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CLEA Software (Version 1.05) Handbook

Better Regulation Science Programme
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- **Delivering information, advice, tools and techniques**, by making appropriate products available to our policy and operations staff.

Steve Killeen

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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, 2009c). Assumptions in the CLEA report (Environment Agency, 2009c) apply to the derivation of **Soil Guideline Values** (SGVs), but offer a useful starting point for assessors developing their own **site-specific assessment criteria**.

The CLEA software (Environment Agency, 2009d) has been updated to reflect the changes to the CLEA model and other changes as well as user feedback on the CLEA v1.03 beta software (Environment Agency, 2005a). The CLEA software replaces the CLEA UK software published in 2005. This report updates and replaces the CLEA software (v1.04) handbook published in January 2009.

The software and this accompanying handbook contain further information on using the CLEA model outside the scope of the CLEA report (Environment Agency, 2009c).

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, 2009c). 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 SGVs, these values are not considered to be SGVs 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 (2009c).

1.2.2 Updates to the software

The CLEA software has changed significantly since 2005 (Environment Agency, 2005a and 2005b), 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, 2009c).

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 pathway**s;
- 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.

In August 2008 we released a beta version of the software (CLEA software version 1.03 beta) for stakeholder evaluation. We updated the software to incorporate comments received from stakeholders and to remove the beta designation of the software. The key updates between version 1.03 beta and 1.04 were:

- we amended the software to allow you to add a user defined effective air permeability to be used within site specific assessment;
- we added an option for you to enter a time average period for surface emissions allowing you to set the time duration in the surface volatilisation factor model on a site-specific basis;
- we added an option for you to enter a chemical-specific correction for the indoor air attenuation factor to account for conservatism in the estimation of indoor vapour intrusion using the Johnson and Ettinger model;
- we restored the pH function in the software, and provided advice for using it in calculating soil-to-plant concentration factors in this handbook;
- we made a number of changes to the user interface to improve its ease of use.

The key updates between version 1.04 and 1.05 are:

- we have added chemical data for the updated TOX and SGV reports that are published to date;
- we have revised the protection scheme to allow the extraction of dioxin exposure factor data for calculation of dioxin site specific assessment criteria using the dioxins, furans and dioxin-like compounds worksheet (Environment Agency, 2009e);
- we have added residential and commercial lifetime exposure data (land use and receptor data) to allow calculation of assessment criteria based on lifetime exposure when appropriate;
- we have replaced the bioaccessibility factor with the relative bioavailability factor and the description in the software and this handbook have been amended accordingly;
- we have corrected an error in the calculation of Exposure Duration which was one year less than it should have been for the following scenarios; ending age class equals 17, starting age class equals 16 or less or ending age class equals 18, starting age class equals 16 or less. This would have a minor effect on assessment criteria calculated using the CLEA software v1.04.

1.2.3 Using this handbook

This is the handbook for the CLEA software version 1.05 (Environment Agency, 2009d). 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.
>
> ⓘ The term 'TOX guidance report' within this handbook refers to reference Environment Agency 2009b. Human health t*oxicological assessment of contaminants in soil*. Science Report SC050021/SR2. Bristol: Environment Agency.
>
> ⓘ The term 'CLEA report' within this handbook refers to reference Environment Agency 2009c. *Updated technical background to the CLEA model*. Science Report SC050021/SR3. Bristol: Environment Agency.

1.3 Technical specification and installation

CLEA Software Version 1.05 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 1.05 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. You will be prompted to either "Disable Macros" or "Enable Macros". You must enable macros for the software to operate.

Note that in order for the 'Find AC' macro to run, “Calculation” in your version of Microsoft Excel needs to be set to automatic.

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 handbook before using the software. 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 model**s than in basic mode.

ⓘ 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.

ⓘ 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, 2009c) 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.

ⓘ Care must be taken to consider whether the algorithms in the CLEA report (Environment Agency, 2009c) 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 data 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 pathway**s (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:

- <u>Step 1: Report Details.</u>
  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. The file name of the software is also included as a header within the output reports.

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

- <u>Step 2: Basic Settings</u>.
  If you want to calculate ADE/HCV ratios for a given **representative site soil concentration** or calculate ADE for dioxins, furans and dioxin-like PCBs, 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’.

- 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.

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

i. Green – the assessment criteria does not exceed the saturated soil concentration

ii. Amber – the assessment criteria does exceed the saturated soil concentration. However, the contribution of the indoor and outdoor vapour pathway to total exposure is less than 10% and it will therefore not affect the assessment criteria significantly

iii. Red – the assessment criteria does exceed the saturated soil concentration and it may significantly affect the interpretation of any exceedances. The contribution of the indoor and outdoor vapour pathway to total exposure is greater than 10%.

See Chapter 5 in the CLEA report and Section 4.12 of this handbook for further discussion and advice on interpreting assessment criteria that exceed the theoretical soil saturation limits.

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, 2009c). 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 765 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 pathway**s (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 3.4).

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
4. 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 3.3).

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

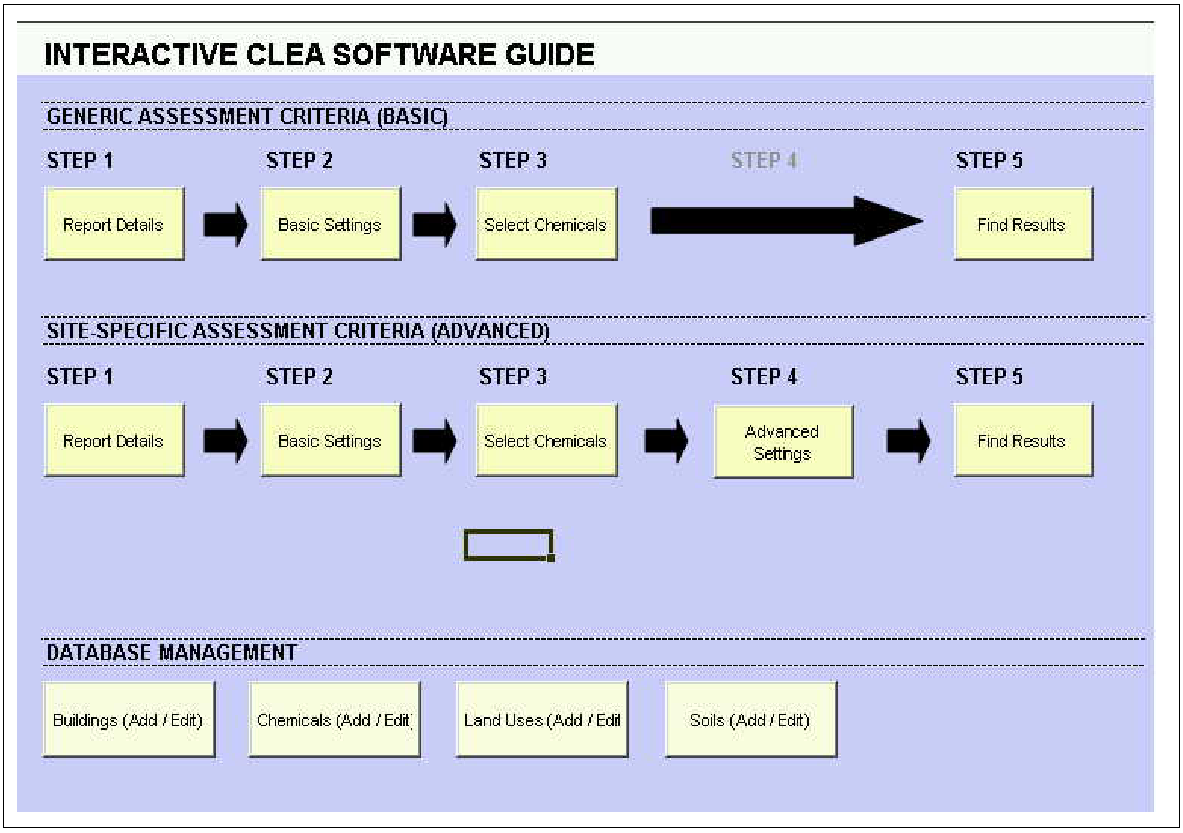

Figure 3.1: Interactive CLEA Software Guide.

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 model**s 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.

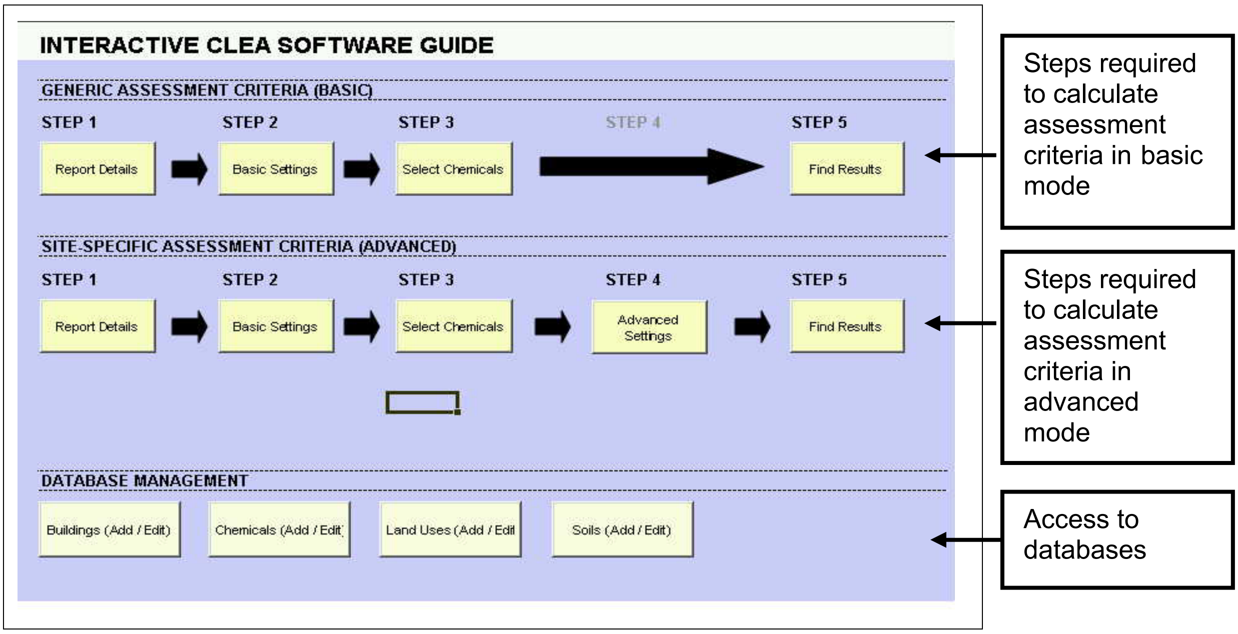

Figure 3.2: The Interactive CLEA Software Guide.

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. The name of the file that you have used to save the CLEA software is also included as a header within the output reports.

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'.

> ⓘ You can go back to Step 1 at any time during the simulation by clicking on the Step 1 button from the 'Interactive CLEA Software Guide'

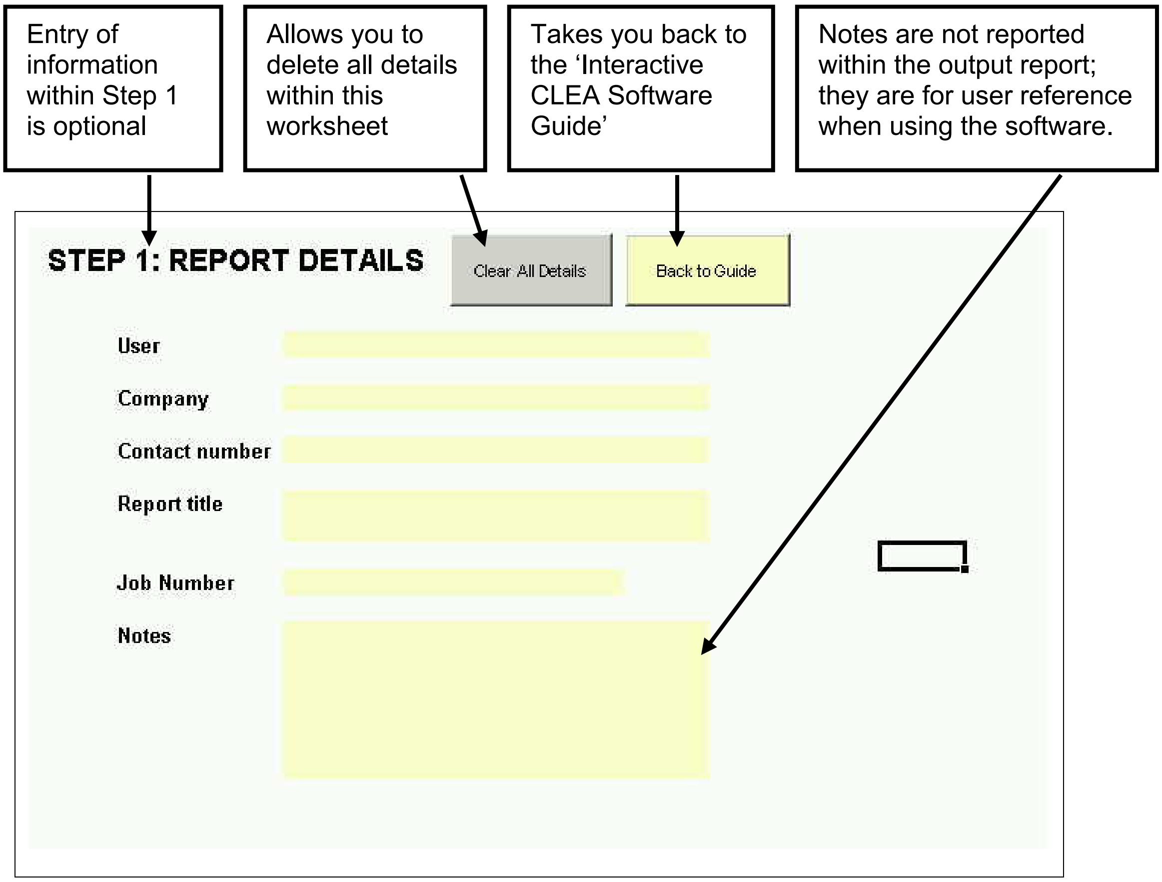

Figure 3.3: Step 1: Report Details worksheet.

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). Ratio mode should also be selected when calculating ADE for dioxins, furans and dioxin-like PCBs (see Environment Agency, 2009f, for guidance on deriving assessment criteria for dioxins, furans and dioxin-like PCBs).

ⓘ In calculating ADE/HCV ratios the 50 per cent rule (see section 4.3.3 for an explanation of this rule) is implemented within the CLEA software as follows; 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 ADE/HCV ratio. Section 4.3.3 provides further 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
- residential (lifetime exposure)
- allotments
- allotments (lifetime exposure)
- commercial
- all user-added land use datasets added to the database (see Section 3.4).

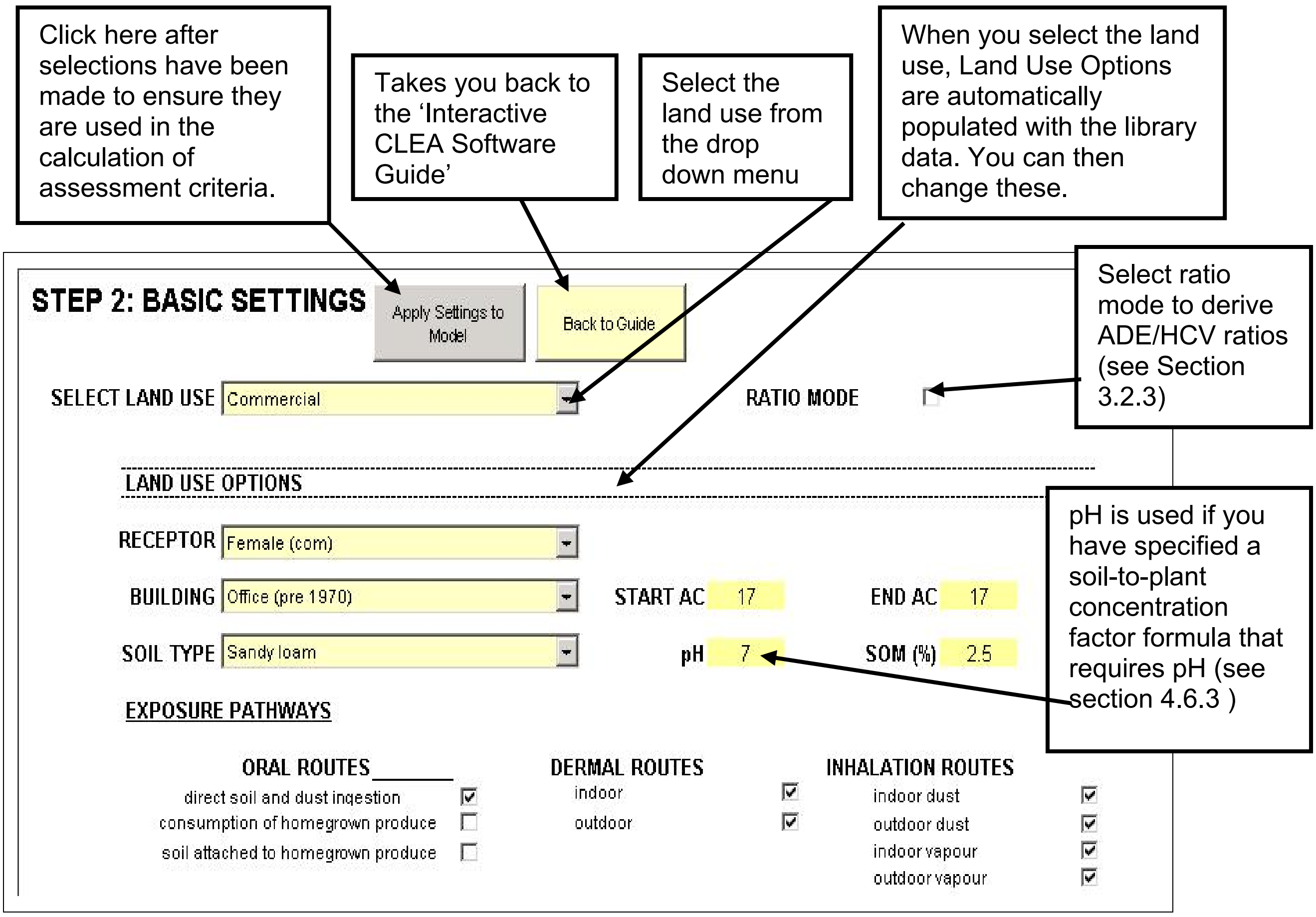

Figure 3.4: **Step 2: Basic Settings worksheet**

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).

ⓘ Soil pH is used within the CLEA model in the calculation of plant uptake of contamination from soil. You are only required to add a value for pH if you have entered a formula to specify the exact calculation of a soil-to-plant concentration factor/s, within the chemicals database worksheet, that require soil pH (see section 4.6.3 for further information).

