The Interdepartmental Group
on Health Risks from Chemicals

Current approaches to **exposure modelling** in UK Government Departments and Agencies

cr15

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The Interdepartmental Group on Health Risks from Chemicals aims to stimulate the development of new, improved approaches to the assessment of risks to human health from chemicals.

The Steering Committee of the Interdepartmental Group on Health Risks from Chemicals comprises participants from the Department for Environment, Food and Rural Affairs, the Department of Health, Health Protection Agency, the Department for Business, Enterprise and Regulatory Reform, the Home Office, the Environment Agency (EA), the Health and Safety Executive (including Chemicals Regulation Directorate), the Food Standards Agency, the Medicines and Healthcare Products Regulatory Agency, the Veterinary Medicines Directorate, the Biotechnology and Biological Sciences Research Council, the Medical Research Council and the Natural Environment Research Council.

The Secretariat is based at the Institute of Environment and Health, Cranfield University.

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Foreword

This document has been produced by the Interdepartmental Group on Health Risks from Chemicals (IGHRC) as part of its Phase 2 work programme (October 2003 to September 2007). A number of government departments and agencies have been involved in the drafting of this document to ensure that the information contained herein reflects the exposure modelling approaches currently in use. The document has been reviewed by the IGHRC Executive Committee to ensure transparency and consistency of the information presented.

The document is intended to demonstrate the different approaches adopted within government for the modelling of exposure and so aid in the reduction of uncertainties inherent in chemical risk assessments. I hope it will provide a useful introduction to the area and assist in the further clarification of what is a complicated area of science.

Professor David R Harper
Chairman of IGHRC
Director General, Health Improvement and Protection

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Executive Summary

UK government departments and agencies are frequently required to assess risks to human health arising from chemical exposures, whether to chemicals in food, beverages and drinking water, household or consumer products, the workplace, or the environment generally. Exposure data are frequently scarce and so exposure models have been developed that can assist in exposure estimation, completing a key stage of the exposure assessment process. Exposure models can be simple, modelling scenarios based upon one chemical, one exposure pathway and one type of receptor, to complex, using groups of chemicals, different routes of exposure and a number of receptors. The different responsibilities of UK government departments and agencies dictate the type of exposure models used and the level of complexity adopted.

The risk assessment requirements of UK government departments and agencies have required the development or adaptation of existing exposure models. It is rare for two departments or agencies to use the same model, due to the very different roles adopted by each of them. Examining models used by three such departments and agencies, it becomes clear that the models utilise different definitions of 'exposure' including intake and even uptake dose; have different capabilities for combining measured, estimated and/or default values; use different modelling methodologies based upon probabilistic (quantitative) or deterministic (descriptive) approaches; use different source, pathway and receptor parameters; and have variable capability to combine exposures to different chemicals in one exposure scenario (aggregate exposure) or one chemical across different scenarios or duration. Nevertheless, all adopt a hierarchy of approach and a tiered methodology to assessment.

The aim of the document is to present examples of exposure models used by three UK government departments and agencies, providing a step-by-step guide to why and how the models are used and the outputs expected. By improving the transparency of the models, it is hoped to demonstrate the underlying similarity in approach adopted, although the individual models may differ in the parameters and scenarios considered. To this end, the models used by these departments, as outlined below, are described and examples provided to show the current exposure modelling approaches used by UK government scientists, regulators and policy makers.

- Environment Agency: Contaminated Land Exposure Assessment (CLEA)
- Health and Safety Executive: Estimation and Assessment of Substance Exposure (EASE), Bayesian Exposure Assessment Toolkit (BEAT), Consumer Exposure (ConsExpo); and also within HSE the Chemicals Regulation Directorate's Predictive Operator Exposure Model (POEM)
- Food Standards Agency: Intake Program (Intake 2)

1 Introduction

A number of UK government departments and agencies are involved in assessing the risks to human health posed by chemicals found in food, beverages and drinking water, household products, the environment or the workplace. The Interdepartmental Group on Health Risks from Chemicals (IGHRC) is an informal group of representatives from the main UK government departments, agencies and research councils with an interest in chemical risk assessment in relation to human health. The general principles involved in quantitative chemical risk assessment are well established, and are based on assessments of the ability of the chemical to cause adverse human health effects, together with quantitative estimates of human exposure. The IGHRC aims to promote coherence and consistency in the practice of chemical risk assessment as used within the different risk management and regulatory frameworks used within government. Achieving coherence and consistency does not mean that all departments should undertake risk assessments in precisely the same way, but rather that they understand where different circumstances require particular approaches and techniques, and are able to explain why this is the case.

Exposure modelling has been defined as 'a conceptual or mathematical representation of exposure' (IGHRC, 2004). Models can use either:

- the more traditional deterministic approach, in which single point estimates of input variables are used to produce single point exposure estimates, or
- probabilistic approaches, which allow input variables to be entered as distributions of possible values, and the outcome generated in the form of an exposure distribution.

Government departments and agencies use a variety of different models for their exposure assessment requirements. Choosing the right model is largely dependent on the route of exposure and the type of exposure data. Existing exposure models have been reviewed in detail by Fryer *et al.* (2004).

A variety of approaches are used within UK government departments and agencies to assess human exposure to chemicals. These can be direct or indirect.

- Direct methods involve measurements of exposure as they occur, for example personal monitoring.
- Indirect methods involve extrapolating exposure estimates from other measurements and existing data, and often involve the application of an appropriate exposure model.

Exposure assessments are generally considered to contribute the greatest uncertainty to risk assessments. The risks characterised from the assessment of environmental exposures to chemicals and their effects on health are usually very low. Therefore, the exposure assessment methodology requires optimal precision and accuracy in order to increase the confidence of the risk estimate. Another contributor to uncertainty in exposure assessment is the lack of good exposure data. It is the poor availability of exposure data and the need for assessments to be carried out in an efficient and cost-effective way that has steered the development of exposure modelling using computer-based software and mathematical modelling.

1.1 Aim of the document

The aim of this report is to summarise current practice in the use of exposure models in risk assessment in different UK government departments and agencies, and explore reasons for the similarities and differences in approach. By increasing transparency on why certain models are used, including their default values and underlying assumptions, it is hoped that the document will facilitate harmonisation of exposure modelling approaches both nationally and internationally.

The purpose of this document is not to prescribe which model(s) each UK department or agency should use, but rather to provide guidance to assist those having to undertake or evaluate exposure assessments. It is directed at risk assessors and policy makers within UK government departments and agencies who need to understand the process involved in obtaining the output from an exposure assessment, and should assist them in making more confident and informed decisions when carrying out quantitative assessments of risks to humans from exposure to chemicals. Discussion is informed by previous IGHRC reports in this area. These include the following.

