA software calculates indoor and outdoor vapour concentrations, assuming a finite source, according to the equations in Sections 4.9.1 and 4.9.2 respectively. The software also assumes that the thickness of the contaminant layer is 200cm unless you have made changes to this within step 4 'Advanced Settings'.
Care should be used in applying the finite source model due to the front loading effect. "Front loading" of exposure is a consequence of using a finite source term over a fixed period of exposure. In deriving assessment criteria the CLEA software averages daily exposure over a fixed duration, any reduction in exposure later in the averaging period may consequently allocate higher exposures earlier in the averaging period. "Front loading" applies only to reduction of the source term (that is, the soil concentration) and not attenuation along the pathway (for example, in the vapour phase). The figure below illustrates the front loading effect of a reducing source term compared with other approaches including an infinite source and a finite-flux model (with very similar outputs on graph).

Potential acute/short-term effects that could be realised earlier in the averaging period must be considered. The potential for acute effects will depend on the toxicity profile of the contaminant, and also the rate of its depletion in soil; that is, the more rapid the rate of depletion, the steeper the depletion(643,848),(998,997)

The potential influence on longer term adverse effects also requires consideration. As stated by the Health Protection Agency, "... high exposures at the beginning of an averaging period are perhaps more significant than the same level of exposure at a later period, at least where long latencies between exposure and evident effects on health (such as cancer) are assumed." (Defra, 2006).

The extent to which "front loading" occurs will depend on how quickly the source is reduced.

### 4.9.1 Indoor vapour concentrations

USEPA (2003) is used as the basis for implementing the Johnson and Ettinger (1991) equations into the CLEA software for calculating indoor vapour concentrations based on a finite source.

Equation 4.2 is used to calculate the time for the source to be depleted by volatilisation.
Equation 4.2

\[ \tau_d = \frac{\left( \frac{d_s}{L_T} + \beta \right)^2 - \beta^2}{2\psi} \]

Where:
- \( \tau_d \) is the time to source depletion, s
- \( d_s \) is the thickness of the contaminant layer, cm
- \( L_T \) is the source-building separation, cm [see Equation 4.2 and 4.3]
- \( \beta \) is an empirical coefficient, dimensionless [see Equation 4.5]
- \( \psi \) is an empirical coefficient, s^{-1} [see Equation 4.6]

The source-building separation is calculated using Equation 4.3 and 4.4 and the empirical coefficients are calculated using Equation 4.5 and 4.6.

Equation 4.3

\[ L_T = L_s - Z_{crack} \]

Where:
- \( L_T \) is the source-building separation, cm
- \( L_s \) is the depth to top of source (beneath building), cm
- \( Z_{crack} \) is the depth below ground to bottom of floor, cm [see Equation 4.4]

One of the fundamental assumptions of Johnson and Ettinger (1991) is that the contaminated layer lies beneath the floor and therefore the source-building separation (\( L_T \)) has a minimum value equal to \( Z_{crack} \) USEPA (2003).

Equation 4.4

\[ Z_{crack} = (H_{cellar} + L_{crack}) \times 100 \text{ cm m}^{-1} \]

Where:
- \( Z_{crack} \) is the depth below ground to bottom of floor, cm
- \( H_{cellar} \) is the living space height (below ground), m
- \( L_{crack} \) is the foundation thickness, m

Equation 4.5

\[ \beta = \left( \frac{D_{eff} A_b}{L_s Q_{soil}} \right) \left[ 1 - \exp \left( -\frac{Q_s L_{crack}}{D_{crack} A_{crack}} \right) \right] + 1 \]

Where:
- \( \beta \) is an empirical coefficient, dimensionless
- \( D_{eff} \) is the effective diffusion coefficient for unsaturated soils, cm² s^{-1}
- \( A_b \) is the area of enclosed floor and walls below ground, cm²
- \( L_T \) is the source-building separation, cm [see Equation 4.2]
- \( Q_s \) is the soil gas ingress rate, cm³ s^{-1}
- \( L_{crack} \) is the foundation thickness, cm
- \( D_{crack} \) is the effective diffusion coefficient through the cracks, cm² s^{-1} [= D_{eff}]
- \( A_{crack} \) is the floor crack area, cm²
Equation 4.6

\[ \psi = \frac{D_{\text{eff}} C_{\text{vap}}}{L_T^2 \rho_s C_s} \]