ⓘ 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 silt 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 sub-divided into age classes which are shown in Table 3.1.

Table 3.1: Age classes used within the CLEA software.

Age Class (AC)	Age (years)	Exposure Duration (years)
1	0 – 1	1
2	1 – 2	1
3	2 – 3	1
4	3 – 4	1
5	4 – 5	1
6	5 – 6	1
7	6 – 7	1
8	7 – 8	1
9	8 – 9	1
10	9 – 10	1
11	10 – 11	1
12	11 – 12	1
13	12 – 13	1
14	13 – 14	1
15	14 – 15	1
16	15 – 16	1
17	16 – 65	49
18	65 – 75	10

ⓘ 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)

ⓘ A complete dataset for the land use and receptor data for the commercial receptor are available within the software for Age Class 17 only. You should not select a commercial receptor for any other Age Class unless you add data for the additional Age Classes selected in step 4 'Advanced Settings'.

ⓘ Land use data for both the residential and allotment land use are available within the software for Age Classes 1 to 6 only. You should not select a residential or commercial land use for any other Age Class unless you add data for the additional Age Classes selected in step 4 'Advanced Settings'. Alternatively you can choose to select the residential (lifetime exposure) or allotment (lifetime exposure) land use and select the Age Classes you require in step 2 'Basic settings'.

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, data for age class 17 is available within the software for the commercial land use and data for all age classes is available within the software for the residential (lifetime exposure) and allotment (lifetime exposure) 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 or soil-derived average daily exposure for dioxins, furans and dioxin-like PCBs (that is, you have selected ‘Ratio Mode’ in Step 2

'Basic Settings'), you must also enter a representative concentration[1] 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.

Chemicals available for selection include:

i. user defined chemicals that have been added to the chemicals database (see section 3.4.5); and

ii. chemical data used to derive Soil Guideline Values that have been published to date. These chemicals are:

- Arsenic
- Cadmium
- Mercury, elemental
- Mercury, inorganic
- Mercury, methyl
- Nickel
- Selenium
- Phenol
- Benzene
- Ethylbenzene
- Toluene
- Xylene, o-
- Xylene, m-
- Xylene, p-
- 2,3,7,8-TCDD [2]
- 1,2,3,7,8-PeCDD [2]
- 1,2,3,4,7,8-HxCDD [2]
- 1,2,3,6,7,8-HxCDD [2]
- 1,2,3,7,8,9-HxCDD [2]
- 1,2,3,4,6,7,8-HpCDD [2]
- OCDD [2]
- 2,3,7,8-TCDF [2]
- 1,2,3,7,8-PeCDF [2]
- 2,3,4,7,8-PeCDF [2]
- 1,2,3,4,7,8-HxCDF [2]
- 1,2,3,7,8,9-HxCDF [2]

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[1] To obtain estimated average daily exposure from soil per unit concentration of the congener in soil, for dioxins, furans and dioxin-like PCBs, the representative concentration that should be used is 1E-06 mg kg^{-1} DW.
[2] You must only use the chemical data for dioxins, furans and dioxin-like compounds to calculate estimated soil-derived average daily exposure per unit concentration of the congener in soil. See the grey text box below.

- 1,2,3,6,7,8-HxCDF [2]
- 2,3,4,6,7,8-HxCDF [2]
- 1,2,3,4,6,7,8-HpCDF [2]
- 1,2,3,4,7,8,9-HpCDF [2]
- OCDF [2]
- PCB-77 [2]
- PCB-81 [2]
- PCB-126 [2]
- PCB-169 [2]
- PCB-105 [2]
- PCB-114 [2]
- PCB-118 [2]
- PCB-123 [2]
- PCB-156 [2]
- PCB-157 [2]
- PCB-167 [2]
- PCB-189 [2]

! You must only use the chemical data for dioxins, furans and dioxin-like compounds to calculate estimated soil-derived average daily exposure, for all relevant pathways, per unit concentration of the congener in soil according to the standard land-use scenario. This calculation is undertaken using ratio mode. Appendix 1 of Environment Agency, 2009f provides guidance on how to calculate and extract the soil-derived average daily exposure from the CLEA software.

! You can use the average daily exposure to derive site specific assessment criteria, including for non standard land uses, using the dioxins, furans and dioxin-like compounds worksheet (Environment Agency, 2009e). Appendix 1 of Environment Agency, 2009f provides guidance on deriving site specific assessment criteria using this workbook.

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 (applies to the infinite source option and to the subsurface model);
- outdoor vapour concentrations;
- indoor vapour concentrations;
- chemical concentrations in edible portions of green vegetables;
- chemical concentrations in edible portions of root vegetables;

- chemical concentrations in edible portions of tuber vegetables;
- chemical concentrations in edible portions of herbaceous fruit;
- chemical concentrations in edible portions of shrub fruit;
- chemical concentrations in edible portions of tree fruit.

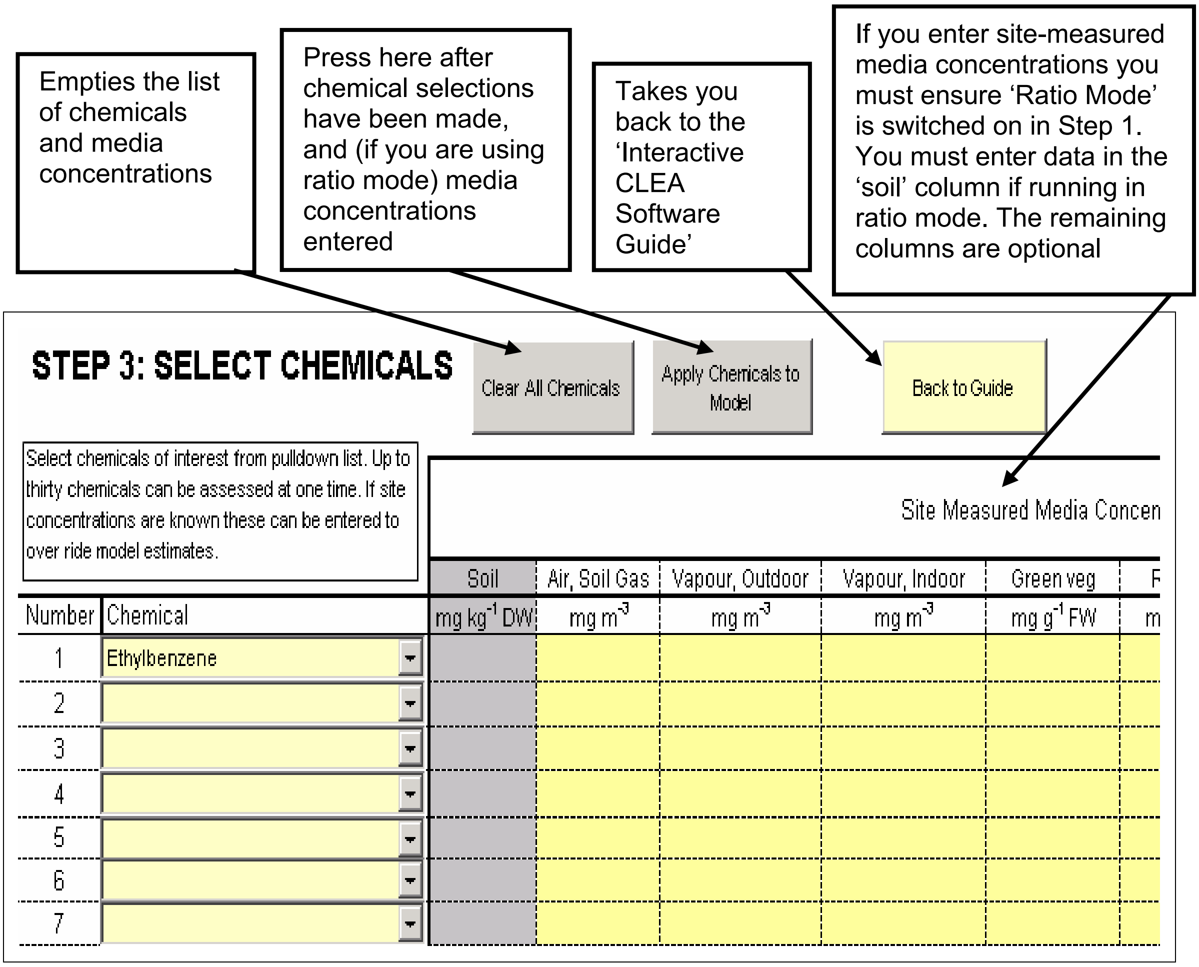


Figure 3.5: Step 3: Select Chemicals worksheet.

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.

ⓘ Neither of the finite source models depend on the soil vapour concentration directly and therefore cannot be used with a fixed soil gas concentration (see Section 4.9).

ⓘ 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 are running a new simulation and chemicals selected within Step 3 from a previous run are present that you want to use again, you do not need to clear all the chemicals and reselect them.

ⓘ 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:

i. Chemical data
ii. Homegrown produce data
iii. Land use and receptor data
iv. 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 relative bioavailability;
- airborne dust relative bioavailability.

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;
- time average period for surface emissions;
- effective air permeability.

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.

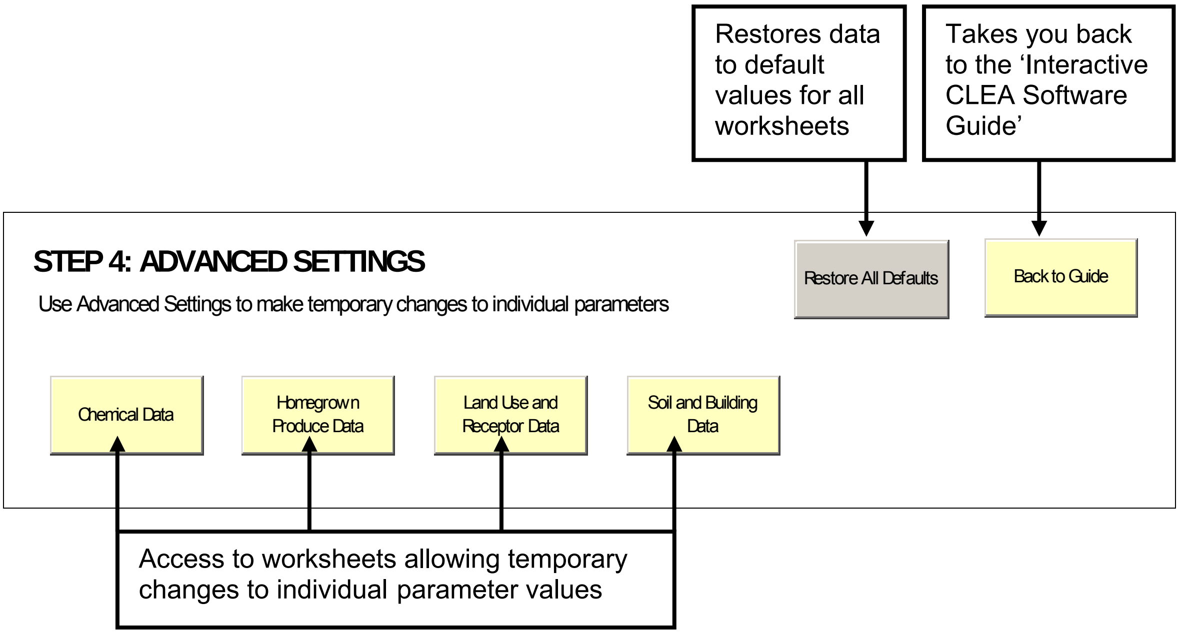


Figure 3.6: Step 4: Advanced Settings worksheet.

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 HCVs	(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.	sub-surface soil to indoor air correction factor	(Section 4.6.7)
xi.	relative bioavailability	(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.

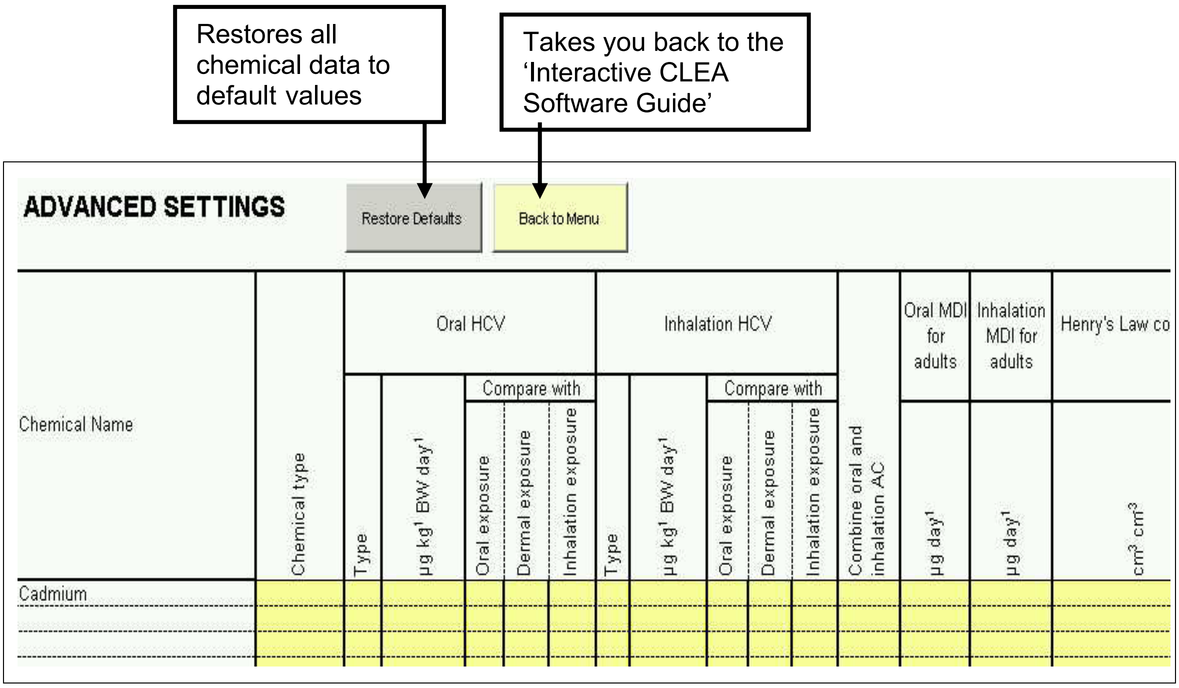
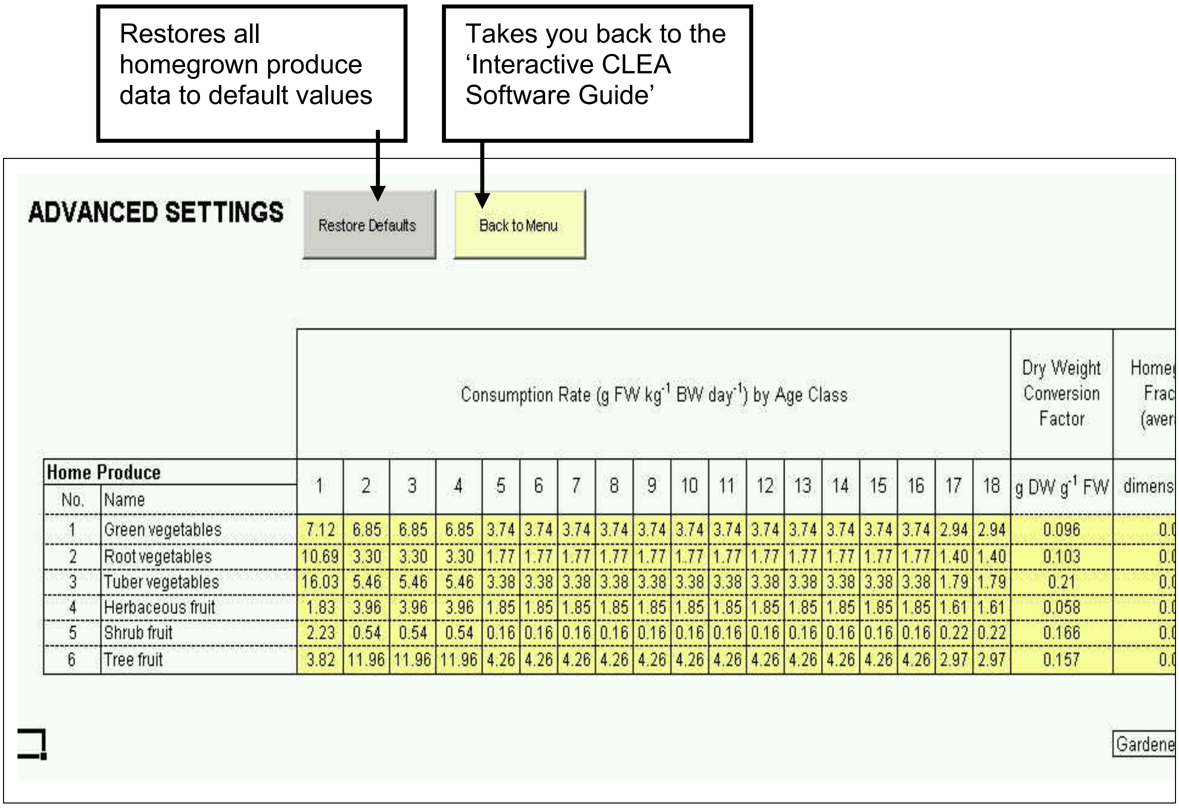


Figure 3.7: Step 4: Advanced Settings Chemical Data.

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.