- Guidelines for Good Exposure Assessment Practice for Human Health Effects of Chemicals (IGHRC, 2004)
- Exposure Assessment in the Evaluation of Risk to Human Health (RATSC, 1999a)
- An IGHRC-commissioned research report: 'Review of Existing Exposure Models', which is included as an Annex in a larger document by Fryer *et al.* (2004). This report cites the need to build upon robust methods for assessing models.
- Risk Assessment Approaches used by UK Government for Evaluating Human Health Effects of Chemicals (RATSC, 1999b)

1.2 Approaches to exposure modelling

This document consists of exposure modelling approaches from the following departments or agencies.

- Environment Agency (EA)
- Health and Safety Executive (HSE)
- Food Standards Agency (FSA)

Other representatives within IGHRC were not able to contribute a chapter for this report because they do not conduct exposure modelling in-house, and contract or collaborate with other departments or agencies to do this type of work if required. Although the following organisations did not contribute a chapter they did review this document prior to publication.

- Department of Health (DH)
- Department for Environment, Food and Rural Affairs (DEFRA)
- Department of Trade and Industry (DTI; now Department for Business, Enterprise and Regulatory Reform; BERR)
- Health Protection Agency (HPA)
- Home Office

References

Fryer ME, Collins CD, Colvile RN, Ferrier H & Nieuwenhuijsen MJ (2004) *Evaluation of currently used exposure models to define a human exposure model for use in chemical risk assessment in the UK: Annex 1, Review of Existing Exposure Models.* Report prepared for IGHRC, MRC Institute for Environment & Health, Leicester UK. Available at: http://ieh.cranfield.ac.uk/ighrc/IEH Final Version 28_04_04.doc [accessed July 2010]

IGHRC (2004) Guidelines for good exposure assessment practice for human health effects of chemicals (cr10). MRC Institute for Environment & Health, Leicester, UK. Available at: http://ieh.cranfield.ac.uk/ighrc/cr10.pdf [accessed July 2010]

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RATSC (1999b) Risk assessment approaches used by UK government for evaluating human health effects of chemicals (cr2). MRC Institute for Environment & Health, Leicester, UK. Available at: http://ieh.cranfield.ac.uk/ighrc/cr12[1].pdf [accessed July 2010]

2 Environment Agency's Approach to Exposure Modelling

2.1 Introduction

Exposure modelling is usually conducted by the Environment Agency (EA) to produce guideline values for the implementation of specific legislation. Exposure assessment and modelling may also be carried out on an *ad hoc* basis for processes and sites where EA is responsible.

Guidance on exposure modelling is provided under three main legislative drivers.

- Environmental Permitting regulations (2007)[1]
- Planning regime
- Contaminated land regime (Part IIA, Environmental Protection Act, 1990)

For the implementation of Environmental Permitting regulations, the EA is continuing to develop environmental assessment levels (EAL) for human receptors, originally begun under the Integrated Pollution Prevention and Control (IPPC) regime. These EAL will be derived for soil, water, and air environmental media. They will be based on toxicity data and simple deterministic exposure modelling. The planning and contaminated land (Part IIA) regimes currently use a set of values for soil that are derived using the Contaminated Land Exposure Assessment (CLEA) model, a deterministic exposure model that is used to derive soil guideline values (SGV).

The CLEA model uses generic assumptions about the fate and transport of chemicals in the environment and generic conceptual exposure models to estimate child and adult exposures to soil contaminants for those living, working and/or playing on contaminated sites over long time periods. The CLEA model is used to produce SGV by comparing the estimated exposure with health criteria values (HCV) that represent tolerable or minimal risk to health from chronic exposure (EA, 2009).

The remainder of this chapter focuses on the exposure assessment carried out for land contamination using the CLEA model. The CLEA model, its underlying assumptions and default parameters values, are described in the Updated Technical Background to the CLEA Model and this chapter draws heavily on this document (EA, 2009). The CLEA software (Version 1.06) was released in support of the implementation of the CLEA model and is freely available (see EA website[2]). Although the CLEA model is used by the EA for generic risk assessment, it can be used for more site-specific risk assessments and exposure modelling. This is in line with the tiered approach to environmental risk assessment outlined in DETR *et al.* (2000).

2.2 Exposure assessment

The aim of the CLEA model is to estimate human exposure to chemicals in soil using relevant HCV (including tolerable daily intake (TDI) and index dose).

The steps used to carry out an exposure assessment are as follows.

- Development of a site conceptual model
- Exposure media concentration measurement or prediction
- Intake calculations from different exposure pathways to calculate average daily exposure (ADE)

[1] Regulatory Guidance for Understanding the Environmental Permitting Regulations, http://www.environment-agency.gov.uk/business/topics/permitting/36419.aspx [accessed July 2010]

[2] http://www.environment-agency.gov.uk/research/planning/33732.aspx [accessed July 2010]

2.2.1 Defining exposure

The CLEA model estimates ADE to a contaminant in soil by using the conceptual exposure models for each standard land use. Each land use scenario considers up to ten exposure pathways according to the following routes of entry into the human body.

- Ingestion of contaminated soil, dust and home-grown produce (oral)
- Inhalation of contaminated dust and vapour (inhalation)
- Absorption of the contaminant through the skin (dermal)

2.2.2 Quantifying exposure

Overall exposure to chemicals in soil for the critical receptor (described more fully in Section 2.3.4) is calculated and compared against an HCV. An HCV represents a tolerable or minimal risk to health from chronic exposure and is derived for each contaminant of concern on the basis of a contaminant's toxicological potency. The overall exposure to the receptor needs to include all the exposure pathways, which are then added for the three routes of exposure: oral, inhalation and dermal. Equation 2.1 illustrates the calculation of ADE for the critical receptor. However, this equation assumes that in the final comparison there is only one HCV for the final assessment against exposure. If an HCV is available for all three exposure routes then the exposure via each route is compared with the most appropriate HCV.

The ADE is the average daily exposure from all exposure routes. It is used to calculate the SGV by comparing it to the HCV. The SGV is the concentration in soil at which ratio of the ADE to the HCV is equal to one. For calculations other than those for the SGV, if the ADE is less than or equal to the HCV then the level of risk is deemed to be minimal or tolerable and no further assessment is required. If this is not the case then risk management measures must be implemented to ensure that the receptor is not adversely affected.

The chemical intake/uptake rate (IR) is calculated from the concentration of a contaminant in the relevant medium (air, soil, water or food) and the daily exposure rate to that medium. For example, the intake rate for cadmium by soil ingestion would depend on the concentration of cadmium in soil and the amount of soil ingested by the critical receptor.