Where:
- \( \psi \) is an empirical coefficient, s\(^{-1}\)
- \( D_{\text{eff}} \) is the effective diffusion coefficient for unsaturated soils, cm\(^2\) s\(^{-1}\)
- \( C_{\text{vap}} \) is the chemical vapour concentration at source, mg cm\(^{-3}\)
- \( L_T \) is the source-building separation, cm [see Equation 4.3]
- \( \rho_s \) is the dry bulk soil density, g cm\(^{-3}\)
- \( C_s \) is the total amount of chemical in soil, mg g\(^{-1}\)

Equations 4.7 and 4.8 describe two methods used for implementing the finite source solution, depending on whether the contamination present in the ground is likely to be depleted over the duration of exposure.

The time-averaged indoor air concentration is calculated using Equation 4.7 when the exposure duration (\( \tau \)) is greater than the time to source depletion (\( \tau_d \)).

Equation 4.7

\[ C_{\text{building}} = \frac{\rho_s C_s d_s A_b}{Q_b \tau} \times 10000000 cm^3 m^{-3} \]

Where:
- \( C_{\text{building}} \) is the time averaged indoor air concentration, mg m\(^{-3}\)
- \( \rho_s \) is the dry soil bulk density, g cm\(^{-3}\)
- \( C_s \) is the total amount of chemical in soil, mg g\(^{-1}\)
- \( d_s \) is the thickness of the contaminant layer, cm
- \( A_b \) is the area of enclosed floor and walls below ground, cm\(^2\)
- \( Q_b \) is the building ventilation rate, cm\(^3\) s\(^{-1}\)
- \( \tau \) is the exposure duration, s

The time-averaged indoor air concentration is calculated using Equation 4.8 when the exposure duration (\( \tau \)) is less than the time to source depletion (\( \tau_d \)). It is assumed that mass depletion occurs slowly and that diffusion continues to take place under steady-state conditions. It is also assumed that source depletion occurs from the top boundary of the contaminated zone closest to the building foundations and 'retreats' from the building with time. This increases the source-building separation over time.

Equation 4.8

\[ \alpha = \left( \frac{\rho_s C_s d_s A_b}{Q_b C_{\text{vap}} \tau} \right) \left( \frac{L_T}{d_s} \right) \left( \sqrt{\beta^2 + 2\psi \tau} \right) - \beta \]

Where:
- \( \alpha \) is the time-averaged finite source attenuation coefficient, dimensionless
- \( \rho_s \) is the dry soil bulk density, g cm\(^{-3}\)
- \( C_s \) is the total amount of chemical in soil, mg g\(^{-1}\)
- \( d_s \) is the thickness of the contaminant layer, cm
- \( A_b \) is the area of enclosed floor and walls below ground, cm\(^2\)
- \( Q_b \) is the building ventilation rate, cm\(^3\) s\(^{-1}\)
- \( C_{\text{vap}} \) is the chemical vapour concentration at source, mg cm\(^{-3}\)
- \( \tau \) is the exposure duration, s
- \( L_T \) is the source-building separation, cm [see Equation 4.3]
- \( \beta \) is the empirical coefficient, dimensionless [see Equation 4.5]
- \( \psi \) is the empirical coefficient, s\(^{-1}\) [see Equation 4.6]
4.9.2 Outdoor vapour concentrations

The modelling of vapour transport for calculating outdoor vapour concentrations using a finite source is implemented within the CLEA software using the ASTM (2004) approach. In modelling outdoor air concentrations, ASTM (2004) recommended a mass balance approach; if the source term is depleted over the exposure duration, the estimated flux is simply averaged over the duration of exposure. The relationship between outdoor air and surface and subsurface soil chemical concentrations is represented by the volatilisation factor (VF). The VF for surface and subsurface soil to ambient vapour inhalation for a finite source is provided in Equation 4.9 (the equation has the same form for both the surface and subsurface VF models).