Home Produce		Consumption Rate (g FW kg^{-1} BW day^{-1}) by Age Class																		Dry Weight Conversion Factor	Homeg Frac (aver
No.	Name	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	g DW g^{-1} FW	dimens
1	Green vegetables	7.12	6.85	6.85	6.85	3.74	3.74	3.74	3.74	3.74	3.74	3.74	3.74	3.74	3.74	3.74	3.74	2.94	2.94	0.096	0.0
2	Root vegetables	10.69	3.30	3.30	3.30	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.40	1.40	0.103	0.0
3	Tuber vegetables	16.03	5.46	5.46	5.46	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	3.38	1.79	1.79	0.21	0.0
4	Herbaceous fruit	1.83	3.96	3.96	3.96	1.85	1.85	1.85	1.85	1.85	1.85	1.85	1.85	1.85	1.85	1.85	1.85	1.61	1.61	0.058	0.0
5	Shrub fruit	2.23	0.54	0.54	0.54	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.22	0.22	0.166	0.0
6	Tree fruit	3.82	11.96	11.96	11.96	4.26	4.26	4.26	4.26	4.26	4.26	4.26	4.26	4.26	4.26	4.26	4.26	2.97	2.97	0.157	0.0

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)

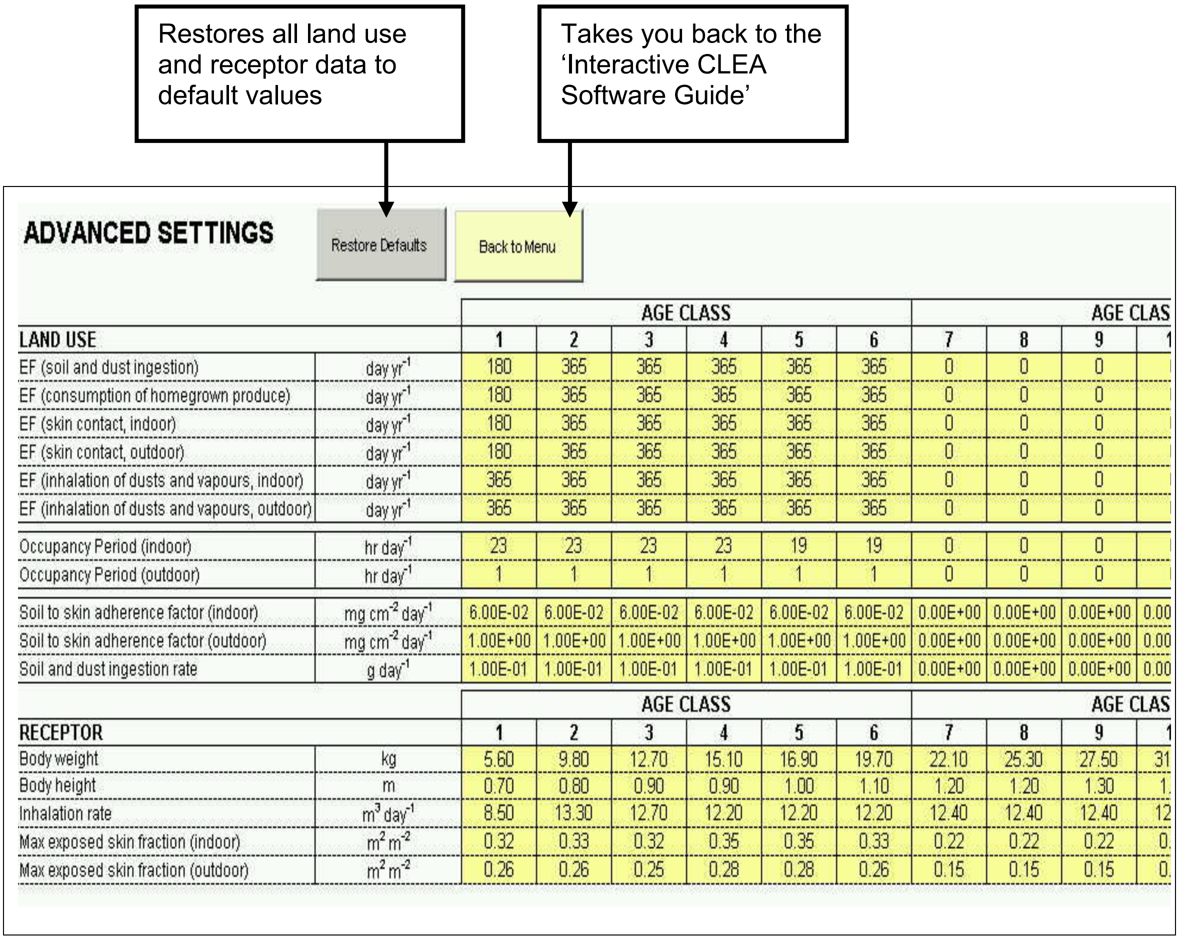
See also Section 4.4.3 on receptor behavioural characteristics for information relating to consumption rates of homegrown produce.

ⓘ 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’.

ⓘ 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.

ⓘ 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.



LAND USE		1	2	3	4	5	6	7	8	9	1
EF (soil and dust ingestion)	day yr^{-1}	180	365	365	365	365	365	0	0	0	
EF (consumption of homegrown produce)	day yr^{-1}	180	365	365	365	365	365	0	0	0	
EF (skin contact, indoor)	day yr^{-1}	180	365	365	365	365	365	0	0	0	
EF (skin contact, outdoor)	day yr^{-1}	180	365	365	365	365	365	0	0	0	
EF (inhalation of dusts and vapours, indoor)	day yr^{-1}	365	365	365	365	365	365	0	0	0	
EF (inhalation of dusts and vapours, outdoor)	day yr^{-1}	365	365	365	365	365	365	0	0	0	
Occupancy Period (indoor)	hr day^{-1}	23	23	23	23	19	19	0	0	0	
Occupancy Period (outdoor)	hr day^{-1}	1	1	1	1	1	1	0	0	0	
Soil to skin adherence factor (indoor)	mg cm^{-2} day^{-1}	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	6.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00
Soil to skin adherence factor (outdoor)	mg cm^{-2} day^{-1}	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00
Soil and dust ingestion rate	g day^{-1}	1.00E-01	1.00E-01	1.00E-01	1.00E-01	1.00E-01	1.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00

RECEPTOR		1	2	3	4	5	6	7	8	9	1
Body weight	kg	5.60	9.80	12.70	15.10	16.90	19.70	22.10	25.30	27.50	31
Body height	m	0.70	0.80	0.90	0.90	1.00	1.10	1.20	1.20	1.30	1.
Inhalation rate	m^3 day^{-1}	8.50	13.30	12.70	12.20	12.20	12.20	12.40	12.40	12.40	12
Max exposed skin fraction (indoor)	m^2 m^{-2}	0.32	0.33	0.32	0.35	0.35	0.33	0.22	0.22	0.22	0.
Max exposed skin fraction (outdoor)	m^2 m^{-2}	0.26	0.26	0.25	0.28	0.28	0.26	0.15	0.15	0.15	0.

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:

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)

Receptor data:

i.	body weight	(
ii.	Table 4.5)	
iii.	body height	(
iv.	Table 4.5)	
v.	inhalation rate	(Sections 4.6.6 to 4.6.8)
vi.	maximum exposed skin fractions	(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**	(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	(Section 4.7)
iv.	van Genuchten shape parameter (*m*)	(Section 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_x)for dust model	(Section 4.6.6)
viii.	ambient soil temperature	(Section 4.7.2)

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.

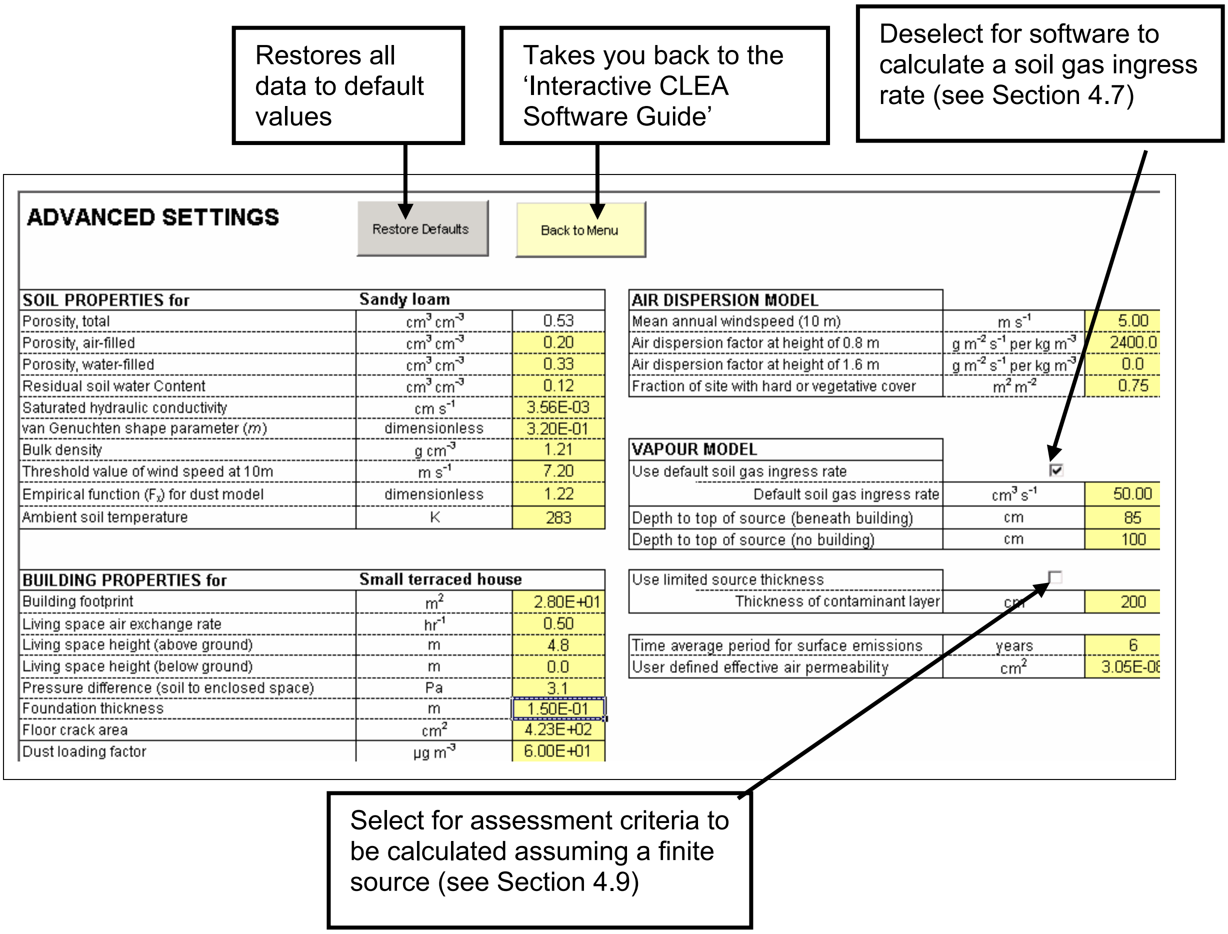


Figure 3.10: Step 4: Advanced Settings Soil and Building Data.

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)
vii.	time average period for surface emissions	(Section 4.11)
viii.	user defined effective air permeability	(Section 4.7)

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’.

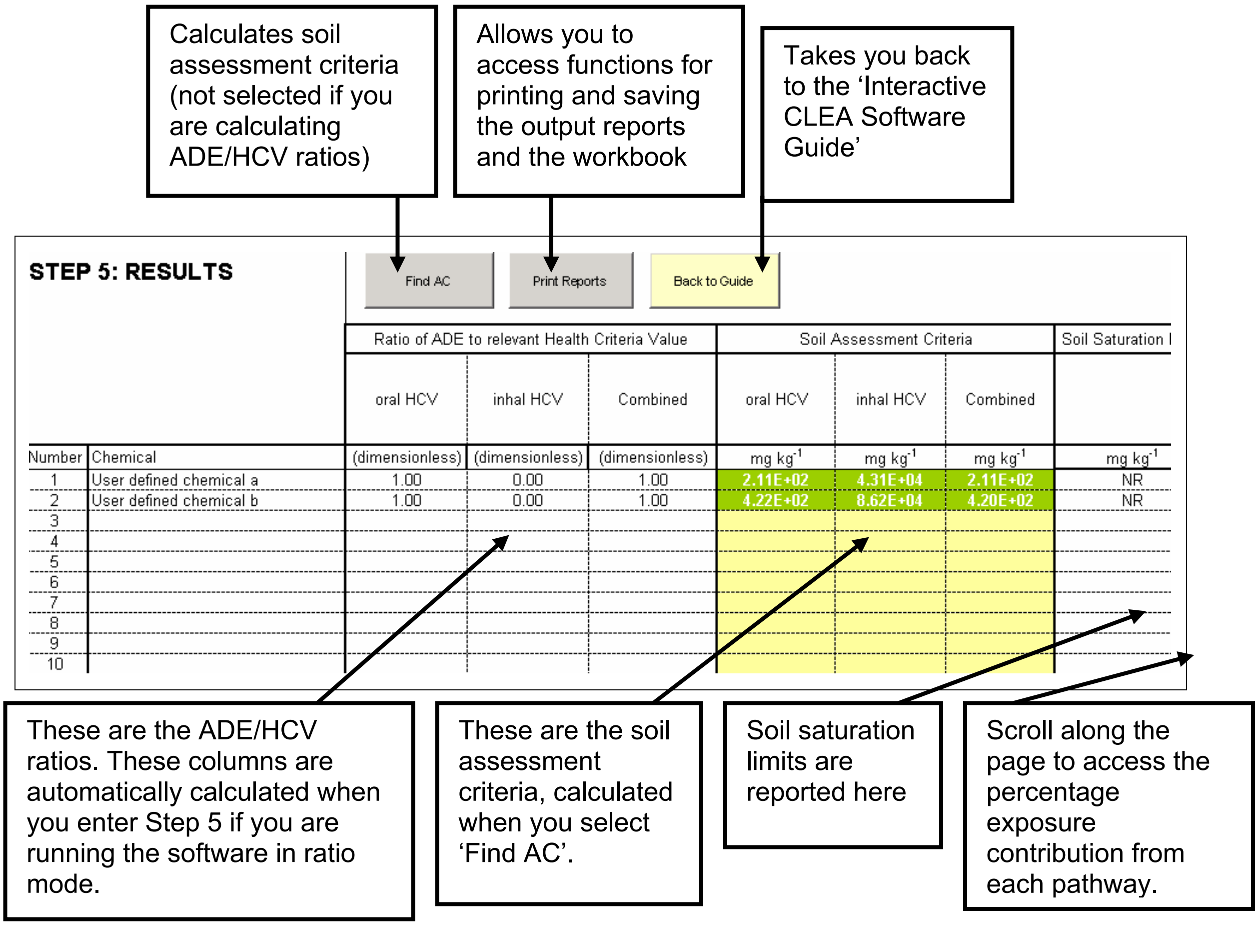


Figure 3.11: Step 5: Find Results worksheet.

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 an assessment criteria has exceeded the saturated soil limits based on theoretical considerations of solubility and vapourisation. The coloured cells within the 'Soil Assessment Criteria' column represent the following:

i. Green – the assessment criteria does not exceed the saturated soil concentration

ii. Amber – the assessment criteria does exceed the saturated soil concentration However, the contribution of the indoor and outdoor vapour pathway to total exposure is less than 10% and it will therefore not affect the assessment criteria significantly

iii. Red – the assessment criteria does exceed the saturated soil concentration and it may significantly affect the interpretation of any exceedances. The contribution of the indoor and outdoor vapour pathway to total exposure is greater than 10%.

See Chapter 5 in the CLEA report and Section 4.12 of this handbook for further discussion and advice on interpreting assessment criteria that exceed the theoretical soil saturation limits.

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 '.

ⓘ If your calculation of the oral assessment criteria does not include vapour pathways then you do not need to consider the solubility or vapour saturation limit.

ⓘ The CLEA software does not cap exposure at the solubility or vapour saturation limits.

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'.

ⓘ 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.

! 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.

ⓘ 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.

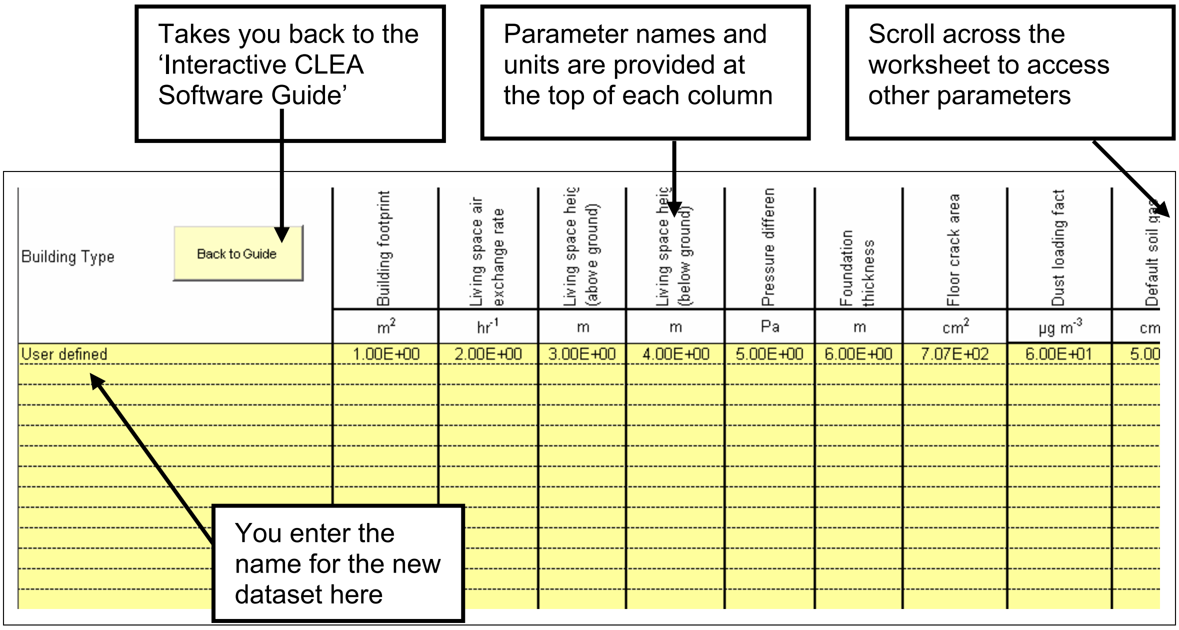


Figure 3.12: Database Management Buildings Database.

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):

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)
ix.	default soil gas ingress rate	(Section 4.6.7)

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

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.

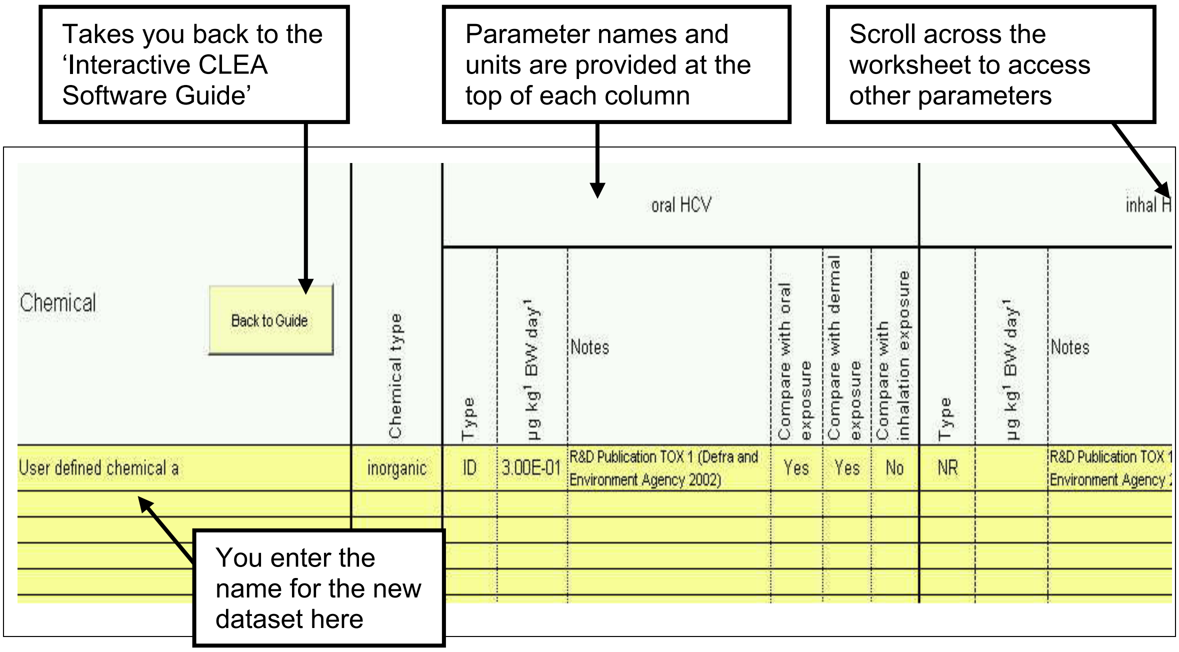


Figure 3.13: Database Management Chemicals Database.