The CLEA model estimates daily exposure from up to ten different pathways based on the concentration of a chemical in the soil. Figure 2.1 illustrates the potential exposure pathways used in the CLEA model to derive SGVs. A different land use and/or different contaminants may result in the selection of different exposure pathways.

Exposure frequency (EF) represents the number of days per year in which a daily exposure event occurs. For example, the EF for inhalation of household dust is 365 days per year. CLEA mostly uses EF that are specific for each land-use scenario (described further in Section 2.5.2).

The ADE is calculated for a specific time period – the exposure duration (ED) – which for CLEA covers chronic exposure. ED can be varied from one year up to 75 years and many human characteristics (e.g. bodyweight) can vary with age. The CLEA model divides a lifetime up in to eighteen age intervals (called age classes) to take account of these variations in exposure characteristics.

The CLEA model estimates an ADE over the period of exposure. The averaging time (AT) is assumed to be equal to ED. For example, exposure during the first six years of a child's life has an AT of 2190 days.

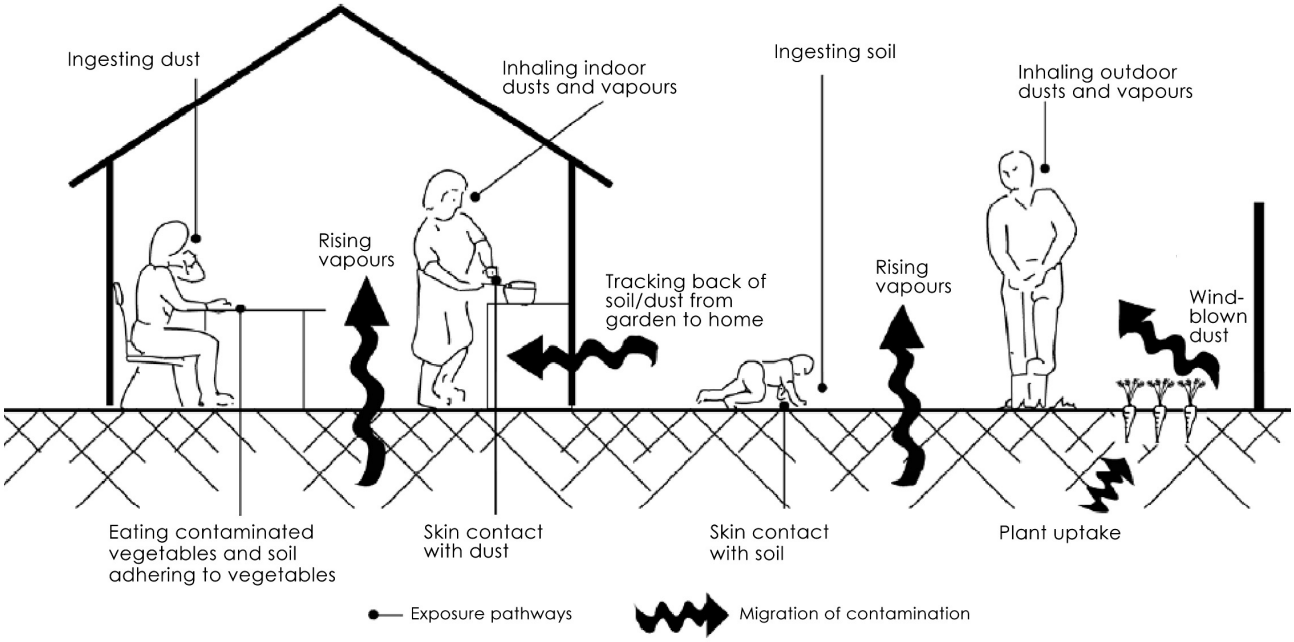
Equation 2.1

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

Where: *ADE* is the average daily human exposure to a chemical from soil, mg kg^{-1} bw day^{-1}
IR is the chemical intake/uptake rate, mg day^{-1}
EF is the exposure frequency, days year^{-1}
ED is the exposure duration, years
BW is human body weight, kg
AT is the averaging time, days

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

Figure 2.1 Illustration of potential exposure pathways in the CLEA model



2.3 Conceptual models and exposure assessment

A conceptual model is an essential element of any risk assessment, qualitative or quantitative. In the context of environmental risk assessment such models are often simple representations of the hypothetical relationships between sources, pathways, and receptors (DETR *et al.,* 2000).

The overall conceptual model takes into consideration the chemical in the soil, how it partitions to air, water and plants, and how people that come into contact with these media are exposed. It also defines the exposure scenario.

The way the land is used helps to describe the type of people that use a site and how they might potentially behave. Factors considered include the age and gender of site users, the number of visits to the site, the duration of each visit, and the likely activities that could bring about contact with the soil. The CLEA model has three types of standard land use, and these are used to define the conceptual exposure model. These land use scenarios are residential, allotment and commercial.

Specific information on the way people behave ('activity patterns') for each of the standard land uses included in CLEA is discussed in the Updated Technical Background to the CLEA Model (EA, 2009). This document should be consulted if further information is required.

2.3.1 Residential land use

The residential site is assumed to consist of a two-storey, small terrace house with a private garden consisting of a lawn, flowerbeds and a small fruit and vegetable patch. The occupants are considered to be parents with small children who make regular use of the garden. It is assumed that the property receives drinking and bathing water through mains supply only (not from a private well or spring, which may itself be contaminated). For the standard residential scenario, the critical receptor is assumed to be a young female child with the duration of exposure covering the first six years of life.

Exposure pathways included for this land use are direct soil and indoor dust ingestion, consumption of home-grown produce, consumption of soil adhering to home-grown produce, skin contact with soils and indoor dust, and inhalation of indoor and outdoor dust and vapours.

2.3.2 Allotment land use

The allotment generic scenario is assumed to consist of approximately 250 m^2 of open space used for growing fruit and vegetables. There is usually more than one plot per site and the overall site area may be more than one hectare in size. The critical receptor is assumed to be a young female child with the duration of exposure covering the first six years of life. The child is assumed to visit the allotment regularly with an adult and consume produce grown in the allotment. We do have evidence that the number of younger allotment gardeners has increased (GLA, 2006) and

that children are likely to be present on a regular but infrequent basis. No buildings are assumed to be on the site (sheds etc. are not considered as buildings for this generic scenario).

Exposure pathways included for this land use are direct soil ingestion, consumption of home-grown produce, consumption of soil adhering to home-grown produce, skin contact with soils, and inhalation of outdoor dust and vapours.

2.3.3 Commercial land use

A typical commercial or light industrial property has been selected to represent the commercial land use. It has a three-story building (pre 1970) where employees spend most of their time indoors involved in office work or light physical activities. A female worker was selected as the critical receptor with ED considered over a working lifetime of 49 years (16 to 65 years).