**Equation 4.9**

\[ VF = \frac{d_s \rho_s}{\frac{Q}{C_{\text{wind}}} \times \tau} \]

Where:  
- \( VF \) is the volatilisation factor from subsurface soil to ambient air, g cm\(^{-3} \)  
- \( d_s \) is the thickness of the contaminant layer, cm  
- \( \rho_s \) is the dry soil bulk density, g cm\(^{-3} \)  
- \( \frac{Q}{C_{\text{wind}}} \) is the air dispersion factor, g m\(^{-2} \) s\(^{-1} \) per g cm\(^{-3} \)  
- \( \tau \) is the exposure duration, s

4.10 Changing the bioaccessible fraction

The soil bioaccessibility fraction (the oral bioaccessibility factor) is the proportion of a chemical that is released from a soil following ingestion and digestion, and enters into solution in the gut, making it available for absorption.

The airborne dust bioaccessibility fraction (the inhalation bioaccessibility factor) is the proportion of a chemical that is released from inhaled respirable dust following inhalation and enters into solution in the lung, making it available for absorption.

The bioaccessibility fraction of a chemical will be between zero (the entire chemical remains bound to the soil or dust) and one (all of the chemical ingested or inhaled is released into solution in the gut or lung).

Bioaccessibility testing uses chemical laboratory methods to attempt to estimate how much of a substance might be available from soils to be absorbed into the human system through either the gastrointestinal tract or the lining of the lung. There are considerable uncertainties in the interpretation of bioaccessibility data.

The assumption in the development of SGVs is that the bioaccessible fraction is one\(^2\).

Changing the bioaccessible fraction adjusts the estimated chemical intake. This is implemented within the CLEA software by multiplying the soil or dust concentration by

---

\(^2\) with only a few notable exceptions such as lead.
the bioaccessible fraction. The soil or dust bioaccessibility fraction is applied only to the direct and indirect soil ingestion pathway and the inhalation bioaccessibility fraction is only applied to the indoor and outdoor dust inhalation pathways.

The bioaccessibility fractions can be changed within Step 4 ‘Advanced Settings – chemical data’.

1 Oral bioaccessibility testing may be applied during a site-specific assessment of land contamination. Information on the Environment Agency’s current view on the use of bioaccessibility data and publications and work programme on bioaccessibility are available on the Environment Agency’s web page at www.environment-agency.gov.uk.

1 There is very little technical guidance concerning inhalation bioaccessibility. You should be cautious when considering changes to this factor within the software.
References


<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AC</td>
<td>Age Class or Acceptance Criteria</td>
</tr>
<tr>
<td>ADE</td>
<td>Average Daily Exposure</td>
</tr>
<tr>
<td>ALARP</td>
<td>As low as reasonably practicable</td>
</tr>
<tr>
<td>ASTM</td>
<td>American Society for Testing and Materials</td>
</tr>
<tr>
<td>AT</td>
<td>Averaging Time</td>
</tr>
<tr>
<td>CLEA</td>
<td>Contaminated Land Exposure Assessment</td>
</tr>
<tr>
<td>DQRA</td>
<td>Detailed Quantitative Risk assessment</td>
</tr>
<tr>
<td>ED</td>
<td>Exposure Duration</td>
</tr>
<tr>
<td>EF</td>
<td>Exposure Frequency</td>
</tr>
<tr>
<td>GAC</td>
<td>Generic Assessment Criteria</td>
</tr>
<tr>
<td>HCV</td>
<td>Health Criteria Values</td>
</tr>
<tr>
<td>ID</td>
<td>Index Dose</td>
</tr>
<tr>
<td>LH</td>
<td>Living Height</td>
</tr>
<tr>
<td>MDI</td>
<td>Mean Daily Intake</td>
</tr>
<tr>
<td>NAPL</td>
<td>Non-Aqueous Phase Liquid</td>
</tr>
<tr>
<td>SGV</td>
<td>Soil Guideline Value</td>
</tr>
<tr>
<td>SOM</td>
<td>Soil Organic Matter</td>
</tr>
<tr>
<td>SSAC</td>
<td>Site-Specific Assessment Criteria</td>
</tr>
<tr>
<td>TDI</td>
<td>Tolerable Daily Intake</td>
</tr>
<tr>
<td>TDSI</td>
<td>Tolerable Daily Soil Intake</td>
</tr>
</tbody>
</table>
## 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.