Default generic datasets are available for selection in basic and advanced mode for the updated TOX and SGV reports that have been published to date, but are hidden within the chemicals database to prevent you from overwriting them.

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 (Section 4.5.5)
ii. oral and inhalation HCVs, type (Section 4.3.3)
iii. oral and inhalation HCVs, value (Section 4.3.3)
iv. comparing HCVs with exposure (Section 2.3.2 of the CLEA report)
v. combine oral and inhalation acceptance criteria (Section 4.3.3)
vi. physical-chemical properties (Section 4.5.3)
vii. dermal absorption fraction (Section 4.6.5)
viii. plant correction factors (Section 4.6.3)
ix. plant concentration factors (Section 4.6.3)
x. soil-to-dust transport factor (Section 4.6.5, 4.6.6)
xi. sub-surface soil to indoor air correction factor (Section 4.6.7)

The relative bioavailability for soil and airborne dust is automatically input as one when you enter a new chemical. The relative bioavailability 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 or enter a formula specifying the exact calculation provided that the answer is not less than zero). See text box for example;
- soil-to-plant concentration factor type (model, numeric dw or number fw);
- soil-to-dust transport factor (enter a value greater than zero);
- sub-surface soil to indoor air correction factor (value must be equal to or greater than one).

ⓘ The formula for the soil-to-plant concentration factor must be entered in the format "= CONST x soil_pH" or "= CONST x som" provided that answer is not less than zero. For example if a soil-to-plant concentration factor for root vegetables for contaminant A is as follows;

$$CF = 11.174 - (1.6461 \text{ x soil pH})$$

You should enter the following into the appropriate cell in the chemical database;

$$= 11.174 - (1.6461 * \text{soil\_pH})$$

ⓘ You can enter a Tolerable Daily Intake (TDI) <u>or</u> 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.

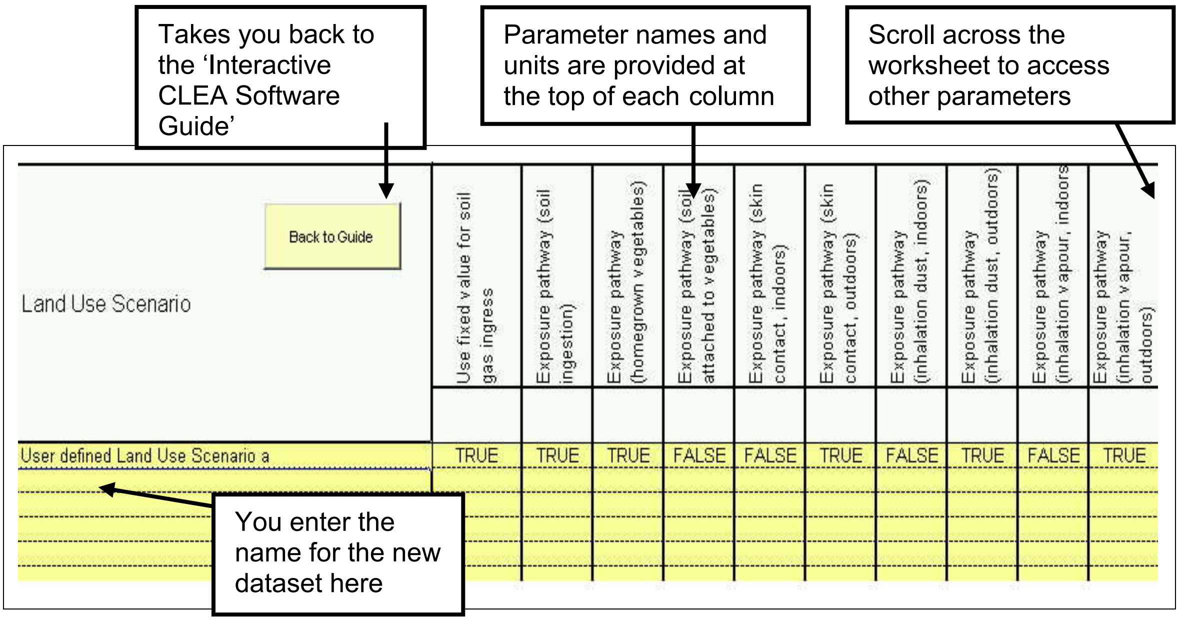


Figure 3.14: Database Management Land Uses Database.

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
- residential (lifetime exposure)
- allotments
- allotments (lifetime exposure)
- 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.

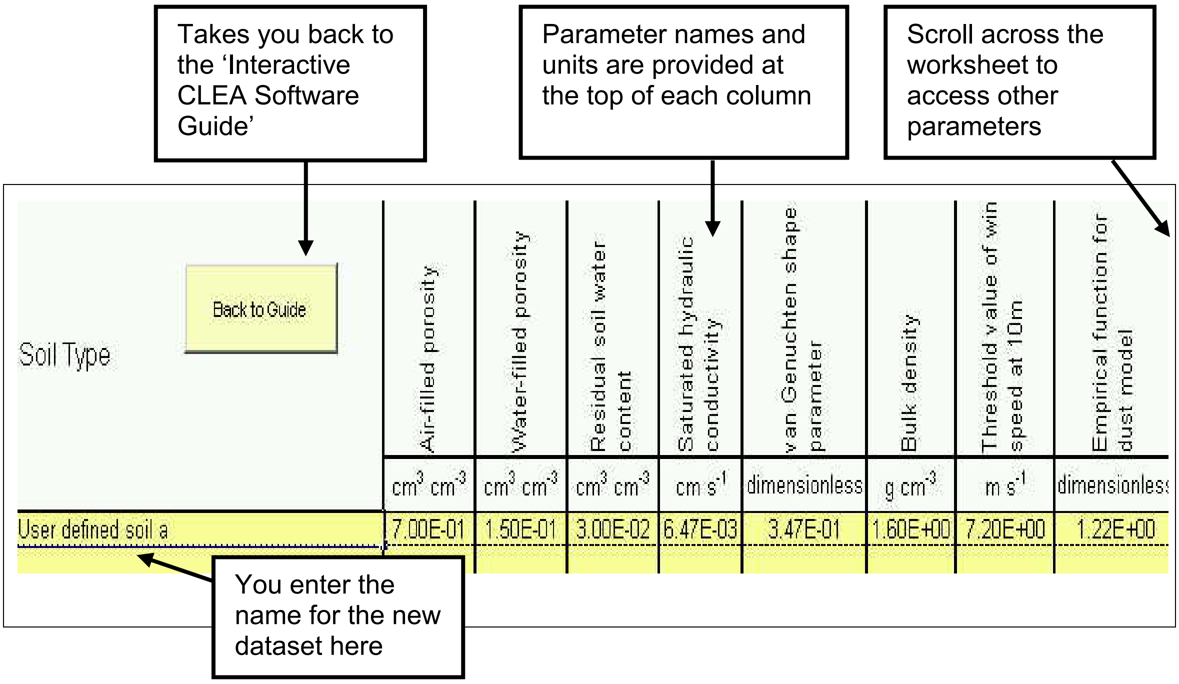


Figure 3.15: Database Management Soils Database.

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 silt 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_x) 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

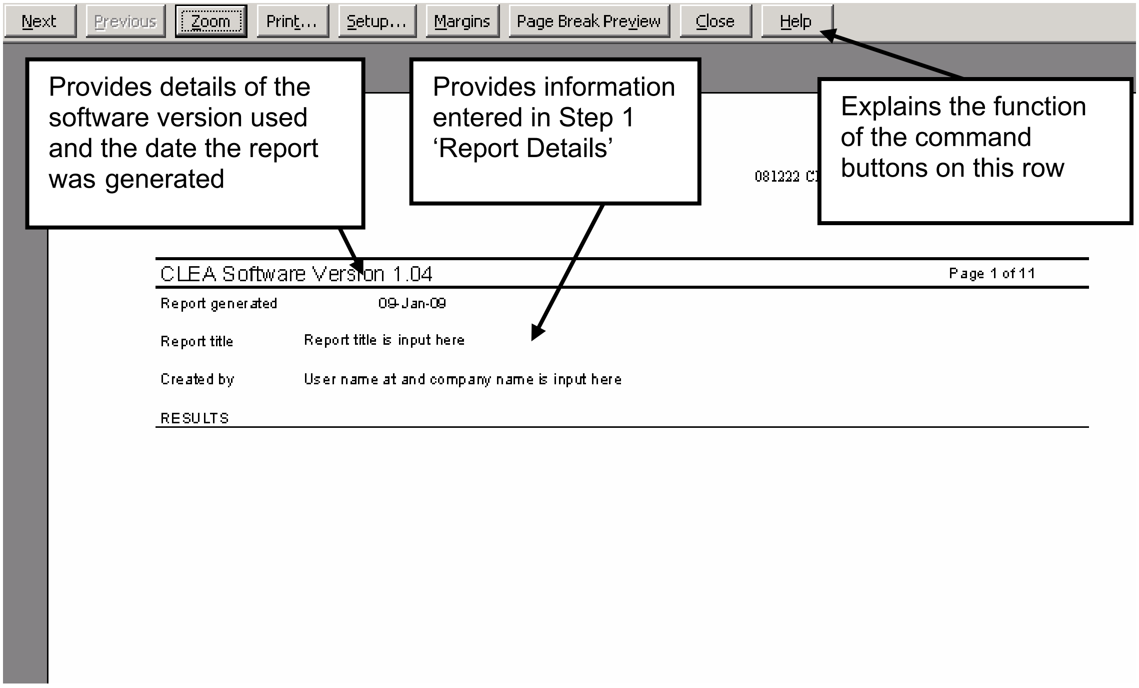


Figure 3.16: 'Print Results' information page.

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		Assessment Criterion (mg kg^{-1})			Ratio of ADE to HCV			Saturation Limit (mg kg^{-1})	50% rule?	
		oral	inhalation	combined	oral	inhalation	combined		Oral	Inhal
1	User derinfed chemical a	1.28E+02	8.26E+00	7.76E+00	0.06	0.94	1.00	5.44E+02 (vap)	No	No
2	User defined chemical b	8.75E+02	7.58E+02	4.06E+02	0.46	0.54	1.00	2.98E+03 (vap)	No	No
3										
4										
5										
6										
7										
8										
9										
10										
11										
12										
13										
14										

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.

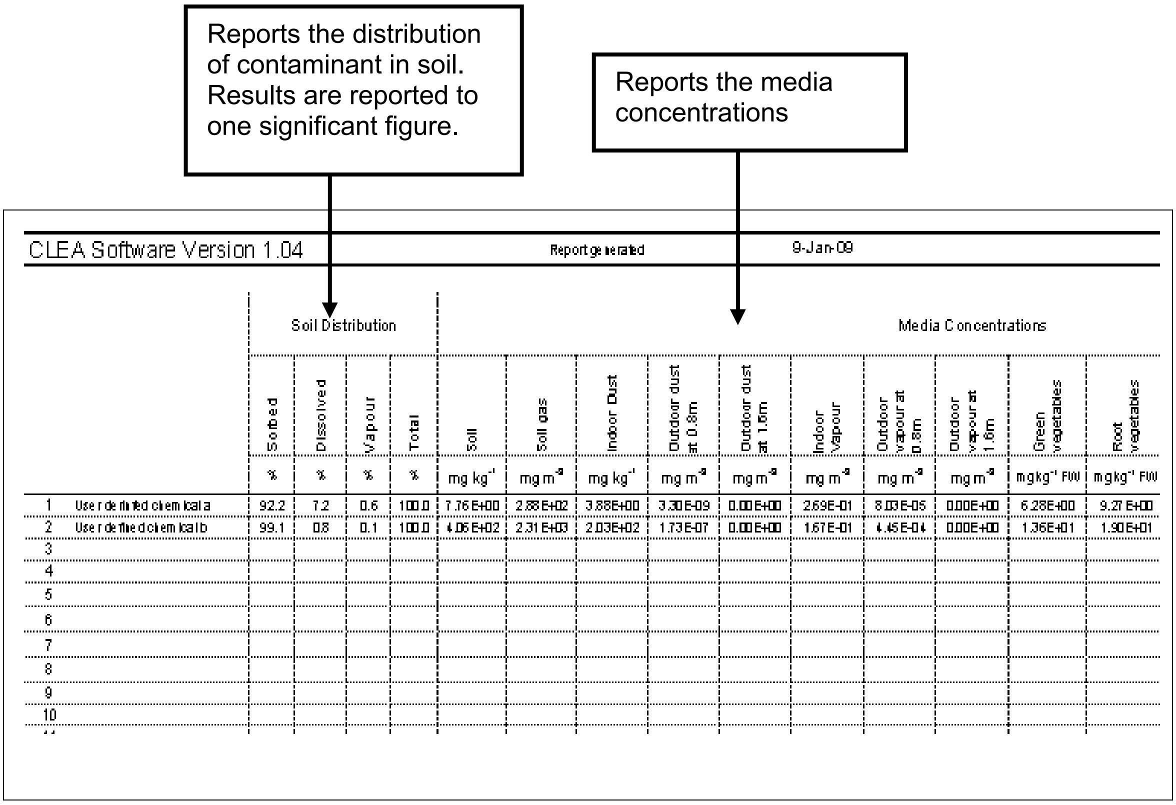
ADE/HCV ratios are reported within the 'Ratio of ADE to HCV' columns.

'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 inhalation 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 (separately 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).



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		Soil Distribution				Media Concentrations									
		Sorbed	Dissolved	Vapour	Total	Soil	Soil gas	Indoor Dust	Outdoor dust at 0.8m	Outdoor dust at 1.6m	Indoor Vapour	Outdoor vapour at 0.8m	Outdoor vapour at 1.6m	Green vegetables	Root vegetables
		%	%	%	%	mg kg^{-1}	mg m^{-3}	mg kg^{-1}	mg m^{-3}	mg m^{-3}	mg m^{-3}	mg m^{-3}	mg m^{-3}	mg kg^{-1} FW	mg kg^{-1} FW
1	User defined chemical a	92.2	7.2	0.6	100.0	7.76E+00	2.88E+02	3.88E+00	3.30E-09	0.00E+00	2.69E-01	8.03E-05	0.00E+00	6.28E+00	9.27E+00
2	User defined chemical b	99.1	0.8	0.1	100.0	4.06E+02	2.31E+03	2.03E+02	1.73E-07	0.00E+00	1.67E-01	4.45E-04	0.00E+00	1.36E+01	1.90E+01
3															
4															
5															
6															
7															
8															
9															
10															

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).

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		Average Daily Exposure (mg kg^{-1} bw day^{-1})							Distribution by Pathway (%)						
		Direct soil ingestion	Consumption of home grown produce and attached soil	Dermal contact with soil and dust	Inhalation of dust	Inhalation of vapour	Background (oral)	Background (inhalation)	Direct soil ingestion	Consumption of home grown produce and attached soil	Dermal contact with soil and dust	Inhalation of dust	Inhalation of vapour (indoor)	Inhalation of vapour (outdoor)	
1	User defined chemical a	5.75E-05	5.06E-03	2.96E-06	2.18E-07	2.49E-01	1.13E-04	5.15E-03	0.02	1.95	0.01	0.00	95.98	0.00	0
2	User defined chemical b	3.01E-03	1.63E-02	1.55E-03	1.14E-06	1.55E-01	1.69E-04	1.52E-03	1.70	9.18	0.87	0.01	87.28	0.01	0
3															
4															
5															
6															
7															
8															
9															
10															
11															
12															
13															
14															

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.

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		Oral Health Criteria Value (µg kg⁻¹ BW day⁻¹)		Inhalation Health Criteria Value (µg kg⁻¹ BW day⁻¹)		Oral Mean Daily Intake (µg day⁻¹)	Inhalation Mean Daily Intake (µg day⁻¹)	Air-water partition coefficient (K_{aw}) (cm³ cm⁻³)	Coefficient of Diffusion in Air (m² s⁻¹)	Coefficient of Diffusion in Water (m² s⁻¹)	log K_{oc} (cm³ g⁻¹)	log K_{ow} (dimensionless)	Dermal Absorption Fraction (dimensionless)	Soil-to-dust transport factor (g g⁻¹ DW)	Sub-surface soil to indoor air correction factor (dimensionless)
1	User defined chemical a	TDI	85	TDI	270	2	85	1.40E-01	4.00E-06	8.00E-10	2	3	0.1	0.5	1
2	User defined chemical b	TDI	45	TDI	290	3	25	2.00E-01	9.00E-06	7.00E-07	3	2	0.1	0.5	10
3															
4															
5															
6															
7															
8															
9															
10															
11															
12															
13															
14															

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		Soil-to-water partition coefficient (cm³ g⁻¹)	Vapour pressure (Pa)	Water solubility (mg L⁻¹)	Soil-to-plant concentration factor for green vegetables (mg g⁻¹ plant DW or FW basis over mg g⁻¹ DW soil)	Soil-to-plant concentration factor for root vegetables (mg g⁻¹ plant DW or FW basis over mg g⁻¹ DW soil)	Soil-to-plant concentration factor for tuber vegetables (mg g⁻¹ plant DW or FW basis over mg g⁻¹ DW soil)	Soil-to-plant concentration factor for herbaceous fruit (mg g⁻¹ plant DW or FW basis over mg g⁻¹ DW soil)
1	User defined chemical a	3.48E+00	5.00E+02	1.50E+02	model	model	model	model
2	User defined chemical b	3.48E+01	4.00E+02	2.00E+02	model	model	model	model
3								
4								
5								
6								
7								
8								
9								
10								
11								
12								
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14								

Figure 3.20: 'Print Results' HCVs, fate and transport data and relative bioavailability.