Exposure pathways included for this land use are direct soil and indoor dust ingestion, skin contact with soils and dust, and inhalation of dust and vapours.

2.3.4 Critical receptors

The critical or most sensitive receptor in the conceptual exposure model is selected on the basis of toxicological sensitivity and the likelihood of greater exposure. Children are often considered to be the critical receptor because their intakes of food, water, air and soil are greater per unit body weight than in adults. In addition, a child's physiology is not the same as that of an adult, and so his or her susceptibility to the effects of a chemical may be different, qualitatively and quantitatively. However realism must also be considered in selection of the critical receptor. A child would be unlikely to spend enough time at a commercial site so a female is usually chosen, due to their lower average body weight than males of the same age.

Therefore the female child is the critical receptor for the residential and allotment land uses and the female adult worker of age 16 to 65 is the critical receptor for the commercial land use.

2.3.5 Exposure media

In Part IIA (the 'contaminated land' regime) the source of exposure is considered to be the historically contaminated soil, and the pathways are the mechanism by which the receptor may come into contact with that contamination. Exposure can occur directly with soil and indirectly by its transport into other environmental media, including air, water and plants. Therefore the CLEA model takes into consideration not just direct soil contamination but also outdoor and indoor air and the potential uptake of contaminants into six types of garden produce groups. However, exposure does not take into consideration any exposure from sources other than the local soil, such as from drinking water.

2.4 Predicting exposure concentrations

An essential step in modelling exposure is to derive a representative concentration of the contaminant in question in air, soil or water. For example, the soil ingestion exposure pathway uses the measured concentration in soil to determine the level of intake for the critical receptor (discussed further in Section 2.5). However, concentrations in vegetables, outdoor air and indoor air are predicted using fate and transport models. It is always preferable to use measured concentrations in the different exposure media rather than rely on modelling; however this is not always possible and so predicted concentrations are used in our exposure assessments.

2.4.1 Outdoor air

Vapour transport in unsaturated soils depends on partitioning of contamination into the vapour phase, and transport of vapours to the surface and into ambient or indoor air (EA, 2002).

The CLEA model assumes that the source of outdoor air contamination is present in the soil from the surface to a depth of 100 cm. It is also assumed that the source is not depleted by volatilisation or by chemical or biological degradation. Chemical transport in the soil is assumed to take place by diffusion within the unsaturated soil pore spaces and not as a result of water evaporation. The overall approach is broadly similar to that of the US EPA (1996) and ASTM (2000).

The outdoor air concentration of a contaminant at the receptor breathing height (C_{air}) is calculated using the ASTM approach for risk-based corrective action at petroleum release sites (ASTM, 2000; Equation 2.2). Contaminant levels in outdoor air are modelled using a volatilisation factor from surface soils to ambient air (VF, Equation 2.3). The diffusion coefficient (D_{eff}) for unsaturated soils is also required to calculate the concentration in ambient air of a chemical (Equation 2.4). This is a complex area of exposure modelling and there is further detail in the Updated Technical Background to the CLEA Model (EA, 2009).

The way CLEA calculates intake from the outdoor air exposure pathway is described in Section 2.5.3 (Equation 2.25).

Equation 2.2

$$C_{air} = C_s \times VF \times 10^6 \text{ cm}^3 \text{ m}^{-3}$$

Where: C_{air} is the ambient air concentration at the receptor height, mg m^{-3}
C_s is the total soil concentration, mg g^{-1}
VF is the volatilisation factor from surface soil to ambient air, g cm^{-3}

Equation 2.3

$$VF = \frac{\rho_s}{\frac{1}{10} \times Q/C_{wind}} \sqrt{\frac{4\,D_{eff}}{\pi\tau \times 3.1536 \times 10^7 \text{ s yr}^{-1}} \times \frac{K_{aw}}{K_{sw}\ \rho_s}}$$

Where: VF is the volatilisation factor from surface soil to ambient air, g cm^{-3}
ρ_s is the dry bulk soil density, g cm^{-3}
Q/C_{wind} is the air dispersion factor, g m^{-2} s^{-1} per kg m^{-3}
D_{eff} is the effective diffusion coefficient for unsaturated soils, cm^2 s^{-1}
τ is the averaging time for surface emission vapour flux, year
K_{aw} is the air–water partition coefficient at ambient temperature, cm^3 cm^{-3}
K_{sw} is the total soil–water partition coefficient, cm^3 g^{-1}

Equation 2.4

$$D_{eff} = D_{air}\ \frac{\theta_a^{3.33}}{\theta_T^2} + D_{water}\ \frac{\theta_w^{3.33}}{K_{aw}\,\theta_T^2} \times 10^4 \text{ cm}^2 \text{ m}^{-2}$$

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

2.4.2 Indoor air

Exposure to indoor air is an important exposure pathway, as many of us spend much of our time indoors. Data on buildings is required by the CLEA model in order to estimate vapour intrusion from contaminated soil into indoor air. The Johnson & Ettinger (1991) screening approach is used and several parameters are required. Default values used for the residential and commercial land uses are shown in Table 2.1. Further detail of the parameters used can be found on p78 of the Updated Technical Background to the CLEA Model (EA, 2009).

The CLEA model assumes that the source of indoor air contamination is at 0.5 m depth below the bottom of the building floor or foundation. As with ambient air, it is assumed that the contamination is not depleted by volatilisation or reduced by chemical or biological degradation. Chemical transport in the soil is assumed to be by diffusion within the unsaturated soil pore spaces. The main route for contamination into the building is assumed to be via cracks in the foundation and between the wall and the edge of the foundation slab.

To calculate the indoor air concentration (C_{air}, Equation 2.7) an attenuation factor between soil and indoor air is needed (α, Equation 2.5); the building ventilation rate (Q_b) is calculated using Equation 2.6.

The indoor air concentration depends strongly on the structure and ventilation performance of the building, as dilution with 'cleaner' outdoor air reduces the contaminant concentration derived from soil contamination.

The way CLEA calculates intake from the indoor air exposure pathway is described in Section 2.5.3 (Equation 2.26).

2.4.3 Ingestion of soil and dust

The CLEA model calculates exposure from direct ingestion of contaminated soil and indoor dust, plus indirect ingestion through consumption of fruit and vegetables. These pathways are modelled separately.