### 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.

### Aerodynamic diameter
The diameter of a sphere with unit density that has aerodynamic behaviour identical to that of the particle in question; an expression of aerodynamic behaviour of an irregularly shaped particle in terms of an idealised particle. Particles having the same aerodynamic diameter may have different dimensions and shapes.

### 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.

### ALARP principle
The ALARP principle ensures that, irrespective of whether a health-based guideline is being breached, exposures must be kept 'as low as reasonably practicable'.

### Algorithms
A well-defined list of mathematical instructions which describe generalised processes.

### Aqueous phase
Chemical dissolved in water.

### 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.

### Average daily exposure (ADE)
The average daily amount of a contaminant per kilogram body weight, 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.

<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Background exposure</td>
<td>The mean daily intake (MDI) for the UK population in terms of the average &quot;background intake&quot; to which that population may be exposed. The MDI is estimated from published information on ambient air concentrations and average concentrations measured in water and food products. Where relevant, other sources are considered.</td>
</tr>
<tr>
<td>Background sources</td>
<td>Sources of human exposure to a chemical other than the soil itself, either directly or indirectly. For example, ambient air, diet, and drinking water.</td>
</tr>
<tr>
<td>Bioaccessibility</td>
<td>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 or is inhaled and enters into solution in the lung.</td>
</tr>
<tr>
<td>Building ventilation</td>
<td>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.</td>
</tr>
<tr>
<td>Carcinogen</td>
<td>An agent capable of inducing tumours and causing cancer</td>
</tr>
<tr>
<td>Cation exchange capacity</td>
<td>A measure of the number of sites on soil surfaces that can retain positively charged ions (cations) by electrostatic forces.</td>
</tr>
<tr>
<td>Chemical intake/uptake rate</td>
<td>The daily amount of a soil contaminant expressed as an intake or an uptake from exposure to chemicals in soil, food, water and air.</td>
</tr>
<tr>
<td>Chemical lipophilicity</td>
<td>A chemical's affinity for, tendency to combine with, or preference to dissolve in lipids (fats).</td>
</tr>
<tr>
<td>Conceptual model</td>
<td>A representation of the characteristics of a site in diagrammatic or written form that shows the possible relationships between contaminants, pathways and receptors.</td>
</tr>
<tr>
<td>Critical adverse effect</td>
<td>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.</td>
</tr>
<tr>
<td>Critical receptor</td>
<td>The individuals or subgroup of the population most likely to be exposed and/or susceptible to the presence of soil contamination.</td>
</tr>
<tr>
<td>Dermal</td>
<td>Of or pertaining to the skin.</td>
</tr>
<tr>
<td>Dermal absorption fraction</td>
<td>An empirical measure of the proportion of chemical compound in soil that is absorbed through the skin by a</td>
</tr>
</tbody>
</table>
typical soilng event.

**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.

**Diffusion coefficient** Proportionality coefficient from Fick’s first law of diffusion.

**Dose** The amount of a substance administered to, taken up by, or absorbed by an organism. See also intake, uptake, and exposure.

**Emission flux** Rate at which particles of dust or vapour are released from a surface.

**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 the 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 (EF)** 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.