Figure 3.20 shows the HCVs, fate and transport data, physical-chemical data, sub-surface soil to indoor air correction factor and relative bioavailability 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

CLEA Software Version 1.04

Report generated	09/01/2009
Report title	Report title is input here
Created by	User name at and company name is input here

BASIC SETTINGS

Land Use	Residential with homegrown produce						
Building	Small terraced house						
Receptor	Female (res)	Start age class	1	End age class	6	Exposure Duration	6 years
Soil	Sandy loam						

Exposure Pathways

Direct soil and dust ingestion	✔	Dermal contact with indoor dust	✔	Inhalation of indoor dust	✔
Consumption of homegrown produce	✔	Dermal contact with soil	✔	Inhalation of soil dust	✔
Soil attached to homegrown produce	✔			Inhalation of indoor vapour	✔
				Inhalation of outdoor vapour	✔

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.

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Land Use Residential with homegrown produce

Age Class	Exposure Frequencies (days yr^{-1}): Direct soil ingestion	Consumption of homegrown produce	Dermal contact with indoor dust	Dermal contact with soil	Inhalation of dust and vapour. Indoor	Inhalation of dust and vapour. outdoor	Occupation Periods (hr day^{-1}): Indoors	Outdoors	Soil to skin adherence factors (mg cm^{2}): Indoor	Outdoor	Direct soil ingestion rate (g day^{-1})
1	180	180	180	180	365	365	23.0	1.0	0.06	1.00	0.10
2	365	365	365	365	365	365	23.0	1.0	0.06	1.00	0.10
3	365	365	365	365	365	365	23.0	1.0	0.06	1.00	0.10
4	365	365	365	365	365	365	23.0	1.0	0.06	1.00	0.10
5	365	365	365	365	365	365	19.0	1.0	0.06	1.00	0.10
6	365	365	365	365	365	365	19.0	1.0	0.06	1.00	0.10
7	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
8	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
9	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00
10	0	0	0	0	0	0	0.0	0.0	0.00	0.00	0.00

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’.

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Receptor Female (res)

Age Class	Body weight (kg)	Body height (m)	Inhalation rate (m^3 day^{-1})	Max exposed skin factor: Indoor (m^2 m^{-2})	Max exposed skin factor: Outdoor (m^2 m^{-2})	Total skin area (m^2)	Consumption rates (g FW kg^{-1} BW day^{-1}): Green vegetables	Root vegetables	Tuber vegetables	Herbaceous fruit	Shrub fruit	Tree fruit
1	5.60	0.7	8.5	0.32	0.26	3.43E-01	7.12	10.69	16.03	1.83	2.23	3.82
2	9.80	0.8	13.3	0.33	0.26	4.84E-01	6.85	3.30	5.46	3.96	0.54	11.96
3	12.70	0.9	12.7	0.32	0.25	5.82E-01	6.85	3.30	5.46	3.96	0.54	11.96
4	15.10	0.9	12.2	0.35	0.28	6.36E-01	6.85	3.30	5.46	3.96	0.54	11.96
5	16.90	1.0	12.2	0.35	0.28	7.04E-01	3.74	1.77	3.38	1.85	0.16	4.26
6	19.70	1.1	12.2	0.33	0.26	7.94E-01	3.74	1.77	3.38	1.85	0.16	4.26
7	22.10	1.2	12.4	0.22	0.15	8.73E-01	3.74	1.77	3.38	1.85	0.16	4.26
8	25.30	1.2	12.4	0.22	0.15	9.36E-01	3.74	1.77	3.38	1.85	0.16	4.26
9	27.50	1.3	12.4	0.22	0.15	1.01E+00	3.74	1.77	3.38	1.85	0.16	4.26
10	31.40	1.3	12.4	0.22	0.15	1.08E+00	3.74	1.77	3.38	1.85	0.16	4.26
11	35.70	1.4	12.4	0.22	0.14	1.19E+00	3.74	1.77	3.38	1.85	0.16	4.26
12	41.30	1.4	13.4	0.22	0.14	1.29E+00	3.74	1.77	3.38	1.85	0.16	4.26
13	47.20	1.5	13.4	0.22	0.14	1.42E+00	3.74	1.77	3.38	1.85	0.16	4.26
14	51.20	1.6	13.4	0.22	0.14	1.52E+00	3.74	1.77	3.38	1.85	0.16	4.26
15	56.70	1.6	13.4	0.21	0.14	1.60E+00	3.74	1.77	3.38	1.85	0.16	4.26
16	59.00	1.6	13.4	0.21	0.14	1.63E+00	3.74	1.77	3.38	1.85	0.16	4.26

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.

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Building Small terraced house

Building footprint (m^2)	2.80E+01
Living space air exchange rate (hr^{-1})	5.00E-01
Living space height (above ground, m)	4.80E+00
Living space height (below ground, m)	0.00E+00
Pressure difference (soil to enclosed space, Pa)	3.10E+00
Foundation thickness (m)	1.50E-01
Floor crack area (cm^2)	4.23E+02
Dust loading factor ($\mu g\ m^{-3}$)	6.00E+01

Soil Sandy loam

Porosity, Total (cm^3 cm^{-3})	5.30E-01
Porosity, Air-Filled (cm^3 cm^{-3})	2.00E-01
Porosity, Water-Filled (cm^3 cm^{-3})	3.30E-01
Residual soil water content (cm^3 cm^{-3})	1.20E-01
Saturated hydraulic conductivity ($cm\ s^{-1}$)	3.56E-03
van Genuchten shape parameter *m* (dimensionless)	3.20E-01
Bulk density ($g\ cm^{-3}$)	1.21E+00
Threshold value of wind speed at 10m ($m\ s^{-1}$)	7.20E+00
Empirical function (F_x) for dust model (dimensionless)	1.22E+00
Ambient soil temperature (K)	2.83E+02
Soil pH	7.00E+00
Soil Organic Matter content (%)	6.00E+00
Fraction of organic carbon ($g\ g^{-1}$)	3.48E-02
Effective total fluid saturation (unitless)	5.12E-01
Intrinsic soil permeability (cm^2)	4.75E-08
Relative soil air permeability (unitless)	6.42E-01
Effective air permeability (cm^2)	3.05E-08

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 and relative soil 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.

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Soil - Vapour Model

Depth to top of source (no building) (cm)	100
Depth to top of source (beneath building) (cm)	85
Default soil gas ingress rate?	Yes
Soil gas ingress rate ($cm^3 s^{-1}$)	5.00E+01
Building ventilation rate ($cm^3 s^{-1}$)	1.87E+04
Averaging time surface emissions (yr)	6
Finite vapour source model?	No
Thickness of contaminated layer (cm)	200

Air Dispersion Model

Mean annual windspeed at 10m ($m s^{-1}$)	5.00
Air dispersion factor at height of 0.8m *	2400.00
Air dispersion factor at height of 1.6m *	0.00
Fraction of site cover ($m^2 m^{-2}$)	0.75

* Air dispersion factor in $g m^{-2} s^{-1}$ per $kg m^{-3}$

Soil - Plant Model	Dry weight conversion factor	Homegrown fraction Average	High	Soil loading factor	Preparation correction factor
	$g DW g^{-1} FW$	dimensionless		$g g^{-1} DW$	dimensionless
Green vegetables	0.096	0.05	0.33	1.00E-03	2.00E-01
Root vegetables	0.103	0.06	0.40	1.00E-03	1.00E+00
Tuber vegetables	0.210	0.02	0.13	1.00E-03	1.00E+00
Herbaceous fruit	0.058	0.06	0.40	1.00E-03	6.00E-01
Shrub fruit	0.166	0.09	0.60	1.00E-03	6.00E-01
Tree fruit	0.157	0.04	0.27	1.00E-03	6.00E-01

Gardener type Average

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, 2009c) 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.

ⓘ The term 'TOX guidance report' within this handbook refers to reference Environment Agency 2009b. *Contaminants in Soil: Collation of Toxicological Data and Intake Values for Humans*. Report SC050021/SR2. Bristol: Environment Agency

ⓘ The term 'CLEA report' within this handbook and within the software refers to reference Environment Agency 2009c. *Updated technical background to the CLEA model*. Report SC050021/SR3. Bristol: Environment Agency

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 1.05) and its key differences to its predecessors (CLEA software version 1.04, CLEA software 1.03 beta and the CLEA UK software). This section of the scientific and technical guide focuses on the principles underpinning the CLEA model (Environment Agency, 2009d) 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 relevant toxicological values that are protective of human health. These are known as **Health Criteria Values (HCVs)** 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 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 HCVs) 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, 2009c).

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 where 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 HCVs, can be found in the TOX guidance report (Environment Agency, 2009b). HCVs describe a level of exposure to a chemical derived from toxicity and/or epidemiology data for the purposes of safeguarding human health. Most HCVs 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}).

HCVs 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 SGVs. 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, 2009c) 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 SGVs on this basis without reserving a minimum proportion of the TDI for exposure from land (Defra, 2008b; Environment Agency, 2009b). In the derivation of SGVs, this minimum proportion is set (Defra, 2008b) at 50 per cent (called the 50 per cent rule). This minimum TDSI for 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 fifty per cent of the TDI for individual assessment criteria, and no greater than that from soil for combined assessment criteria, ensuring that soil always contributes a minimum of half of the total exposure when combining pathways.

The TDSI calculation is implemented within the CLEA software as follows:

- In calculating the soil assessment criteria, the objective is to find the combination of soil ADE that equals the TDSI. 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 seek to run smoothly for both the individual and combined AC.

- If only a single HCV is known and it is a TDI, then the TDSI is calculated including background exposure from all routes.

- If an oral and an inhalation HCV is known and they are both a TDI, the oral background ADE is used in calculation of the oral TDSI and the inhalation background ADE is used in the calculation of the inhalation TDSI.

- The TDSI is calculated by subtracting the weighted average background exposure for all age classes included in the assessment from the relevant TDI. Varying proportions of background exposure may occur for individual age classes.

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

- In calculating ADE/TDSI ratios (in ratio mode), the soil ADE is fixed by the user-entered site data.

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, 2009b).

ⓘ 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	(Section 3.2 of CLEA report)
ii.	allotment land use	(Section 3.3 of CLEA report)
iii.	commercial land use	(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 pathway**s and a defined **critical receptor**.

For some contaminants, it might be appropriate to derive ,assessment criteria for the residential and allotment land use assuming lifetime exposure (age classes 1 to 18). One such example is cadmium, because it is the kidney burden of cadmium, accumulated over a prolonged period which is the key determinant of cadmium's toxicity to the kidney (Environment Agency 2009h and 2009i). The CLEA software includes a residential (lifetime exposure) or allotment (lifetime exposure) land use. The parameter values that describe each of these land uses are based on estimates representative of lifetime exposure.

The residential and allotment land use scenarios presented in the CLEA report include recommended values for estimating exposure for young children only (age classes 1 to 6). However, the report contains additional information on receptor and exposure characteristics that are appropriate for estimating lifetime exposure (age classes 1 to 18) for these standard land use scenarios.

This additional information has been used to estimate lifetime exposure characteristics; these exposure characteristics are summarised in Table 4.1 and Table 4.2. Where exposure characteristics for older children are not in the CLEA report, often because of a lack of underlying data, it has been assumed that:

- for children up to the age of 12 (age classes 7 to 12) the data for young children are most applicable;
- for children aged 12 to 16 (age classes 13 to 16) behaviour will be similar to adults.

Table 4.1 Default exposure characteristics for lifetime exposure for the standard residential land use.

Age class	Exposure frequencies (day year^{-1}) Soil / dust ingestion	Homegrown produce	Dermal Indoor	Dermal Outdoor	Inhalation Indoor	Inhalation Outdoor	Occupancy periods (hours day^{-1}) Garden	Indoor	Soil-to-skin AF (mg cm^{-2}) Indoor	Outdoor	Soil and dust ingestion rates (g day^{-1})
1	180	180	180	180	365	365	1	23	0.06	1	0.1
2	365	365	365	365	365	365	1	23	0.06	1	0.1
3	365	365	365	365	365	365	1	23	0.06	1	0.1
4	365	365	365	365	365	365	1	23	0.06	1	0.1
5	365	365	365	365	365	365	1	19	0.06	1	0.1
6	365	365	365	365	365	365	1	19	0.06	1	0.1
7	365	365	365	365	365	365	1	19	0.06	1	0.1
8	365	365	365	365	365	365	1	19	0.06	1	0.1
9	365	365	365	365	365	365	1	19	0.06	1	0.1
10	365	365	365	365	365	365	1	19	0.06	1	0.1
11	365	365	365	365	365	365	1	19	0.06	1	0.1
12	365	365	365	365	365	365	1	19	0.06	1	0.1
13	365	365	365	365	365	365	1	15	0.06	0.3	0.05
14	365	365	365	365	365	365	1	15	0.06	0.3	0.05
15	365	365	365	365	365	365	1	15	0.06	0.3	0.05
16	365	365	365	365	365	365	1	15	0.06	0.3	0.05
17	365	365	365	365	365	365	1	16	0.06	0.3	0.05
18	365	365	365	365	365	365	1	16	0.06	0.3	0.05

Table 4.2 Default exposure characteristics for lifetime exposure for the standard allotment land use.

Age class	Exposure frequencies (day year^{-1}) Soil / dust ingestion	Homegrown produce	Dermal Indoor	Dermal Outdoor	Inhalation Indoor	Inhalation Outdoor	Occupancy period (hours day^{-1}) Allotment	Soil-to-skin AF (mg cm^{-2}) Outdoor	Soil and dust ingestion rates (g day^{-1})
1	25	180	0	25	0	25	3	1	0.1
2	130	365	0	130	0	130	3	1	0.1
3	130	365	0	130	0	130	3	1	0.1
4	130	365	0	130	0	130	3	1	0.1
5	65	365	0	65	0	65	3	1	0.1
6	65	365	0	65	0	65	3	1	0.1
7	65	365	0	65	0	65	3	1	0.1
8	65	365	0	65	0	65	3	1	0.1
9	65	365	0	65	0	65	3	1	0.1
10	65	365	0	65	0	65	3	1	0.1
11	65	365	0	65	0	65	3	1	0.1
12	65	365	0	65	0	65	3	1	0.1
13	25	365	0	25	0	25	3	0.3	0.05
14	25	365	0	25	0	25	3	0.3	0.05
15	25	365	0	25	0	25	3	0.3	0.05
16	25	365	0	25	0	25	3	0.3	0.05
17	258	365	0	258	0	258	3	0.3	0.05
18	258	365	0	258	0	258	3	0.3	0.05

Table 4.3 presents default inhalation rates for all age classes according to age and sex for the allotment land use based on short-term exposure. This table extends the data presented in Table 4.15 in the CLEA report and has been calculated using the same methodology (Lordo *et al*., 2006; Environment Agency, 2009c).

Table 4.3 Default inhalation rates according to age and sex for the allotment land use, based on short-term exposure [1].

Age class	Inhalation rate [2] ($m^3\ day^{-1}$)	
	Female	Male
1	10.3	12.5
2	18.8	19.7
3	20.7	20.4
4	19.1	20.6
5	21.3	22.9
6	24.9	25.5
7 [3]	17.6	18.5
8 [3]	20.2	20.5
9 [3]	21.8	22.7
10 [3]	25.0	26.8
11 [3]	28.4	28.7
12 [3]	19.8	21.2
13 [3]	22.7	23.3
14 [3]	24.5	26.5
15 [3]	27.2	31.2
16 [3]	28.3	32.4
17 [4]	27.4	35.7
18 [4]	25.4	34.5

Notes: [1] This table extends information found in Table 4.15, of the CLEA report, to all age classes.
[2] Assuming an hourly rate for 24 hours.
[3] Assumes the balance between light and moderate activity is half-and-half.
[4] Assumes an adult spends two-thirds of their time undertaking moderate intensity activities and one-third light activities.

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 individuals 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 4.4. 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 4.4 Critical receptors used in the CLEA software.

Standard land use	Critical receptor	Age class
Residential	0 to 6-year old female child	1 to 6
Residential (lifetime exposure)	0 to 75-year old female	1 to 18
Allotments	0 to 6-year old female child	1 to 6
Allotments (lifetime exposure)	0 to 75-year old female	1 to 18
Commercial	16 to 65-year old female working adult	17

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

ⓘ Receptor data for the residential and allotment land uses are available within the software for all age classes. Residential and allotment land use data is available for age classes 1 to 6 only unless you select the lifetime exposure land use for which data is available for age classes 1 to 18.

ⓘ Complete data sets for commercial receptors are available within the software for age class 17 only. You should therefore not select a commercial receptor for any other age class unless you add the land use and receptor 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. Section 4.11 provides guidance on changing the default time period for calculation of the surface volatilisation factor.

> ⓘ 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 4.5.

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 4.5: Physiological characteristics.

Physiological characteristic	Description of use within the CLEA software
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 HCVs, 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 and for the allotment lifetime exposure land use, Table 4.3 of this report, the CLEA software handbook)	• 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 4.6.

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 4.6 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 4.6: Behavioural characteristics.

Land use characteristics	Description of use within the CLEA software
Exposure frequency (Section 2.1.2 and Section 3 of the CLEA report and for lifetime exposure land uses, section 4.3.4 of this report, the CLEA software handbook)	• 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 and for lifetime exposure land uses, section 4.3.4 of this report, the CLEA software handbook)	• 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.
Soil-skin adherence factor, indoors and outdoors (Section 8.1.1 of the CLEA report and for lifetime exposure land uses, section 4.3.4 of this report, the CLEA software handbook)	• Provides information on the amount of soil adhered to, or in intimate contact with the skin, over the contact period for a single event. • Used to estimate exposure to soil contamination from **dermal absorption**.
Soil and dust ingestion rate (Section 6.1 of the CLEA report and for lifetime exposure land uses, section 4.3.4 of this report, the CLEA software handbook)	• Provides information on the amount of soil and indoor dust ingested on a daily basis. • Used to estimate exposure to soil contamination from ingestion of soil and indoor dust (outdoors and indoors).
Consumption rate of homegrown produce (Section 4.4.5 of the CLEA report)	• Provides information on the amount of homegrown fruit and vegetables consumed per day. • Used to estimate exposure to soil contamination from consumption of contaminated homegrown produce.

ⓘ 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. Default generic datasets are provided in the software for chemicals for which updated TOX and SGV reports have been published to date. Physical-chemical properties 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). This can be corrected for in the CLEA software using the sub-surface soil to indoor air correction factor (see Section 4.6.7).

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 coefficient**s 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 (CIRIA, in press).

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).

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 decide which broad category a soil falls into based, for example, on trial pit logs or particle size determination. Figure 4.1 in the CLEA report has been provided for illustrative purposes only, further guidance on using the UK system can be found in Hodgson, 1997. 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.

The chemical concentration in soil solution is determined by the soil-water partition coefficient (K_d) and depends on soil type and pH (Environment Agency, 2009c). If you have entered a formula to specify the calculation of a **soil-to-plant concentration factor**/s that relies on SOM, SOM is used within the software to calculate plant uptake of contamination from soil (see section 4.6.3 for further information).

The default value used within the CLEA software (and in the derivation of Soil Guideline Values) is SOM content of 6 per cent. This is an average value for sandy loam soil calculated from analysis of the HORIZON Hydraulics library data held by the National Soil Resources Institute (NSRI) based at Cranfield University. The NSRI holds very detailed descriptions of soil property data for a large number of soils sampled across England and Wales.