Direct soil and dust ingestion

The ingestion of soil and indoor dust are important exposure pathways (especially for children) for non-

Table 2.1 Default values for building data according to residential and commercial building type

Building type	Building footprint	LS air exchange rate	Building height	Storeys	Storey height	LS height	Press diff	Found thick	Floor crack area
	m^2	$hour^{-1}$	m	–	m	m	Pa	m	cm^2
Residential									
Bungalow	78.0	0.5	2.4	1	2.4	2.4	2.6	0.15	706.5
Small terraced house	28.0	0.5	4.8	2	2.4	4.8	3.1	0.15	423.3
Medium/large terrace house	44.0	0.5	4.8	2	2.4	4.8	3.1	0.15	530.7
Semi-detached house	43.0	0.5	4.8	2	2.4	4.8	3.1	0.15	524.6
Detached house	68.0	0.5	4.8	2	2.4	4.8	3.1	0.15	659.7
Commercial									
Warehouse (pre-1970)	1089.0	1.0	5.2	1	4.6	4.6	3.2	0.15	2640.0
Warehouse (post-1970)	1914.0	1.0	5.9	1	5.1	5.1	3.4	0.15	3499.9
Office (pre-1970)	424.0	1.0	10.2	3	3.2	9.6	4.4	0.15	1647.3
Office (post-1970)	610.0	1.0	13.0	4	3.2	12.8	5.1	0.15	1975.9

LS, Living space; Press diff, negative pressure difference; Found thick, Foundation thickness

volatile contaminants such as polycyclic aromatic hydrocarbons (PAH), arsenic and lead. Modelling these pathways is not simple and there are significant uncertainty issues. Most tracer studies do not differentiate between occasional deliberate ingestion of soil (pica) and inadvertent ingestion (e.g. hand to mouth ingestion). It is also difficult to distinguish between soil-derived dust and ingestion of outdoor soil. The CLEA model therefore uses default values that are combined soil and dust ingestion rates (shown in Table 2.2) with the soil concentration used to calculate an intake by this exposure pathway.

Table 2.2 Default values for the combined soil and dust ingestion rate by age

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

Indirect soil ingestion via fruit and vegetables

The ingestion of entrained soil from home-grown produce is usually unavoidable. Fine particles of soil can adhere to the skin and leaves of fruit and vegetables grown in the garden or allotment via direct contact with the soil or by aerial deposition onto leaves. This soil can remain on the skins of potatoes and carrots, for example, even after washing and cooking. Soil loading and preparation factors used by the CLEA model are shown in Table 2.3. The way CLEA calculates intake from the indirect ingestion of soil exposure pathway is described in Section 2.5.3 (Equation 2.27).

Table 2.3 Default values for entrained soil according to produce category

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

dw, dry weight; fw, fresh weight

Soil and dust properties for fate and transport modelling

Soil characteristics such as moisture content, texture, particle size etc. can have an effect on the intake of a chemical. The CLEA model uses a range of soil and chemical defaults which are described fully in the Updated Technical Background to the CLEA Model

Equation 2.5

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

Where: α is the steady-state attenuation coefficient between soil and indoor air, dimensionless
D_{eff} is the effective diffusion coefficient for unsaturated soils, $cm^2\ s^{-1}$
A_B is the area of enclosed floor and walls below ground, cm^2
Q_b is the building ventilation rate, $cm^3\ s^{-1}$
L_T is the source–building separation, cm
Q_s is the volumetric flow rate of soil gas into the enclosed space, $cm^3\ s^{-1}$ [25 to 150]
L_{crack} is the foundation slab thickness, cm
A_{crack} is the floor crack area, cm^2
D_{crack} is the effective diffusion coefficient through the cracks, $cm^2\ s^{-1}$ [= D_{eff}]

Equation 2.6

$$Q_b = \left(H \times A_{foot} \times Ex\right) \times 10^6\ cm^3\ m^{-3}\ \ \frac{1}{3600}\ s\ hr^{-1}$$

Where: Q_b is the building ventilation rate, $cm^3\ s^{-1}$
H is height of living space, m
A_{foot} is the building footprint, m^2
Ex is the building air exchange rate, $hour^{-1}$

Equation 2.7

$$C_{air} = \alpha\, C_{vap} \times 10^6\ cm^3\ m^{-3}$$

Where: C_{air} is the indoor air concentration, $mg\ m^{-3}$
α is steady-state attenuation coefficient between soil and indoor air, dimensionless
C_{vap} is the soil vapour concentration, $mg\ cm^{-3}$

(EA, 2009). Default soil properties used by CLEA are shown in Table 2.4.

2.4.4 Ingestion of fruit and vegetables

The concentration in the edible parts of fruit and vegetables can be predicted from relationships between the soil and the plant; soil-to-plant concentration factor (CF) is calculated using Equation 2.8.

Equation 2.8

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

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

The CLEA model uses concentration factors in fresh weight units (fw) but many concentration factors are reported on a dry weight basis (dw) and need to be converted. The CLEA model includes a range of dry weight conversion factors for all the fruit and vegetables used by the model (EA, 2009, p 100).

The literature reports large variations in the uptake of contaminants from soil, so a deliberately cautious approach has been taken for the CLEA model, which is different for organic and inorganic chemicals and different vegetable produce groups. The derivation and use of soil-to-plant concentration factors is fully described in the Updated Technical Background to the CLEA Model (EA, 2009), but is summarised here.

Uptake of inorganic chemicals

The generic model used by the EA is consistent with the approach used by the Food Standards Agency

Table 2.4 Default properties according to soil type

Soil type[1]	Property: Bulk density	Porosity ($cm^3\ cm^{-3}$)			Residual water content	Saturated hydraulic conductivity	van Genuchten a	van Genuchten m
	($g\ cm^{-3}$)	Air	Water	Total	($cm^3\ cm^{-3}$)	($cm\ s^{-1}$)	(cm^{-1})	(dimensionless)
Clay	1.07	0.12	0.47	0.59	0.24	9.93×10^{-4}	0.0385	0.2972
Silty clay	0.94	0.12	0.51	0.63	0.26	1.17×10^{-3}	0.0541	0.3155
Silty clay loam	1.07	0.12	0.46	0.58	0.21	1.17×10^{-3}	0.0291	0.3072
Clay loam	1.14	0.14	0.42	0.56	0.19	1.51×10^{-3}	0.0437	0.3039
Sandy clay loam	1.20	0.16	0.37	0.53	0.15	2.37×10^{-3}	0.0560	0.3098
Silt loam	1.09	0.14	0.44	0.58	0.18	1.58×10^{-3}	0.0375	0.3078
Sandy silt loam	1.19	0.14	0.38	0.52	0.15	2.20×10^{-3}	0.0410	0.3174
Sandy loam[2]	1.21	0.20	0.33	0.53	0.12	3.56×10^{-3}	0.0689	0.3201
Sand	1.18	0.30	0.24	0.54	0.07	7.36×10^{-3}	0.1221	0.3509

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

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

(PRISM v2, Thorne *et al.*, 2004, 2005). Equation 2.9 describes the soil-to-root concentration factor (CR).