**Free product** Chemical present in soil or water in its natural physical form under ambient conditions, for example, solid, liquid or gas. (See also non-aqueous phase liquid.)
<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Generic assessment criteria</td>
<td>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.</td>
</tr>
<tr>
<td>Geophagia</td>
<td>A specific type of pica behaviour (see also pica) that applies to the persistent and purposeful ingestion of soil. It is considered to occur rarely in the general population in most industrialised countries.</td>
</tr>
<tr>
<td>Generic quantitative risk assessment</td>
<td>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.</td>
</tr>
<tr>
<td>Genotoxic carcinogenesis</td>
<td>The production of a malignant tumour by a chemical via a mechanism involving damage to the genetic material.</td>
</tr>
<tr>
<td>Geometric mean</td>
<td>The $n^{th}$ root of the product of all the numbers of a dataset.</td>
</tr>
<tr>
<td>Hazard</td>
<td>The set of inherent properties of a substance or mixture of substances that makes it capable of causing adverse effects to humans, other organisms or the environment.</td>
</tr>
<tr>
<td>Health Criteria Values (HCV)</td>
<td>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).</td>
</tr>
<tr>
<td>Index Dose (ID)</td>
<td>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.</td>
</tr>
<tr>
<td>Inhalable particle</td>
<td>A particle the size of which dictates that when inhaled, it only reaches the upper respiratory tract. These particles generally have an aerodynamic diameter of 10-100 $\mu$m. Following deposition in the lung, they may be subject to mucociliary clearance, swallowing and oral absorption (cf. respirable particle).</td>
</tr>
<tr>
<td>Intake</td>
<td>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.</td>
</tr>
<tr>
<td>Mean daily intake (MDI)</td>
<td>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.</td>
</tr>
<tr>
<td>Non-aqueous phase liquid (NAPL)</td>
<td>A term which refers to contamination present within the soil or groundwater, which is neither adsorbed to the soil surface nor dissolved in the groundwater (not in the</td>
</tr>
</tbody>
</table>
Non-threshold health effects

Contaminant for which there is not a threshold level of toxicant that needs to be exceeded to produce an adverse effect. Any exposure to these chemicals, no matter how small, will carry some level of risk.

Organic carbon fraction

Amount of organic carbon in soil expressed as a mass fraction.

Partition coefficient

The experimental or calculated ratio of the concentrations of the same chemical species in two phases.

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.

Porosity

Fraction of void space within a porous media such as a rock or soil.

Ratio mode

An assessment of whether estimated average daily exposure of actual representative concentrations of contaminants at a specific site would exceed the relevant health criteria values. This is also known as the “hazard quotient” since in risk assessment, it is usual to compare the exposed dose with the relevant health criteria value(s).

Representative site soil concentration

Soil data representative of the body of soil being assessed.

Respirable dust

A particle that is able to reach the deep lung and alveoli. For humans, respirable particles generally have an aerodynamic diameter of less than 10 μm. (cf. inhalable particle).

Risk

The possibility that a harmful event (death, injury or loss) arising from exposure to a chemical or physical agent may occur under specific conditions.

Route of exposure

The way a chemical enters an organism after contact (for example, ingestion, inhalation or dermal absorption).

Route-to-route extrapolation

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 Saturation Limit: The concentration at which soil is saturated with the chemical and the adsorptive limits of the soil and volatility in air have been reached.

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.

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 (TDI): 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.

Toxicity: The inherent property of a substance to cause injury or an adverse effect in a living organism.

Threshold health effects: Contaminant for which there is a threshold level of toxicant that needs to be exceeded to produce an adverse effect.

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 reaches the circulating blood having been absorbed by the body through the skin, the gastrointestinal system and/or the pulmonary system (lungs).
Appendix 1

Software familiarisation walk-through

The following walk-through is provided to help familiarise you with the main functions of the software. You will need a copy of the software installed on a computer (see Section 1.3).

The walk-through is designed to take you through adding a chemical to the database and producing generic assessment criteria by following the instructions below. You can also refer to sections of this handbook where necessary.

Add a chemical to the database

Using the CLEA software you are going to add chemical A to the database, Table A1 contains the data that you have collected for Chemical A.

To add the chemical to the database you press the 'Chemicals' button on the Interactive CLEA software guide, See Figure A1. This takes you to the chemicals database

![Interactive CLEA software guide]