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

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

ⓘ 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.

ⓘ 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.

ⓘ 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 (f_{oc}). 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 f_{oc}, the conversion used is:

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

ⓘ % 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 (2008), 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 relative bioavailability is one (that is, the absolute bioavailability of the chemical in the soil sample is the same as the absolute bioavailability in the media used in the relevant toxicological studies on which the HCV is based). You can find further information on these terms and their use in land contamination risk assessments on the Environment Agency's website at www.environment-agency.gov.uk.

ⓘ Unlike CLEA 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 m^3 mol^{-1}. You can calculate the air-water partition coefficient (K_{aw}), in units of cm^3 cm^{-3}, at ambient soil temperature, 283K, and enter this value directly into the CLEA software chemical database. Environment Agency (2008) provides methods for calculating K_{aw} at ambient soil temperature. (K_{aw} was formerly referred to as HLC dimensionless within the CLEA model).

ⓘ 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 4.7.

Table 4.7: Exposure pathways in the CLEA software.

Routes of entry	Exposure pathways
Oral	Direct soil ingestion
	Direct dust ingestion
	Consumption of homegrown produce
	Consumption of soil attached to homegrown produce
Dermal	Indoor dermal uptake
	Outdoor dermal uptake
Inhalation	Indoor dust inhalation
	Outdoor dust inhalation
	Indoor vapour inhalation
	Outdoor vapour inhalation

ⓘ 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/showering 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. The data is contained within the 'Land Uses' database.

- In the context of land contamination, relative bioavailability is the comparison of the extent of absorption between two or more forms of the same chemical (such as lead carbonate versus lead acetate), or the same chemical administered in different media (such as food, soil, water) or at different doses. The software assumes that the soil relative bioavailability is one (that is, the absolute bioavailability of the chemical in the soil sample is the same as the absolute bioavailability in the media used in the relevant toxicological studies on which the HCV is based). The data is contained within the 'Chemicals' database of the CLEA software. See Section 4.1 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 Uses' 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 relative bioavailability by:

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

ⓘ 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.

ⓘ 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.

ⓘ 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.

ⓘ 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.

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.

Inorganic chemicals:
We recommend that you always review the plant uptake behaviour of the contaminant of concern and use literature or site-based data, if available. PRISM is a conservative generic model. We recommend that a review of the plant uptake literature will greatly assist its parameterisation.

The section 'How parameter values can be changed in the software' includes an explanation of how you can add a formula into the software to calculate soil-to-plant concentration factors (that rely on soil pH or SOM) or add a site-measured media chemical concentration according to the fruit or vegetable type.

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 H_20. 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 (K_d) 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:
The section 'How parameter values can be changed in the software' includes an explanation of how you can add a formula into the software to calculate soil-to-plant concentration factors (that rely on soil pH or SOM) or add a site-measured media chemical concentration according to the fruit or vegetable type.

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. The default value used in the derivation of SGVs is SOM content of 6 per cent (see Section 4.5.4). The SOM value used within the software is 6 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_20. 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.

Further information on the approach for organic chemicals is provided in Section 7.2.2 of the CLEA report.

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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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 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 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 and root-shoot/root-root/root-tuber/root-fruit correction 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 soil organic matter (SOM) or soil pH by:

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

You can change parameter values for the soil-to-plant concentration factor or you can add the chemical concentrations for the appropriate fruit and vegetable types from site-specific studies by:

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

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

iii. entering site-measured chemical concentrations for the edible portions of the fruit and vegetable types from site-specific studies, 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. Site-measured fruit and vegetable chemical concentrations entered in Step 3 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.

iv. In both the 'Chemicals' database and 'Chemical Data' you can either:
    1. make changes to the parameter data that is used to calculate a soil-to-plant concentration factor; or
    2. add a numerical value for a soil-to-plant concentration factor; or
    3. add a formula to specify the exact calculation that relies on either pH or the Soil Organic Matter content. Formulas must be entered in the format "= CONST x soil_pH" or "= CONST x som" provided that answer is not less than zero.

    An example is provided in a grey text box in Section 3.4.5.

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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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.

- In the context of land contamination, relative bioavailability is the comparison of the extent of absorption between two or more forms of the same chemical (such as lead carbonate versus lead acetate), or the same chemical administered in different media (such as food, soil, water) or at different doses. The software assumes that the soil relative bioavailability is one (that is, the absolute bioavailability of the chemical in the soil sample is the same as the absolute bioavailability in the media used in the relevant toxicological studies on which the HCV is based). The data is contained within the 'Chemicals' database of the CLEA software. See Section 4.1 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 relative bioavailability 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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 0.5. 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.

ⓘ The maximum soil-to-skin adherence factor that is used within the software for a standard land use is 1 mg cm^2. 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 cm^2. 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.

ⓘ 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.

ⓘ 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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, Table 4.15 for allotment land use and Table 4.3 of this report, the CLEA software handbook, for the allotment lifetime exposure 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 (m^3 $hour^{-1}$) for each hour of **site occupancy**. By averaging over 24 hours, a daily inhalation rate of air at the site can be calculated (m^3 day^{-1}).

- In the context of land contamination, airborne dust relative bioavailability is the comparison of the extent of absorption between two or more forms of the same chemical (such as lead carbonate versus lead acetate), or the same chemical administered in different media (such as food, soil, water) or at different doses. The software assumes that the airborne dust relative bioavailability is one (that is, the absolute bioavailability of the chemical in the respirable fraction of a soil sample is the same as the absolute bioavailability in the media used in the relevant toxicological studies on which the HCV is based). The data is contained within the 'Chemicals' database of the CLEA software. See Section 4.1 for further information.

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 further information. In the absence of literature values, the CLEA model uses a generic value of 0.5. 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 relative bioavailability 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. For further guidance on the site-specific assessment of this pathway please refer to *The VOCs Handbook* (CIRIA, in press). 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 CIRIA, in press, and use additional lines of evidence.

! The vapour intrusion of soil gas from the subsurface into overlying buildings remains a highly uncertain scientific area (CIRIA, in press).

! 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 and CIRIA, in press, for further information). The CLEA software provides the user with an option to correct for this over prediction but extreme caution should be used.

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

ⓘ Advective 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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_20. Air-filled porosity is the remainder of the pore space. Porosity is important for the mobility of a chemical through soil by diffusion or **advection** transport processes. 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.
- Effective air permeability of soil varies according to its properties including porosity, hydraulic conductivity, and water content (Environment Agency, 2002; CIRIA, in press). Advective air movement of chemicals within unsaturated soils is controlled by its effective air permeability. It is used to calculate the steady-state attenuation coefficient between soil and indoor air. Generic values within the software are calculated using the soil properties of the soil type selected. Equations for calculating the effective air permeability are provided in Appendix 1 of the CLEA report.
- 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 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, Table 4.15 for allotment land use and Table 4.3 of this report, the CLEA software handbook, for the allotment lifetime exposure 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 (m^3 $hour^{-1}$) for each hour of **site occupancy**. By averaging over 24 hours, a daily inhalation rate of air at the site can be calculated (m^3 day^{-1}).

- <u>Occupancy period (indoors)</u> 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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 <u>air-filled and water-filled soil porosity</u> 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 <u>diffusion coefficient in air and water</u> and <u>air-water partition coefficient</u> 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 <u>living space height (above/below ground)</u>, <u>building footprint</u>, <u>living space air exchange rate</u>, <u>foundation thickness,</u> and <u>floor crack area</u> 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 <u>effective air permeability</u> and <u>depth to top of source (beneath building)</u> by:

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

You can change parameter values for <u>default soil gas ingress rate</u> 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).

You can change parameter values for <u>inhalation rate</u> 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.

ⓘ 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 (2008) 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.

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

Accounting for conservatism in the estimation of indoor vapour intrusion

Many environmental models, including the CLEA model, predict chemical partitioning in soil systems using Henry's Law constant (Environment Agency, 2009c). Using Henry's Law constant to model partitioning into the soil vapour phase results in a significant over prediction of the attenuation coefficient for petroleum hydrocarbons by at least a factor of ten higher (and up to a factor of one thousand higher) than are likely to be measured on site (CIRIA, in press; Environment Agency, 2009c).

The CLEA software provides you with an option to correct the predicted finite source attenuation coefficient to account for conservatism in the estimation of indoor vapour intrusion using the Johnson and Ettinger model.

You can choose to calculate the predicted finite source attenuation factor using an empirical correction factor 'Sub-surface soil to indoor air correction factor'. You can do this in the following ways;

1. You can add a chemical specific empirical correction factor into the chemical database. A value of 1 assumes there is no correction. A value greater than 1 reduces the attenuation factor by division.
2. You can derive site specific assessment criteria based on temporary amendments to the chemical specific empirical correction factor in 'Chemical Data' in advanced mode, Step 4.

4.6.8 Outdoor vapour inhalation

The approach to modelling ambient vapour inhalation used for Soil Guideline Values is described in Section 10 of the CLEA report.

In the derivation of Soil Guideline Values, the CLEA model assumes that the source of outdoor air contamination is present as a continuous layer from the surface to a depth of 100cm (Environment Agency, 2009c). Vapour emissions to air are modelled using the surface vaporisation model developed by the USEPA for the derivation of Soil Screening Levels (USEPA, 1996) and based on the earlier work of Jury *et al*. (1983 and 1990).

An important factor in the surface emission model is the time period over which the calculated emission flux is averaged. The recommended default value is the exposure duration (USEPA, 1996; Environment Agency, 2009c) although the software includes the option to change this value independently (see Section 4.11). In the infinite source model, the soil vapour is assumed to diffuse to the soil surface to replace that lost by volatilisation to the atmosphere. As noted by USEPA (1996) the model predicts an exponential decay curve over time once system equilibrium has been achieved. As surface concentrations are depleted, the high initial flux rate decreases and the slower long-term flux is characterised by the rate of diffusion from deeper soil layers. It is the slower flux that is important for assessing long-term exposure. However, it is important to note that the algorithm will tend to under predict emissions during the initial release period and may not be suitable for use in some circumstances (such as in the assessment of fresh spills).

The CLEA software also includes an algorithm suitable for estimating vapour emissions from a sub-surface vapour source. This is based on the screening algorithm recommended in the Risk-Based Corrective Action (RBCA) guidance (ASTM, 2000). An important assumption in using a sub-surface vapour source is that the soil layer between the surface and top of contamination is uncontaminated. The validity of this assumption is often difficult to check where the sub-surface source is assumed to be close to the surface.

The CLEA software assumes that the sub-surface emission model should be applied when the depth to the top of source exceeds 100cm. At shallower depths, the surface emission model will be used. This is a relatively arbitrary choice of depth that allows for a smooth transition in calculated air concentrations between the two emission algorithms. At very shallow depths, the sub-surface model estimates higher outdoor air concentrations than the surface model which is counter intuitive.

In addition to the infinite source options described above, the CLEA software allows the user to specify whether a finite source is assumed.

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:

- <u>Exposure frequency of inhalation of vapours outdoors</u> 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. The data is contained within the 'Land Uses' database of the CLEA software.
- <u>Air-filled and water-filled soil porosity</u> 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 H_20. Air-filled porosity is the remainder of the pore space. Porosity is important for the mobility of a chemical through soil by diffusion or advection transport processes. 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.
- <u>Diffusion coefficients in air and water</u> 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 software.
- <u>Air-water partition coefficient</u> 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.

- Time average period for surface emissions is the averaging time for surface emission vapour flux and is used to calculate the volatilisation factor from surface soil to ambient air. It describes the period over which the average emission flux is calculated. The default is to assume that this averaging time is equal to the exposure duration, for example, for the residential and allotment land-use scenarios the value used is six years. However, this emission period may be calculated separately from exposure duration. The data is contained within the 'Soil and Building Data' in advanced mode Step 4 of the software. Section 4.11 provides further information.

- 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, Table 4.15 for allotment land use and Table 4.3 of this report, the CLEA software handbook, for the allotment lifetime exposure 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 ($m^3\ hour^{-1}$) for each hour of site occupancy. By assuming an hourly rate for 24 hours, a daily inhalation rate can be calculated ($m^3\ day^{-1}$).

- 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 and for lifetime exposure land uses, Table 4.1 and Table 4.2 of this report, the CLEA software handbook. 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 10 cm, which is broadly consistent with the contamination being at the surface (see also Section 10.2 of the CLEA report). Up to a depth of 100 cm, the surface vapour model is assumed. Where this value is changed to be greater than the generic value of 100 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:

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 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 values for depth to top of source (no building) and time average period for surface emissions 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, 2008).

ⓘ 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. Soil gas ingress rate used to calculate the steady-state attenuation coefficient (alpha) between soil and indoor air.

You can chose 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 25 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 loam 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 150 $cm^3 s^{-1}$ 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 loam 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.

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 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.

- 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 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.

- 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 4.8 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. The default depth of 65cm within the software is calculated by adding 50cm (the default depth from beneath the building to the top of contamination) to 15cm (the default value for the foundation slab thickness).

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. 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 0 cm for depth to the top of the contaminant source (depth to top of source, no building) can be temporarily changed. Note that this will have no effect on the choice of vapour model until the depth exceeds 100 cm. Up to 100 cm, the surface vapour model described in Section 10 of the CLEA report is used. At depths greater than 100 cm, the sub-surface vapour model described in Equation 4.1 below is used in preference to the surface model. Below 100 cm, the depth will not affect the estimated vapour concentration because the surface emission model assumes a continuous layer from the surface. At depths greater than 100 cm, the estimated vapour concentration will decrease with increasing depth. The subsurface volatilisation factor (VF) is calculated with Equation 4.1 implemented within the CLEA software using the ASTM (2000) approach.

You should only change the depth to the top of the contaminant source (depth to top of source, no building) to a value greater than 100cm if there is no contamination between the sub-surface contaminant source (at a depth greater than 100 cm) and the soil surface.

Equation 4.1

$$VF = \frac{1}{1 + \dfrac{\mathrm{Q/C_{wind}}\ L_s \times \dfrac{1}{10000} m^2 cm^{-2} \times 1000000\, cm^3 m^{-3} \times \dfrac{1}{1000} kg\ g^{-1}}{D_{eff}} \dfrac{K_{sw}}{K_{aw}}}$$

Where: VF is the volatilisation factor from subsurface to ambient air, g cm^{-3}
Q/C_{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_{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 does not depend on the soil vapour concentration directly and therefore cannot be used with a fixed soil gas concentration.

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.

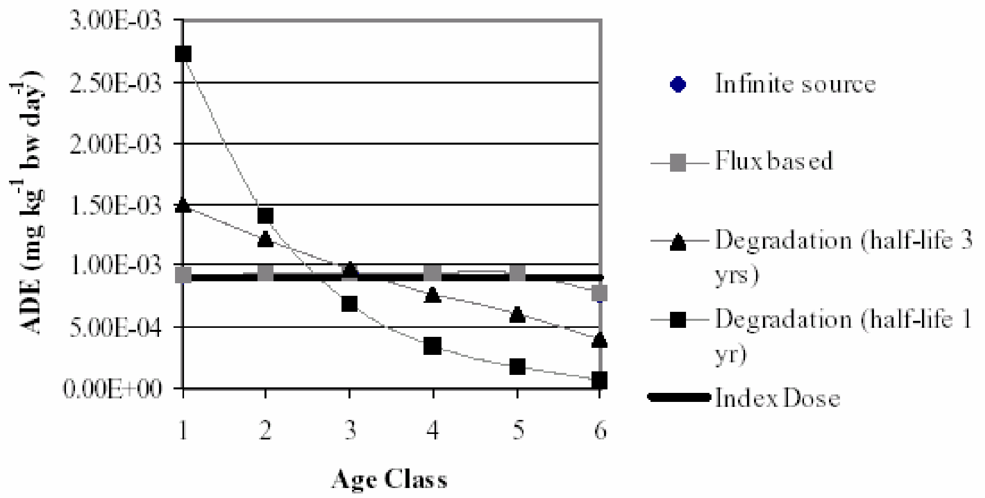
The CLEA software calculates indoor and outdoor vapour concentrations, assuming a finite source, according to the equations in Sections 4.9.1 and 4.9.2 respectively. The software also assumes that the thickness of the contaminant layer is 200cm unless you have made changes to this within step 4 'Advanced Settings'.

ⓘ The finite source model does not depend on the soil vapour concentration directly and therefore cannot be used with a fixed soil gas concentration.

ⓘ 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 curve and the greater the front loading (and the initial exposure) will be compared to the, for example, estimated 6-year average.

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: τ_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 4.3 and 4.4]
β is an empirical coefficient, dimensionless [see Equation 4.5]
ψ 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

$$Z_{crack} = (H_{cellar} + L_{crack}) \times 100 \, cm \, m^{-1}$$

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

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

Where: β is an empirical coefficient, dimensionless
D_{eff} is the effective diffusion coefficient for unsaturated soils, $cm^2\ s^{-1}$
A_b is the area of enclosed floor and walls below ground, cm^2
L_T is the source-building separation, cm [see Equation 4.3]
Q_s is the soil gas ingress rate, $cm^3\ s^{-1}$
L_{crack} is the foundation thickness, cm
D_{crack} is the effective diffusion coefficient through the cracks, $cm^2\ s^{-1}$ [= D_{eff}]
A_{crack} is the floor crack area, cm^2

Equation 4.6

$$\psi = \frac{D_{eff} C_{vap}}{L_T^{\ 2} \rho_s C_s}$$

Where: ψ is an empirical coefficient, s^{-1}
D_{eff} is the effective diffusion coefficient for unsaturated soils, $cm^2\ s^{-1}$
C_{vap} is the chemical vapour concentration at source, $mg\ cm^{-3}$
L_T is the source-building separation, cm [see Equation 4.3]
ρ_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 (τ) is greater than the time to source depletion (τ_d).

Equation 4.7

$$C_{building} = \frac{\rho_s C_s d_s A_b}{Q_b \tau} \times 1000000\ cm^3 m^{-3}$$

Where: $C_{building}$ is the time averaged indoor air concentration, $mg\ m^{-3}$
ρ_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, $cm^3\ s^{-1}$
τ is the exposure duration, s

The time-averaged indoor air concentration is calculated using Equation 4.8 when the exposure duration (τ) is less than the time to source depletion (τ_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

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

Where: α is the time-averaged finite source attenuation coefficient, dimensionless
ρ_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_{vap} is the chemical vapour concentration at source, mg cm^{-3}
τ is the exposure duration, s
L_T is the source-building separation, cm [see Equation 4.3]
β is the empirical coefficient, dimensionless [see Equation 4.5]
ψ is the empirical coefficient, s^{-1} [see Equation 4.6]

ⓘ Johnson and Ettinger (1991) identified limitations in the applicability of their finite source solution; most notable was the conclusion that it represented "*a reasonable assumption for diffusion-dominated transport to the building-soil interface, but not valid for convection-dominated transport from contaminated soil adjacent to a building floor*."