Equation 2.9

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

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

Note: Thorne *et al.* (2005) CR is presented in units of Bq kg^{-1} fw plant per Bq kg^{-1} dw soil.

The transport of inorganic chemicals within the plant, that is from the root zone to the edible fruits, leaves or root storage organs and tubers, was also considered by Thorne *et al.* (2005) requiring a correction factor to be applied to the calculated value of *CR* from Equation 2.9. To derive a soil-to-plant concentration factor (*CF*), Equation 2.10 is used.

Equation 2.10

$$CF = CRf_{int}$$

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

Uptake of organic chemicals

Several models have been developed to predict the uptake of organic chemicals into plants, although overall performance of these models is inconsistent (EA, 2006). The CLEA model therefore uses a cautious approach when using these generic uptake models; those adopted are shown in Table 2.5.

Table 2.5 Generic models for predicting soil-to-plant concentration factors according to produce groups for organic contaminants

Produce group	Generic model
Green vegetable	Ryan *et al.* (1988)
Root vegetable	Trapp (2002)
Tuber vegetable	Trapp *et al.* (2007)
Herbaceous fruit	No model found
Shrub fruit	No model found
Tree fruit	Trapp *et al.* (2004)

Produce included in each group of fruit and vegetables are as follows.

- Green vegetable: beans, Brussels sprouts, cabbage, cauliflower, lettuce, spinach, peas, broccoli, celery, asparagus and herbs
- Root vegetable: beetroot, carrot, garlic, parsnip, radish, sweet potato, turnip, swede, onion, leek and rhubarb
- Tuber vegetable: potato
- Herbaceous fruit: cucumber, marrow, courgette, aubergine, pumpkin, tomato and strawberry
- Shrub fruit: blackberry, cranberry, gooseberry, loganberry, raspberry, blackcurrant and red currant
- Tree fruit: apple, pear, plum, cherry, apricot and peach

Soil-to-plant concentration factor for green vegetables

Equation 2.11

$$CF = \left(10^{0.95\log K_{ow}-2.05} + 0.82\right)\left(0.784 \times 10^{-0.43(\log K_{ow}-1.78)^2 / 2.44}\right)\frac{\rho_s}{\left(\theta_w + \rho_s K_{oc} f_{oc}\right)}$$

Where: CF is the calculated soil-to-plant concentration factor for green vegetables, mg g^{-1} fw plant per mg g^{-1} dw soil
K_{ow} is the octanol–water partition coefficient for the chemical, dimensionless
ρ_s is the dry soil bulk density, g cm^{-3}
θ_w is the soil water content by volume, cm^3 cm^{-3}
K_{oc} is the organic carbon–water partition coefficient for the contaminant, cm^3 g^{-1} dw
f_{oc} is the fraction of organic carbon in the soil, dimensionless

Soil-to-plant concentration factor for root vegetables

The Trapp model (2002) used here proposes that uptake by roots is due to diffusion through the peel and by preferential partitioning of organic chemicals in the xylem stream to cell lipids. To calculate the soil-to-plant concentration factor (Equation 2.13), K_{rw}, the equilibrium partition coefficient between roots and water is required, using Equation 2.12.

Equation 2.12

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

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

Equation 2.13

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

Where: CF is the calculated soil-to-plant concentration factor for root vegetables, mg g^{-1} fw plant per mg g^{-1} dw soil
K_d is the sorbed soil–water partition coefficient, cm^3 g^{-1} dw
K_{rw} is the equilibrium partition coefficient between root and water, cm^3 g^{-1} fw
Q is the transpiration stream flow rate, cm^3 day^{-1} (1000)
ρ_p is the plant root density, g cm^{-3} (1)
V is the root volume, cm^3 (1000)
K_g is the first order growth rate constant, day^{-1} (0.1)
K_m is the first order metabolism rate constant, day^{-1} (0)

Soil-to-plant concentration factor for tuber vegetables

The potato is the most important vegetable grown in Europe and is a tuber vegetable. The potato is a storage organ of the stem and not the root, so root uptake models are not relevant to potatoes. To calculate the soil-to-plant concentration factor (CF) for potatoes (Equation 2.17) first requires the potato-to-water partition coefficient (K_{pw}, Equation 2.14), and also the balance of the rate of diffusion into the potato (k_1, Equation 2.15) and out of the potato (k_2, Equation 2.16), plus a correction factor for dilution due to plant growth (k_g, 0.0014 hour^{-1}).

Soil-to-plant concentration factor for tree fruit

Many plant uptake models have focused on uptake in to the leaves, but there is evidence that persistent organic chemicals may accumulate in fruit which can then be eaten (often without peeling). The relationship of the chemical in the wood and in the water is key here (K_{wood}, Equation 2.18). To calculate the soil-to-plant concentration factor for tree fruit ($CF_{treefruit}$, Equation 2.21) several other factors are required, such as the chemical concentration in the xylem flowing into the stem (C_{xy}, Equation 2.19) and the steady-state concentration in the stem (C_{stem}, Equation 2.20).

Once chemical concentrations are modelled for the different produce types this information is combined with the amount of produce ingested by the receptor to calculate the exposure from this pathway (Section 2.5.3, Equation 2.29).

2.4.5 Inhalation of dust

Dust is not made up of just soil particles but can include clothing fibres, hair, moulds, pollen, bacteria and skin. Not all particles are important in terms of health impact and particle size is the key parameter. Particles of less than 150 µm can be breathed in by adults and children, but most particles greater than 10 µm are trapped in the nose or throat.

The CLEA model only considers dust arising from soil. The fraction of outdoor soil that contributes to

Equation 2.14

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

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

Equation 2.15

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

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

Equation 2.16

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

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

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

Equation 2.17

$$CF_{tuber\ vegetables} = \frac{k_1}{k_2 + k_g}$$

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

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

Equation 2.18

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

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

Equation 2.19

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

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

Equation 2.20

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

Where: C_{stem} is the chemical concentration in the woody stem, $mg\ g^{-1}$ dw
C_{Xy} is the chemical concentration in the xylem sap, $mg\ cm^{-3}$
Q is the transpiration stream flow rate, $cm^3\ year^{-1}$ [2.5×10^7]
M is the mass of the woody stem, g dw [5.0×10^4]
K_{wood} is the wood–water partition coefficient, $mg\ g^{-1}$ dw wood per $mg\ cm^{-3}$ water
k_e is the rate of chemical metabolism, $year^{-1}$ [0]
k_g is the rate of dilution due to wood growth, $year^{-1}$ [0.01]

Equation 2.21

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

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

indoor dust, and the tracking back of contamination into buildings, is a difficult process to model. There is a detailed discussion in the Updated Technical Background to the CLEA Model (EA, 2009).