Figure A1: Enter the ‘Chemicals’ database
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical Name</td>
<td>Chemical A</td>
<td></td>
</tr>
<tr>
<td>Chemical Type</td>
<td>organic</td>
<td></td>
</tr>
<tr>
<td>Oral HCV Type</td>
<td>TDI</td>
<td></td>
</tr>
<tr>
<td>Oral HCV value</td>
<td>1.00E+02</td>
<td>µg kg⁻¹ BW day⁻¹</td>
</tr>
<tr>
<td>Compare oral HCV with oral exposure</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>Compare oral HCV with dermal exposure</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>Compare oral HCV with inhalation exposure</td>
<td>No</td>
<td></td>
</tr>
<tr>
<td>Inhalation HCV Type</td>
<td>TDI</td>
<td></td>
</tr>
<tr>
<td>Inhalation HCV value</td>
<td>1.00E+02</td>
<td>µg kg⁻¹ BW day⁻¹</td>
</tr>
<tr>
<td>Compare inhalation HCV with oral exposure</td>
<td>No</td>
<td></td>
</tr>
<tr>
<td>Compare inhalation HCV with dermal exposure</td>
<td>No</td>
<td></td>
</tr>
<tr>
<td>Compare inhalation HCV with inhalation exposure</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>Combine oral and inhalation AC</td>
<td>Yes</td>
<td></td>
</tr>
<tr>
<td>Oral MDI for adults</td>
<td>5.00E+00</td>
<td>µg day⁻¹</td>
</tr>
<tr>
<td>Inhalation MDI for adults</td>
<td>1.30E+02</td>
<td>µg day⁻¹</td>
</tr>
<tr>
<td>Air-water partition coefficient (Kaw)</td>
<td>1.52E-01</td>
<td>cm³ cm⁻³</td>
</tr>
<tr>
<td>Diffusion coefficient in air</td>
<td>7.50E-06</td>
<td>m² s⁻¹</td>
</tr>
<tr>
<td>Diffusion coefficient in water</td>
<td>7.80E-10</td>
<td>m² s⁻¹</td>
</tr>
<tr>
<td>Relative molecular mass</td>
<td>1.06E+02</td>
<td>g mol⁻¹</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>6.38E+02</td>
<td>Pa</td>
</tr>
<tr>
<td>Water solubility</td>
<td>1.80E+02</td>
<td>mg L⁻¹</td>
</tr>
<tr>
<td>Koc</td>
<td>2.64E+00</td>
<td>Log (cm³ g⁻¹)</td>
</tr>
<tr>
<td>Kow</td>
<td>3.13E+00</td>
<td>Log (dimensionless)</td>
</tr>
<tr>
<td>Dermal absorption fraction</td>
<td>1.00E-01</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Soil - plant availability correction</td>
<td>Not relevant</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Root - shoot correction factor</td>
<td>Not relevant</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Root - root store correction factor</td>
<td>Not relevant</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Root - tuber correction factor</td>
<td>Not relevant</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Root - fruit correction factor</td>
<td>Not relevant</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Soil-to-plant concentration factor (green vegetables)</td>
<td>model</td>
<td></td>
</tr>
<tr>
<td>Soil-to-plant concentration factor (root vegetables)</td>
<td>model</td>
<td></td>
</tr>
<tr>
<td>Soil-to-plant concentration factor (tuber vegetables)</td>
<td>model</td>
<td></td>
</tr>
<tr>
<td>Soil-to-plant concentration factor (herbaceous fruit)</td>
<td>6.83E-04</td>
<td>mg g⁻¹ plant (FW basis) over mg g⁻¹ DW soil</td>
</tr>
<tr>
<td>Soil-to-plant concentration factor (shrub fruit)</td>
<td>3.50E-04</td>
<td>mg g⁻¹ plant (FW basis) over mg g⁻¹ DW soil</td>
</tr>
<tr>
<td>Soil-to-plant concentration factor (tree fruit)</td>
<td>model</td>
<td></td>
</tr>
<tr>
<td>Soil-to-dust transport factor</td>
<td>0.7</td>
<td>g g⁻¹ DW</td>
</tr>
</tbody>
</table>
You enter the chemical name in the first available row in the first column and then you move through the columns, from left to right, adding the chemical data. You will use the user help text (shown as a pop up box when selecting each parameter data field) to assist you in entering correct information if data is not relevant or is to be modelled. This is what the screen should look like as you are adding the data.

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Type</th>
<th>Notes</th>
<th>Oral LD50</th>
<th>Oral LD100</th>
<th>TDI</th>
<th>CLEA software handbook (2009)</th>
<th>Genotoxic with oral exposure</th>
<th>Carcinogenic with oral exposure</th>
<th>Chronic with oral exposure</th>
<th>Inhalation with oral exposure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical A</td>
<td>organic</td>
<td>1.00E+02</td>
<td>1.00E+02</td>
<td>1.00E+02</td>
<td>TDI</td>
<td>CLEA software handbook (2009)</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>

**Figure A2: Chemical database**

When you have added the data for chemical A, press the ‘Back to Guide’ button to take you back to the 'Interactive CLEA software guide'. Save the spreadsheet so that Chemical A is permanently stored within the chemical database.