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

$$VF = \frac{\mathrm{d}_s \rho_s}{Q / C_{wind} \times \tau}$$

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
ρ_s is the dry soil bulk density, g cm^{-3}
Q/C_{wind} is the air dispersion factor, g m^{-2} s^{-1} per g cm^{-3}
τ is the exposure duration, s

4.10 Changing the relative bioavailability

4.10.1 Introduction

The scientific assessment of the risks posed to human health by soil contamination involves consideration of both chemical toxicity and estimated or observed levels of exposure.

Health criteria values (HCVs) are toxicological benchmarks or guidelines to a risk assessor on the level of long-term exposure to individual chemicals in soil that are tolerable or pose a minimal risk (Environment Agency, 2009b). They are established from a review of the evidence from occupational and environmental epidemiological studies, animal studies, and from scientific understanding of the mechanisms of absorption, transport, metabolism, excretion and toxicity of chemicals within the human body.

Combined with estimates or measurements of exposure (such as those generated by the CLEA Software), HCVs can be used by risk assessors and risk managers to consider whether land affected by contamination requires further investigation, assessment, and/or remediation (Environment Agency, 2009a, 2009c). Based on these principles, we have published a series of Soil Guideline Values (SGVs) for use in human health risk assessment. SGVs are an example of generic assessment criteria, which can be used to screen out sites where a significant risk to health is unlikely, as part of a tiered approach to assessing land contamination (Defra and Environment Agency, 2004).

Further information on how SGVs have been derived can be found in *Using Soil Guideline Values* (Environment Agency, 2009a), and the framework documents *Updated technical background to the CLEA model* (Environment Agency, 2009c) and *Human health toxicological assessment of contaminants in soil* (Environment Agency, 2009c).

4.10.2 Human exposure and bioavailability

Humans may be exposed to chemicals via a number of routes and the various physicochemical and biological factors that may affect absorption mean that different chemicals will gain entry to the body to different extents (Environment Agency, 2009b). For example, following ingestion, unless the chemical is readily absorbed through the lining of the mouth it will be swallowed and move through the gastrointestinal tract. From there it may be absorbed into the body and transported to the liver, or it may be excreted. Some chemicals are more readily absorbed from the gut than others, and there are a number of factors (such as the presence or absence of food in the gut) that can influence the extent of absorption. Once in the liver, some chemicals will be largely returned to the gastrointestinal tract via bile, while others will mostly enter the systemic circulation.

When investigating a chemical's toxicity and considering how the degree of exposure affects the biological response produced, a suitable measure for quantifying the exposure is needed. The most commonly used measure of exposure in toxicology is the intake dose (usually abbreviated to "dose"). This is normally expressed on a bodyweight basis, i.e. the amount of chemical per unit of bodyweight, for example, milligrams per kilogram bodyweight per day (Environment Agency, 2009b). However, toxicologically, it is the exposure of the target tissue or organ that is the actual determinant of toxicity (Environment Agency, 2009b). If a chemical is poorly absorbed by the gut, or returned to the gut in the bile after absorption, only a small amount will be available within the body to cause toxicity at the target organ.

The proportion of an intake dose of a chemical that is absorbed by the body and reaches systemic circulation unchanged (that is, without undergoing first-pass metabolism) is referred to as the chemical's bioavailable fraction, or ***absolute bioavailability*** (ABA) (Environment Agency, 2009b). The amount of chemical that this fraction represents is known as the systemic dose. Hence, the absolute bioavailability of a chemical will be between zero (if none of a chemical reaches the systemic circulation intact) and one (if all of the chemical reaches the systemic circulation intact), although it can also be reported as a percentage (Environment Agency, 2009b).

Absolute bioavailability is the fraction of a chemical that is absorbed by the body through the gastrointestinal system, pulmonary system, and/or the skin. It can be expressed as the ratio of the absorbed dose to the intake dose.

$$ABA = \frac{D_s}{D_i}$$

Where ABA is the absolute bioavailability of a chemical in dimensionless form, D_s is the absorbed dose in mg kg^{-1} BW day^{-1}; and D_i is the intake dose in mg kg^{-1} BW day^{-1}.

4.10.3 Relative bioavailability

There is increasing interest in many countries in the potential for information on the bioavailability of a chemical to be used to refine risk assessments. However, in many cases we know little about the absolute bioavailability of chemicals in environmental media such as soil and dust.

Like other toxicological exposures, HCVs are usually reported in terms of an intake dose. Oral HCVs are often derived from studies in which the intake dose is reported as the amount of chemical ingested via the diet or drinking water. In assessing risks from soil using such HCVs, we therefore implicitly assume that the chemical will be taken up into the body from soil to the same extent as from the medium of exposure (for example from food or water) in the study used to derive the HCVs (Environment Agency, 2009b). Yet, we know that for many chemicals, absolute bioavailability (ABA) varies due to differences in media characteristics and the physical and chemical form of the substance (USEPA, 2007a). This is especially true for metals and metalloids (USEPA, 2007a). As a result, the ABA of a chemical in soil may be higher or lower than its ABA from the test media used in the relevant toxicological study, leading to an over- or under-estimation of risk.

In assessing risks from soil contamination, we are therefore interested in whether the absolute bioavailability of the chemical in the soil sample (ABA_{soil}) is greater or less than that measured in the media used for the toxicological study (ABA_{tox}). The relationship between these two bioavailabilities is also known as the ***relative bioavailability*** of a chemical (RBA), with the comparison of absorption based on differences in media, chemical form or concentration (USEPA, 2007a). While the ABA can never exceed one (i.e. 100 per cent), RBA may be either greater than or less than one (USEPA, 2007a). [3]

[3] Relative bioavailability may also be referred to as the relative absorption fraction (RAF) or the relative bioavailability adjustment (RBA) in some references.

Relative bioavailability is the comparison of the extent of absorption between two or more forms of the same chemical (such as lead carbonate versus lead acetate), or the same chemical administered in different media (such as food, soil, water) or at different doses.

$$RBA_{soil,tox} = \frac{ABA_{soil}}{ABA_{tox}}$$

Where $RBA_{soil,tox}$ is the bioavailability from the soil sample relative to the bioavailability from the media used in the toxicological studies in dimensionless form; ABA_{soil} is the absolute bioavailability of the chemical in soil in dimensionless form; and ABA_{tox} is the absolute bioavailability of the chemical in the media used in the toxicological studies in dimensionless form.

When a reliable site-specific RBA value has been determined, it may be used to adjust the estimated exposure from soil by the relevant pathways before comparison with the applicable HCVs. For example, a site-specific $RBA_{soil,tox}$ based on ingested soil and dust is applicable only to relevant chemical forms and the direct soil and dust ingestion exposure pathway for comparison (usually) with the oral HCVs. It would not be appropriate to apply the same $RBA_{soil,tox}$ either to other oral pathways such as the consumption of homegrown produce, even though it is also an ingestion pathway, or to dermal or inhalation routes.

In the context of the CLEA software, the $RBA_{soil,tox}$ value for the oral route applies only to the direct soil and dust ingestion pathway and the indirect ingestion of soil attached to vegetables pathway. Similarly, a $RBA_{soil,tox}$ value for the inhalation route applies only to the inhalation of soil-derived dust either indoors or outdoors. The $RBA_{soil,tox}$ value can be used to adjust the average daily exposure (ADE) from soil according to the equation in the textbox below, which has been adapted from Environment Agency (2009c).

Adjusting exposure estimates with relative bioavailability (RBA) values

The CLEA software takes into account $RBA_{soil,tox}$ for the oral and inhalation routes in calculating average daily exposure (ADE) using the expanded equation below, which is adapted from Equation 2.1 in *Updated technical background to the CLEA model* (Environment Agency, 2009c). Dermal uptake is already accounted for by using the dermal absorbed fraction (ABS_d). The $RBA_{soil,tox}$ is not applied to all ingestion and inhalation pathways.

$$ADE = \frac{(IR_{ing} \times RBA_{soil,tox} \times EF_{ing} \times ED_{ing})}{BW \times AT} + \frac{(IR_{inh} \times RBA_{soil,tox} \times EF_{inh} \times ED_{inh})}{BW \times AT} + \frac{(IR_{derm} \times ABS_d \times EF_{derm} \times ED_{derm})}{BW \times AT}$$

Where ADE is the average daily human exposure to a chemical from soil, mg kg^{-1} bw day^{-1}
IR is the chemical intake rate, mg day^{-1}
EF is the exposure frequency, days $year^{-1}$
ED is the exposure duration, year
BW is the human body weight, kg
AT is the averaging time, days
$RBA_{soil,tox}$ is the bioavailability from the soil sample relative to the bioavailability from the media used in the toxicological studies in dimensionless form. $RBA_{soil,tox}$ applies only to the chemical intake rate (IR) via specified exposure pathways and differs between oral and inhalation routes
ABS_d is the dermal absorption fraction, dimensionless

The subscripts *ing*, *inh*, and *derm* apply to the ingestion, inhalation and dermal contact routes respectively.

Absolute and relative bioavailability testing involves *in vivo* (live animal model) studies. For example, the USEPA recommend a juvenile swine test for use in estimating the bioavailability of lead in soil to children (USEPA, 2007b). The *in vivo* test involves administering lead-contaminated soil to juvenile swine and measuring the resultant lead concentration in a number of body compartments including blood, liver, kidney, and bone (USEPA, 2007b). However, for many contaminated sites *in vivo* testing would be impractical because of time and cost constraints. In addition, it also raises ethical issues. The concept of *in vitro* (artifical, non-animal) testing has therefore been of increasing interest to researchers and regulatory authorities as a surrogate for animal testing.

4.10.4 Bioaccessibility and *in vitro* tests

Over the past decade, there has been considerable interest from regulators and researchers in developing tests that might quantify the potentially decreased bioavailability of chemicals in soil compared to other media (such as food, drinking water), so that this can be taken into account in health risk assessments (Ruby *et al*., 1999; Environment Agency and British Geological Survey, 2003a, 2003b; DHI, 2005; USEPA, 2007a). In the UK, there has been a particular interest in the bioavailability of arsenic in soils because of the large areas of land where its concentration is (naturally) elevated (Farago *et al*., 2003; Palumbo-Roe *et al*., 2005; Cave *et al*., 2007; Wragg *et al*., 2007; Appleton *et al*., 2008).

The most commonly used site-specific approach to considering arsenic bioavailability in soil is an *in vitro* test (Environment Agency and British Geological Survey, 2003a, 2003b; Environment Agency, 2006a). Two different types of *in vitro* test have been proposed:

- chemical extraction tests that equate to 'easily extractable metals';
- tests that try to mimic biochemical conditions in the human/animal gastrointestinal tract.

In vitro tests such as those used for arsenic or lead do not measure directly the absolute or relative bioavailability of a chemical in soil. The aim of these tests is to try to measure the ***bioaccessibility*** of a chemical (F_B), which is defined as the fraction released from soil by physiological processes (such as digestion) into solution and which is potentially available for subsequent absorption by the body through for example, the linings of the gut or lung wall (Environment Agency and British Geological Survey, 2003a; Oomen *et al*., 2006; USEPA, 2007a).

Oral bioaccessibility (F_B) is the fraction of a substance that is released from the soil during processes like digestion into solution, making it available for uptake by the body (Environment Agency and British Geological Survey, 2003a).

Oral bioaccessibility can be expressed as an absolute bioaccessible concentration in soil (e.g., mg kg^{-1}) or as a fraction of the total concentration in soil.

$$F_B = \frac{C_{released}}{C_{soil}}$$

Where F_B is the oral bioaccessible fraction of a chemical in soil; $C_{released}$ is the amount of chemical released from soil in mg kg^{-1} soil; and C_{soil} is the initial total amount of a chemical in soil in mg kg^{-1}.

Bioaccessibility is relevant to bioavailability, since it represents a step in the overall process of human absorption of a chemical (USEPA, 2007a; Hagens *et al*., 2008). Since solubilisation is usually required for absorption of a substance across a biological membrane, poorly soluble forms of a chemical, with low measured bioaccessibility, may also have low bioavailability (USEPA, 2007a). In certain circumstances, if the solubility of a substance is the controlling factor in overall absorption then bioaccessibility may be a good predictor of bioavailability (USEPA, 2007a).

Oomen *et al*. (2006) proposed that the oral bioavailability of a substance could be divided conceptually into three major processes (see also text box below). This could apply to the ingestion of any contaminated media including food, drinking water, and soil. After soil ingestion, the chemical may be partially or totally released into solution from soil during digestion in the gastrointestinal system. This is the oral bioaccessible fraction (F_B) and represents the maximum amount of the substance available for absorption through the gastro-intestinal wall. However, not all released substance may be transported across the gastrointestinal wall. F_A is the fraction of bioaccessible chemical that is absorbed across the gastrointestinal wall and transported to the liver. Contaminants may be metabolised within the gastrointestinal wall or the liver, which is referred to as first-pass metabolism, or they may be excreted. F_H is the fraction of a chemical that passes through the liver intact and enters systemic circulation, where it may be distributed to other parts of the body. Collectively, these three processes combine to represent the ABA of a chemical from a specific media (Oomen *et al*., 2006).

Oral bioaccessibility and bioavailability

Oomen *et al*. (2006) proposed that the absolute oral bioavailability of a substance (ABA) could be mathematically described by three major processes. This could apply to the ingestion of any contaminated media, including food, drinking water, and soil:

$$ABA_{soil} = F_B \times F_A \times F_H$$

Where ABA_{soil} is the absolute oral bioavailability of a chemical in soil in dimensionless form; F_B is the oral bioaccessible fraction of a chemical in soil; F_A is the fraction of a solubilised chemical transported across the gastrointestinal wall into systemic circulation; and F_H is the fraction absorbed that does not undergo first pass metabolism in the intestinal epithelium and/or the liver.

The Oomen *et al*. (2006) approach can also be expressed in terms of relative bioavailability by substituting for ABA_{soil}.

$$RBA_{soil,tox} = \frac{F_B \times F_A \times F_H}{ABA_{tox}}$$

Where $RBA_{soil,tox}$ is the relative bioavailability between the soil sample and the media used in the toxicological studies in dimensionless form; ABA_{soil} is the absolute bioavailability of the chemical in soil in dimensionless form; F_B is the oral bioaccessible fraction of a chemical in soil; F_A is the fraction of a solubilised chemical transported across the gastrointestinal wall into systemic circulation; F_H is the fraction absorbed that does not undergo first pass metabolism in the intestinal epithelium and/or the liver; and ABA_{tox} is the absolute bioavailability of the chemical in the media used in the toxicological studies in dimensionless form.

Example application: Arsenic
In the specific case of arsenic, the terms oral bioaccessible fraction (F_B) and relative bioavailability ($RBA_{soil,tox}$) are used by some practitioners interchangeably. In general this is incorrect because these terms do not share the same definition. However, in the particular case of arsenic the mathematical relationship between the two parameters can be simplified to demonstrate that they are approximately equivalent.

The oral Index Dose (ID) for arsenic is based on the epidemiology of arsenic in drinking water. Absorption of soluble arsenic salts in drinking water is understood to be high, perhaps more than 95% (ATSDR, 2007; Environment Agency, 2009g). Therefore, the absolute bioavailability of arsenic (ABA_{tox}) in the studies on which the ID is based can be assumed to be close to 1 (or 100 per cent). If ABA_{tox} is close to 1, then it follows that bioaccessibility of arsenic from water (F_B), absorption of arsenic in solution within the gastro-intestinal system (F_A) and the fraction of the absorbed dose that reaches the systemic circulation (F_H) must all also be approximately 1. As a result, using the relationship proposed by Oomen *et al*. (2006) it can be shown that for arsenic in soil:

$$RBA_{soil,tox} = \frac{F_B \times 1 \times 1}{1}$$

This equation simplifies to:

$$RBA_{soil,tox} = F_B$$

For other substances the relationship is not so straightforward (Ruby *et al*., 1999).

The approach proposed by Oomen *et al*. (2006) can also be used to derive a relationship between the relative bioavailability of a chemical ($RBA_{soil,tox}$) and its bioaccessibility (F_B). (See the textbox 'Oral bioaccessibility and bioavailability'). This equation demonstrates that it is not a straightforward task to use bioaccessibility data from soils as a surrogate for relative bioavailability in refining health risk assessments, particularly as in many cases parameters such as F_B, F_A, F_H, and even ABA_{tox}, are poorly understood for many chemicals.

ⓘ Information on the Environment Agency's current view on the use of *in vitro* tests in the assessment of risks to health from chemicals in soil are available on our website at www.environment-agency.gov.uk.

ⓘ The terms oral bioaccessibility and relative bioavailability are often used interchangeably. In general this is incorrect as these two terms do not share the same definition. However, in the specific case of arsenic, the mathematical relationship between the two parameters can be simplified to demonstrate that they are approximately equivalent.

ⓘ There is very little technical guidance concerning inhalation bioaccessibility, which is the bioaccessibility of the respirable fraction of the soil. You should be very cautious when considering changes to this airborne dust relative bioavailability within the software.

4.11 Changing the default time period for calculation of the surface volatilisation factor

In the derivation of Soil Guideline Values, the CLEA model assumes that the source of outdoor air contamination is present as a continuous layer from the surface to a depth of 100cm (Environment Agency, 2009c). Vapour emissions to air are modelled using the surface vaporisation model developed by the USEPA for the derivation of Soil Screening Levels (USEPA, 1996) and based on the earlier work of Jury *et al*. (1983 and 1990).

An important factor in the surface emission model is the time period over which the calculated emission flux is averaged. The recommended default value is the exposure duration (USEPA, 1996; Environment Agency, 2009c) and the software includes the option to change this value independently.

In the infinite source model, the soil vapour is assumed to diffuse to the soil surface to replace that lost by volatilisation to the atmosphere. As noted by USEPA (1996), the model predicts an exponential decay curve over time once system equilibrium has been achieved. As surface concentrations are depleted, the high initial flux rate decreases and the slower long-term flux is characterised by the rate of diffusion from deeper soil layers. It is the slower flux that is important for assessing long-term exposure. However, it is important to note that the algorithm will tend to under predict emissions during the initial release period and may not be suitable for use in some circumstances (such as in the assessment of fresh spills).

Within the CLEA software you can set the exposure duration that is used in the surface soil volatilisation factor model independently from the exposure duration that is calculated using the selections for Age Class that you have made in Step 2. You can do this in site-specific assessment, advanced mode, Step 4 Soil and Building Data by changing the time average period for emission fluxes. By making changes to this value the CLEA software will over ride the default exposure duration for calculation of the surface soil volatilisation factor.

ⓘ Only the volatilisation factor for surface soils depends explicitly on the exposure duration. Controlling physical factors for sub-surface sources including the models for indoor and ambient air used in the CLEA software assume a steady-state system for the rate of diffusion through the environment and do not involve a time-based numerical solution.