In the CLEA model it is assumed that the indoor dust concentration of a chemical from soil is related to the soil concentration by a transport factor (TF) calculated by Equation 2.22.

Equation 2.22

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

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

2.5 Exposure modelling

Fate and transport modelling is used to calculate exposure point media concentrations when data are not available for the media of concern. However, the calculation of human exposure levels also requires data on the receptor, including activity patterns and physiological parameters. A summary of these default parameters is included here, and more detail can be found in the Updated Technical Background to the CLEA Model (EA, 2009). The methods of modelling intake for each CLEA exposure scenario are described in Section 2.5 3 onwards.

2.5.1 Physiological parameters

CLEA uses a variety of key physiological parameters, including:

- body weight and height (kg and m)
- inhalation rate (m^3 hour^{-1})
- exposed skin area (cm^2) and soil-to-skin adherence factors (mg soil cm^{-2} skin)
- vegetable/fruit consumption rate (g fw kg^{-1} bw day^{-1})
- home-grown fraction fruit and vegetables consumed.

Body weight and height

The CLEA model uses body weights and heights from the Health Survey for England 2003 (NCSR & UCL, 2003). Table 2.6 lists body weight and heights for males and females for each age class. In the generic CLEA model, the mean female weights and heights are used as default values (Jeffries, 2009).

Table 2.6 Mean body weights and heights for males and females from the 2003 Health Survey for England (Jeffries, 2009)

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

Body weights are used in determining intakes via different routes of exposures and are therefore used in all the intake equations found in the following sections.

Inhalation rate

Inhalation rate is key to the estimation of intake for many exposure assessments. The usual method for measuring inhalation rate is the minute volume as litres of air per minute (US EPA, 1997). Inhalation rate depends on characteristics such as age, sex, fitness level and activity or work rate.

Table 2.7 gives the default values used in the CLEA model for the residential and commercial land uses. Table 2.8 gives inhalation rates for the allotment land use where the default site occupancy rate is three hours per day. The younger child (aged 0 to 3 years) is assumed to spend two hours undertaking light activity and one hour on moderate activity while on site. For the older child (aged 4 to 6 years) it is half and half.

Exposed skin area, soil–to–skin adherence factors and skin absorption

Exposed skin area

CLEA uses a relationship between height and weight to estimate total skin area, see Equation 2.23. Not all skin will be exposed however. Equation 2.24 is used to calculate the exposed skin area (m^2) for each age class modelled by CLEA.

The maximum exposed fraction of skin (ϕ_{max}) varies with age, and with land use and activity (indoors or

Table 2.7 CLEA default inhalation rates for the residential and commercial land uses, based on long-term exposure

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

Table 2.8 CLEA default inhalation rates according to age and sex for the allotment land use, based on short-term exposure

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

[1] Assuming an hourly rate for 24 hours

outdoors). Table 2.9 gives estimates of exposed skin fraction for the residential and allotment scenarios and Table 2.10 for the commercial scenario.

CLEA uses exposed skin area (SE, Equation 2.24) for each land use; the values used are shown in Table 2.11.

Soil-to-skin adherence factors

Exposure to contaminated soil is particularly sensitive to the amount of soil adhered to the skin over the contact period, but there is considerable uncertainty in deriving soil-to-skin adherence factors. Soil loading is highly variable and varies with soil properties, especially texture and moisture content. The CLEA model uses the default values in Table 2.12 for soil-to-skin adherence factors.

Contamination absorbed through the skin

The layers of the skin (dermis and epidermis) provide a physical barrier to the absorption of chemicals into the body. A number of factors affect the absorption process,

Equation 2.23

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

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

Equation 2.24

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

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

including age, soil type and the solubility of the contaminant in fat. There are significant uncertainties in understanding the extent to which a chemical is absorbed by the skin and how it partitions from the soil to skin. The dermal absorption factor (ABS_d) used by the CLEA model for generic assessment, is 0.1 for all organic chemicals and zero for inorganic chemicals (in the absence of a literature value).

Consumption rate and home–grown fraction

Both the residential and allotment exposure scenarios take account of consumption of home-grown fruit and vegetables, which have been included in accordance with the FSA PRISM model (Thorne *et al.*, 2004) and are listed in Section 2.4.3. Consumption rates (at the 90th percentile) have also been suggested by the FSA and have been taken from a variety of dietary surveys (Table 2.13). For ages one-and-a-half upwards, the National Diet and Nutrition Survey (NDNS) has been used. The NDNS has not yet considered younger children so an older survey has been used. Further details are listed in the Updated Technical Background to the CLEA Model (EA, 2009).

To calculate a chemical intake via ingestion of fruit and vegetables, the proportion of produce that is home grown is also required. The evidence for this parameter is not as robust as that for consumption rates. The majority of the UK population grows little or no produce (either fruit or vegetable): the Defra Expenditure and Food Survey supports this (Defra, 2007). Table 2.14 gives the average fraction of home-grown produce (i.e. non-purchased) for each fruit and vegetable group. There are subgroups of the population that do grow their own fruit and vegetables (e.g. allotment holders) and they could be expected to consume a much higher proportion of their intake from their own produce. Table 2.15 gives home-grown fractions (HF) for an average and a high-end consumer for each produce group.

Table 2.9 Estimates of maximum exposed skin fraction during indoor and outdoor activities for the residential and allotment land uses

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

Table 2.10 Estimates of maximum exposed skin fraction during indoor and outdoor activities for commercial land use

Age class	Outdoors coverage	ϕmax (m^2 m^{-2})	Indoors coverage	ϕmax (m^2 m^{-2})
17	Assumes face and hands exposed	0.08	Assumes face and hands exposed	0.08

Table 2.11 Calculated exposed skin values by age, sex, and land use

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

[1] Only age class 17, i.e. people of working age, are considered as part of the commercial land use scenario.

Table 2.12 Default values for soil-to-skin adherence factors by age and land use

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

2.5.2 Activity parameters

Specific activities of land use and duration are critical parameters when modelling exposure using CLEA.

Exposure frequency

Table 2.16 shows the exposure frequencies for each exposure pathway modelled as part of the residential exposure scenario, Table 2.17 for the allotment scenario and Table 2.18 for the commercial scenario.

Occupancy period

Table 2.19 gives the default site occupancy periods used in the CLEA model for the residential land use, Table 2.20 for the commercial land use and Table 2.21 for the allotment land use.

2.5.3 Intake calculations for exposure pathways

Inhalation of vapours: Outdoors and indoors

The chemical exposure rate for the inhalation of contamination from soil-derived vapours is shown in Equation 2.25 for *ambient* air. The inhalation rate, V_{inh} and the outdoor site occupancy rate (T_{site}) were described in sections 2.5.1 and 2.5.2, respectively.