**Calculate Generic Assessment Criteria**

Using the software you are going to follow the steps provided within the 'Interactive CLEA software guide' to derive generic assessment criteria for chemical A for a residential land use with gardens used to grow vegetables.

Follow the steps for generic assessment criteria within the 'Interactive CLEA software guide'.

1) Press the 'Report Details' button and add any detail that you wish to record. Go back to the 'Interactive CLEA software guide'.

2) Press the 'Basic Settings' button and select the land use 'Residential with homegrown produce'. You will see that the software automatically selects default settings for the remainder of the information on this worksheet. You can assume, for the purposes of this walk-through, that the conceptual exposure model set out in the CLEA report for the 'residential with homegrown produce' land use is appropriate for this assessment. Go back to the 'Interactive CLEA software guide'.

3) Press the 'Select Chemicals' button and use the drop down menu to select chemical A. Apply the chemical to the model. You have not made any changes in 'Advanced Settings 4' as you are carrying out a generic assessment so you select to continue. When you have received confirmation that the chemical data is loaded, go back to the 'Interactive CLEA software guide'.
4) Press the 'Find Results' button select the 'Find AC' button. If you have saved any previous assessments you choose to continue. You will receive confirmation when the generic assessment criteria have been calculated. The calculated information within this worksheet is shown in Table A2.

Table A2: Results of calculation of generic assessment criteria for chemical A

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ratio of ADE to relevant Health Criteria Value: oral HCV</td>
<td>0.05</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Ratio of ADE to relevant Health Criteria Value: inhal HCV</td>
<td>0.95</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Ratio of ADE to relevant Health Criteria Value: combined</td>
<td>1.00</td>
<td>dimensionless</td>
</tr>
<tr>
<td>Soil Assessment Criteria: oral HCV</td>
<td>2.47E+02</td>
<td>mg kg⁻¹</td>
</tr>
<tr>
<td>Soil Assessment Criteria: inhalation HCV</td>
<td>1.31E+01</td>
<td>mg kg⁻¹</td>
</tr>
<tr>
<td>Soil Assessment Criteria: Combined</td>
<td>1.24E+01</td>
<td>mg kg⁻¹</td>
</tr>
<tr>
<td>Soil Saturation Limit</td>
<td>1.19E+03</td>
<td>mg kg⁻¹</td>
</tr>
<tr>
<td>Pathway contribution; direct soil ingestion</td>
<td>0.09</td>
<td>%</td>
</tr>
<tr>
<td>Pathway contribution; consumption of homegrown produce and attached soil</td>
<td>4.85</td>
<td>%</td>
</tr>
<tr>
<td>Pathway contribution; dermal contact (indoor)</td>
<td>0.00</td>
<td>%</td>
</tr>
<tr>
<td>Pathway contribution; dermal contact (outdoor)</td>
<td>0.05</td>
<td>%</td>
</tr>
<tr>
<td>Pathway contribution; inhalation of dust (indoor)</td>
<td>0.00</td>
<td>%</td>
</tr>
<tr>
<td>Pathway contribution; inhalation of dust (outdoor)</td>
<td>0.00</td>
<td>%</td>
</tr>
<tr>
<td>Pathway contribution; inhalation of vapour (indoor)</td>
<td>86.90</td>
<td>%</td>
</tr>
<tr>
<td>Pathway contribution; inhalation of vapour (outdoor)</td>
<td>0.00</td>
<td>%</td>
</tr>
<tr>
<td>Pathway contribution; oral background</td>
<td>0.28</td>
<td>%</td>
</tr>
<tr>
<td>Pathway contribution; inhalation background</td>
<td>7.83</td>
<td>%</td>
</tr>
</tbody>
</table>

5) When you have derived the generic assessment criteria you can view (and save) detailed results and the selections made for calculation of the criteria by pressing the 'Print Reports' button and selecting the appropriate button.
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