ⓘ When you run the software for a single age class, you are assuming an exposure duration of one year, unless you select Age Class 17 or 18 which assume exposure durations of 49 years and 10 years respectively.

ⓘ Each individual run of the software is independent of other Age Classes, for example, the run at Age Class 3 does not assume that the emission flux started at Age Class 1.

ⓘ For short exposure periods you must consider the effect of aggregating exposures (see Figure 2.3 in Environment Agency, 2009c).

4.12 Interpreting assessment criteria that exceed the theoretical soil saturation limits

An important assumption used in the CLEA model is that of simple linear partitioning of a chemical in the soil between the sorbed, dissolved, and vapour phases (Environment Agency, 2009c). The theoretical upper boundaries to this behaviour are represented by the maximum aqueous solubility and pure saturated vapour concentration of the chemical. The CLEA report presents equations for using these chemical properties to estimate the saturated soil concentrations where these limits are reached (Environment Agency, 2009c). These boundaries are important when considering vapour phase transport of chemicals into ambient and indoor air.[4]

As noted in Section 3.3.3, Step 5, the CLEA software uses a traffic-light system to identify when individual and/or combined assessment criteria exceed the lower of either the aqueous or vapour based saturation limit (the lower saturation limit). There are two factors considered:

- Whether the assessment criterion exceeds the lower of the two saturation limits
- Whether the vapour pathway is an important contributor to exposure

Where the individual assessment criteria and/or the combined criterion are highlighted in green, the lower saturation limit has not been exceeded. Even though the individual oral and inhalation assessment criteria may be red, a green combined assessment criterion can still be used in a risk assessment since combining exposures often represents a soil concentration that may be much lower than the individual assessment criteria. Combined exposure is estimated independently of the individual assessment criteria.

It is important to note that not all exposure pathways depend on the partitioning calculations within the CLEA software and will therefore not be affected by exceeding the saturation limit. In the software, such assessment criteria are highlighted in orange / amber. Where contamination is present at the surface, the direct contact pathways including soil ingestion, skin contact, and the inhalation of dust are independent of partitioning behaviour and will not be affected by exceeding the saturation limit. However, the potential presence of free phase contamination at the surface should be considered qualitatively as part of the risk assessment. In many cases, assessment criteria highlighted in amber can be treated as if they were highlighted in green.

Only where the assessment criterion exceeds the lower saturation limit and the vapour pathway is an important contributor to exposure will the result be red. When this is the case the following should be considered:

- Free phase contamination may be present
- Exposure from the vapour pathways will be over predicted
- Where the vapour pathway dominates exposure (greater than 90 per cent) then it is unlikely that the relevant HCV will be exceeded at soil concentrations at least a factor of ten higher than the relevant HCV.

Where the vapour pathway is the only exposure route considered and the resulting assessment criterion is highlighted in red the following should be considered:

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[4] In theory, maximum aqueous solubility is also a potential limit on the passive uptake of chemicals by plants. However, there are many examples where plant concentrations exceed the overall concentration in surrounding soil. It is also worth noting that Environment Agency (2006b) found that the Ryan algorithm compared better with observed case study data when the artificial limit on solubility was removed.

- Exposure is unlikely to reach the relevant HCV and the risk based on the assumed conceptual model is likely to be negligible
- Vapour pathway exposure should be calculated using algorithms suitable for free phase or NAPL sources[5]
- Screening could be considered using the lower saturation limit, which is the approach adopted by the USEPA. However, this may not be practical in many cases because of very low limits and is in any case highly conservative.

Where the vapour pathway is only one of the exposure pathways considered then it may still be possible to calculate an effective assessment criterion manually:

1. Determine the relevant ADE / HCV ratio at the lower saturation limit by manually entering this as a soil concentration
2. Estimate the relevant contribution required from other pathways by subtracting the value in (1) from one.
3. Determine the soil concentration (by manually editing the soil concentration in Step 3 until the relevant ratio is achieved) from considering other pathways at which the relevant ADE/HCV ratio is equal to the value in (2). Check this soil concentration exceeds the lower saturation limit (since we are assuming that the contribution from vapour pathways is constant above the lower saturation limit)
4. Check that the soil concentration in (3) does not exceed combined assessment criterion based on all non-vapour pathways only.
5. Effective assessment criterion is the lower of 3 and 4.

The example below has been worked through for Chemical X, using the physical-chemical and toxicological parameters given in Table 4.8. In this example, Chemical X has an oral, inhalation, and combined assessment criteria based on a commercial scenario. In Step 5 'Results', the oral, inhalation and combined assessment criterion are highlighted in red, indicating that the assessment criterion exceeds the lower saturation limit and the vapour pathway is an important contributor to exposure. The vapour pathway contributes 96 per cent to total exposure.

Step 1: Enter the saturation limit as a soil concentration manually in the Select Chemicals page of the software and note the resulting inhalation ADE / HCV ratio on the Results page. Record this value, for example, 0.36. For this example, the saturation limit is 2840 mg kg^{-1}.

Step 2: Calculate the contribution from other pathways as one minus the ratio from step 1. For this example, this is 1 – 0.36 = 0.64.

Step 3: Manually adjust the soil concentration until the resulting oral ADE / HCV ratio on the Results page equals the ratio value determined in Step 2. Record this soil concentration. For this example, the oral ADE / HCV ratio equals 0.64 at a soil concentration of 121,000 -122,000 mg kg^{-1}. This concentration is higher than the lower saturation limit.

Step 4: Switch off the vapour pathways on the Basic Settings tab and recalculate the assessment criteria. Find the combined assessment criterion and compare this value to the soil concentration estimated in Step 3. If dust inhalation is significant compared to the oral and dermal routes then this value will be lower. For this example, the combined assessment criterion with the vapour pathways switched off is 190,000 mg kg^{-1} and therefore dust inhalation is relatively unimportant.

[5] For example; USEPA,2003 or CIRIA, in press.

Step 5: Compare the soil concentrations from Step 3 and Step 4. Select the lowest value as an effective combined assessment criterion. For this example, the soil concentration of 121,000 mg kg^{-1} is the lowest value.

Table 4.8: Physical-chemical and toxicological parameters for Chemical X.

Parameter	Value	Units
Chemical Name	Chemical X	
Chemical Type	organic	
Oral HCV Type	TDI	
Oral HCV value	1.00E+02	μg kg-1 BW day-1
Compare oral HCV with oral exposure	Yes	
Compare oral HCV with dermal exposure	Yes	
Compare oral HCV with inhalation exposure	No	
Inhalation HCV Type	TDI	
Inhalation HCV value	1.70E+02	μg kg-1 BW day-1
Compare inhalation HCV with oral exposure	No	
Compare inhalation HCV with dermal exposure	No	
Compare inhalation HCV with inhalation exposure	Yes	
Combine oral and inhalation AC	Yes	
Oral MDI for adults	5.00E+00	μg day^{-1}
Inhalation MDI for adults	1.30E+02	μg day^{-1}
Air-water partition coefficient (Kaw)	1.39E-01	cm^3 cm^{-3}
Diffusion coefficient in air	7.04E-06	m^2 s^{-1}
Diffusion coefficient in water	5.31E-10	m^2 s^{-1}
Relative molecular mass	1.06E+02	g mol-1
Vapour pressure	5.53E+02	Pa
Water solubility	1.80E+02	mg L^{-1}
Koc	2.65E+00	Log (cm^3 g^{-1})
Kow	3.15E+00	Log (dimensionless)
Kd	Not relevant	cm^3 g^{-1}
Dermal absorption fraction	1.00E-01	dimensionless
Soil - plant availability correction	Not relevant	dimensionless
Root - shoot correction factor	Not relevant	dimensionless
Root - root store correction factor	Not relevant	dimensionless
Root - tuber correction factor	Not relevant	dimensionless
Root - fruit correction factor	Not relevant	dimensionless
Soil-to-plant concentration factor (green vegetables)	Model	
Soil-to-plant concentration factor (root vegetables)	Model	
Soil-to-plant concentration factor (tuber vegetables)	Model	
Soil-to-plant concentration factor (herbaceous fruit)	Model [1]	
Soil-to-plant concentration factor (shrub fruit)	Model [1]	
Soil-to-plant concentration factor (tree fruit)	Model	
Soil-to-dust transport factor	0.5	g g^{-1} DW
Sub-surface soil to indoor air correction factor	1	dimensionless

Note: [1] Algorithms are not present in the CLEA software for herbaceous and shrub fruit. Exposure from these pathways is therefore not considered in the derivation of assessment criteria for organic chemicals.

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List of abbreviations

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

Glossary

Absolute bioavailability	The proportion of an intake dose of a chemical that is absorbed by the body and reaches systemic circulation unchanged; that is, without undergoing first-pass metabolism.
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.
Background exposure	The mean daily intake (MDI) for the UK population in terms of *the average "background intake" 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.
Background sources	Sources of human exposure to a chemical other than the soil itself, either directly or indirectly. For example, ambient air, diet, and drinking water.
Bioaccessibility	The degree to which a chemical is released from soil into solution (and thereby becomes available for absorption) when that soil is ingested and undergoes digestion or is inhaled and enters into solution in the lung.
Bioavailable fraction	See Absolute bioavailability
Building ventilation	The exchange of indoor and outdoor air through circulation within the building either naturally through cracks in doors and windows or mechanically by air conditioning or fans.
Carcinogen	An agent capable of inducing tumours and causing cancer
Cation exchange capacity	A measure of the number of sites on soil surfaces that can retain positively charged ions (cations) by electrostatic forces.
Chemical intake/uptake rate	The daily amount of a soil contaminant expressed as an intake or an uptake from exposure to chemicals in soil, food, water and air.
Chemical lipophilicity	A chemicals affinity for, tendency to combine with, or preference to dissolve in lipids (fats).
Conceptual model	A representation of the characteristics of a site in diagrammatic or written form that shows the possible relationships between contaminants, pathways and receptors.
Critical adverse effect	The adverse effect judged to be the most important for setting a **Health Criteria Value**. This is usually the most sensitive adverse effect (that is, the lowest effect level) or sometimes a more serious effect, not necessarily having the lowest effect level.
Critical receptor	The individuals or subgroup of the population most likely

	to be exposed and/or susceptible to the presence of soil contamination.
Dermal	Of or pertaining to the skin.
Dermal absorption fraction	An empirical measure of the proportion of chemical compound in soil that is absorbed through the skin by a typical soiling event.
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.)
Generic assessment criteria	Criteria derived using largely generic assumptions about the characteristics and behaviour of sources, pathways and receptors. These assumptions will be conservative in a defined range of conditions.
Geophagia	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.
Generic quantitative risk assessment	The purpose of generic quantitative risk assessment is to establish whether generic assessment criteria and assumptions are appropriate for assessing the risks, and, if so, to apply them to establish whether there are actual or potential unacceptable risks.
Genotoxic carcinogenesis	The production of a malignant tumour by a chemical via a mechanism involving damage to the genetic material.
Geometric mean	The n^{th} root of the product of all the numbers of a dataset.
Hazard	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.
Health Criteria Value (HCV)	A generic term used in this report to describe a benchmark level of exposure to a chemical derived from available toxicity data for the purposes of safeguarding human health (for example, a **Tolerable Daily Intake**).
Index Dose (ID)	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.
Inhalable particle	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 μm. Following deposition in the lung, they may be subject to mucociliary clearance, swallowing and oral absorption (cf. **respirable particle**).
Intake	Amount of a chemical entering the human body at the point of entry (that is, mouth, nose or skin) by ingestion, inhalation, or skin contact.

Mean daily intake (MDI)	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.
Non-aqueous phase liquid (NAPL)	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 aqueous phase).
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).
Relative bioavailability	The comparison of the extent of absorption between two or more forms of the same chemical (such as lead carbonate versus lead acetate), or the same chemical administered in different media (such as food, soil, water) or at different doses.
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

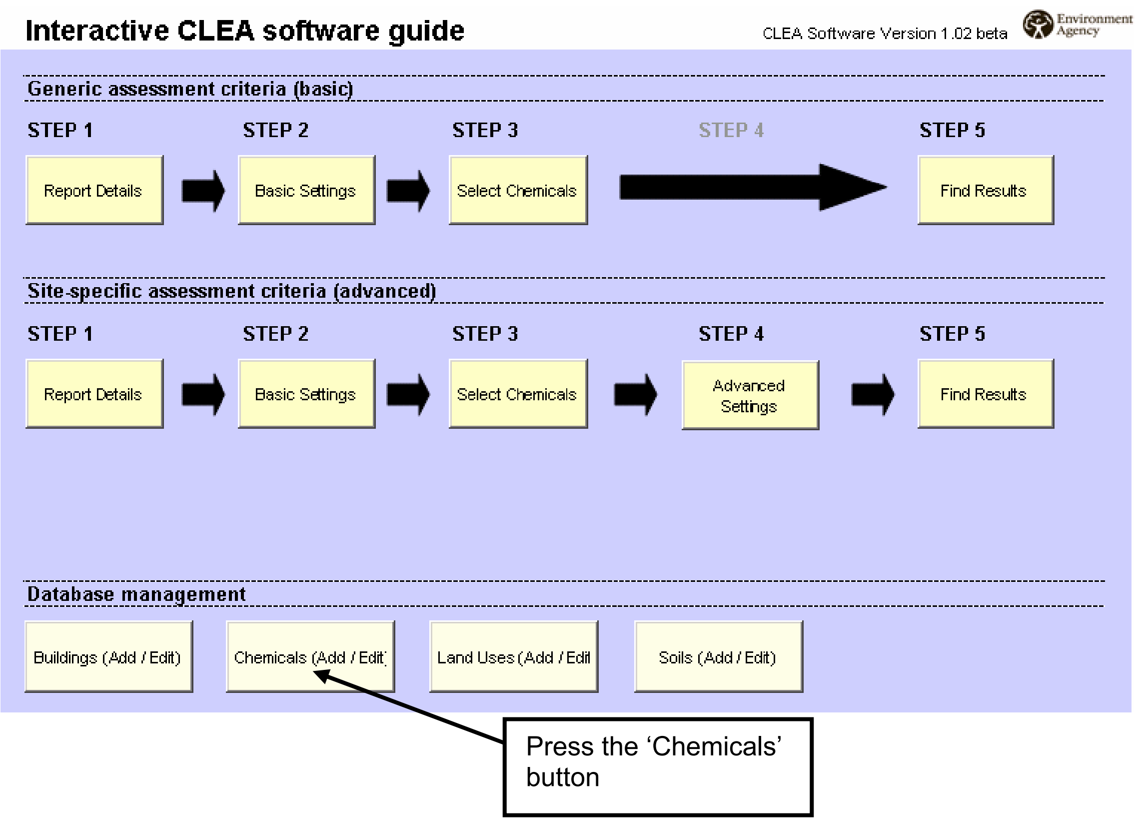

Figure A1: Enter the ‘Chemicals’ database.

Table A1 Information collated for chemical A

Parameter	Value	Units
Chemical Name	Chemical A	
Chemical Type	organic	
Oral HCV Type	TDI	
Oral HCV value	1.00E+02	µg kg-1 BW day-1
Compare oral HCV with oral exposure	Yes	
Compare oral HCV with dermal exposure	Yes	
Compare oral HCV with inhalation exposure	No	
Inhalation HCV Type	TDI	
Inhalation HCV value	1.00E+02	µg kg-1 BW day-1
Compare inhalation HCV with oral exposure	No	
Compare inhalation HCV with dermal exposure	No	
Compare inhalation HCV with inhalation exposure	Yes	
Combine oral and inhalation AC	Yes	
Oral MDI for adults	5.00E+00	µg day^{-1}
Inhalation MDI for adults	1.30E+02	µg day^{-1}
Air-water partition coefficient (Kaw)	1.52E-01	cm^3 cm^{-3}
Diffusion coefficient in air	7.50E-06	m^2 s^{-1}
Diffusion coefficient in water	7.80E-10	m^2 s^{-1}
Relative molecular mass	1.06E+02	g mol-1
Vapour pressure	6.38E+02	Pa
Water solubility	1.80E+02	mg L^{-1}
Koc	2.64E+00	Log (cm^3 g^{-1})
Kow	3.13E+00	Log (dimensionless)
Kd	Not relevant	cm^3 g^{-1}
Dermal absorption fraction	1.00E-01	dimensionless
Soil - plant availability correction	Not relevant	dimensionless
Root - shoot correction factor	Not relevant	dimensionless
Root - root store correction factor	Not relevant	dimensionless
Root - tuber correction factor	Not relevant	dimensionless
Root - fruit correction factor	Not relevant	dimensionless
Soil-to-plant concentration factor (green vegetables)	Model	
Soil-to-plant concentration factor (root vegetables)	Model	
Soil-to-plant concentration factor (tuber vegetables)	Model	
Soil-to-plant concentration factor (herbaceous fruit)	6.83E-04	mg g-1 plant (FW basis) over mg g^{-1} DW soil
Soil-to-plant concentration factor (shrub fruit)	3.50E-04	mg g-1 plant (FW basis) over mg g^{-1} DW soil
Soil-to-plant concentration factor (tree fruit)	Model	
Soil-to-dust transport factor	0.7	g g^{-1} DW
Sub-surface soil to indoor air correction factor	1	dimensionless

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.

Chemical (Back to Guide)	Chemical type	oral HCV					
		Type	$\mu g\ kg^{-1}\ BW\ day^{-1}$	Notes	Compare with oral exposure	Compare with dermal exposure	Compare with inhalation exposure
Chemical A	organic	TDI	1.00E+02	CLEA software handbook (2009)	Yes	Yes	No

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. Press the 'Apply settings to model' button. 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 for calculation of generic assessment criteria - chemical A.

Parameter	Value	Units
Ratio of ADE to relevant Health Criteria Value: oral HCV	0.06	dimensionless
Ratio of ADE to relevant Health Criteria Value: inhal HCV	0.94	dimensionless
Ratio of ADE to relevant Health Criteria Value: combined	1.00	dimensionless
Soil Assessment Criteria: oral HCV	5.61E+02	mg kg^{-1}
Soil Assessment Criteria: inhalation HCV	3.44E+01	mg kg^{-1}
Soil Assessment Criteria: Combined	3.24E+01	mg kg^{-1}
Soil Saturation Limit	2.79E+03	mg kg^{-1}
Pathway contribution; direct soil ingestion	0.24	%
Pathway contribution; consumption of homegrown produce and attached soil	5.36	%
Pathway contribution; dermal contact (indoor)	0.01	%
Pathway contribution; dermal contact (outdoor)	0.12	%
Pathway contribution; inhalation of dust (indoor)	0.00	%
Pathway contribution; inhalation of dust (outdoor)	0.00	%
Pathway contribution; inhalation of vapour (indoor)	86.17	%
Pathway contribution; inhalation of vapour (outdoor)	0.00	%
Pathway contribution; oral background	0.28	%
Pathway contribution; inhalation background	7.82	%

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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