Equation 2.25

$$IR = C_{air} V_{inh} \left(\frac{T_{site}}{24} \right)$$

Where: IR is the chemical intake rate from inhalation of vapour from ambient air, mg day^{-1}
C_{air} is the ambient air concentration of the chemical, mg m^{-3}
V_{inh} is the daily inhalation rate, m^3 day^{-1}
T_{site} is the outdoor site occupancy period, hour day^{-1}

The chemical exposure rate for the inhalation of contamination from soil-derived vapours is shown in Equation 2.26 for *indoor* air. The indoor inhalation rate, V_{inh} and the indoor site occupancy rate (T_{site}) were described in sections 2.5.1 and 2.5.2.

Equation 2.26

$$IR = C_{air} V_{inh} \left(\frac{T_{site}}{24} \right)$$

Where: IR is the chemical intake rate from inhalation of vapour from indoor air, mg day^{-1}
C_{air} is the indoor air concentration of the chemical, mg m^{-3}
V_{inh} is the daily inhalation rate, m^3 day^{-1}
T_{site} is the indoor site occupancy period, hour day^{-1}

Table 2.13 Consumption rates for produce categories by age class

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

[1] Not a NDNS survey

Table 2.14 Estimated proportion of home–grown fruit and vegetables from the Expenditure and Food Survey 2004/05

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

Table 2.15 Generic values of home–grown fraction for average and high–end scenarios (such as allotment holders)

Produce type		Home–grown fraction	
		Average	High
Vegetables			
	Green	0.05	0.33
	Root	0.06	0.40
	Tuber	0.02	0.13
Fruit			
	Herbaceous	0.06	0.40
	Shrub	0.09	0.60
	Tree	0.04	0.27

Ingestion of soil and dust

Direct soil and dust ingestion

The chemical exposure rate for the direct ingestion of soil and indoor dust is calculated by the CLEA model using Equation 2.27. Default soil and dust ingestion rates were discussed in Section 2.4.3.

Indirect soil ingestion

The chemical exposure rate for the indirect ingestion of soil attached to home-grown produce is calculated by CLEA using Equation 2.28. The soil loading (SL_x) and preparation (PF_x) factors were discussed in Section 2.4.3.

Ingestion of fruit and vegetables

The chemical intake rate for the consumption of home-grown produce is calculated in CLEA using Equation 2.29. The soil-to-plant concentration factors (CF) have been described in Section 2.4.1, consumption rates (CR) and the home-grown fraction (HF) in Section 2.5.1.

Table 2.16 Default exposure frequencies for each pathway for age classes 1 to 6: Residential land use

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

[1] It is assumed that an infant has limited contact with garden soils or household dust for the first six months of life.
[2] Department of Health (2006) recommends that infants are introduced to solid food from about age six months, starting with pureed fruit and vegetables such as pear, carrot and potato.

Table 2.17 Default exposure frequencies per pathway for age classes 1 to 6: Allotment land use

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

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

Table 2.18 Default exposure frequencies for each pathway for age class 17: Commercial land use

	Standard commercial land use exposure frequency (days year^{-1})
Soil and dust ingestion	230
Dermal contact with indoor dust	230
Dermal contact with soil	170
Inhalation of dust and vapours from indoor air	230
Inhalation of dust and vapours from ambient air	170

Equation 2.27

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

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

Table 2.19 Default site occupancy periods for age classes 1 to 6: Residential land use

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

[1] It is assumed that the child is at school for 7 hours per day for 180 days per year, and at home for 24 hours per day on non-school days.

Table 2.20 Default site occupancy periods for commercial land use

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

[1] It is assumed that the worker spends 230 days per year on site, but only goes outside on 170 days per year for no more than 1 hour per day – all activities are passive.

Table 2.21 Default on–site occupancy periods for age classes 1–6: Allotment land use

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

Dermal absorption

In contrast to other exposure pathways included in the CLEA model, this exposure route is measured as uptake rather than intake. The chemical uptake rate for dermal contact with soil and dust is calculated in the CLEA model for outdoor (Equation 2.30) and indoor exposure (Equation 2.31). The exposed skin area (A_{skin}) dermal absorption fraction (ABS_d) and soil-to-skin adherence factor (AF) were discussed in Section 2.5.1.

Inhalation of dust: Indoors and outdoors

For ambient air the chemical intake is calculated in CLEA by Equation 2.32. The daily inhalation rate (V_{inh}) and the site occupancy rate (T_{site}) were described in sections 2.5.1 and 2.5.2, respectively. The particulate emission factor (PEF) has not been discussed here, but details can be found in the Updated Technical Background to the CLEA Model (EA, 2009).

For indoor air, the chemical intake rate from inhalation of dust from indoor air is calculated in the CLEA model using Equation 2.33.

2.6 Case study

An initial site investigation at a commercial site found chromium concentration in soils at the 95% upper confidence limit of 3338 mg kg^{-1}. The soil at the site was characterised as a typical UK sandy soil with a pH of 6.0 and a total soil organic matter content of 6%. Given the site use, the commercial conceptual model was selected in the CLEA software. The exposure pathways for the site users were selected as:

- direct soil ingestion
- skin contact with soil-derived contaminants
- inhalation of soil-derived indoor dust
- inhalation of soil dust.

Other pathways included in CLEA, such as ingestion of fruit and vegetables, are not applicable for this land use and are excluded.

The chromium at the site was analysed and reported as Cr(VI), the more toxic of the two types of chromium found in soils. Therefore the HCV used is that derived for Cr(VI). The applicable HCV for use in land contamination assessments needs to consider the background exposure of the receptor to non-soil sources of contamination. Therefore the HCV used for the oral and inhalation exposures are 2.8 and 0.001 µg kg^{-1} bw day^{-1}, respectively.

Using the CLEA UK software and the information below (Table 2.22), it was determined that the oral exposure pathway was the dominant exposure. This pathway alone contributed almost 100% of the total exposure. The inhalation of dust had minimal contributions to overall exposure. The calculated ADE_{oral} and ADE_{inh} were 1.807 µg kg^{-1} bw day^{-1} and 3.45×10^{-4} µg kg^{-1} bw day^{-1}, respectively. The

ADE_{oral}/HCV_{oral} ratio (1.807/2.8) was calculated to be 0.65, and the ADE_{inh}/HCV_{inh} ratio ($3.45 \times 10^{-4}/0.001$) was 0.345. The cumulative *ADE* to *HCV* ratio is 0.995 (EA, 2005). Therefore, the risk to the receptor from chromium at the site is considered to be minimal.

Equation 2.28

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

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

Equation 2.29

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

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

Equation 2.30

$$IR = C_s\ n\ AF\ ABS_d\ A_{skin} \times \frac{1}{10^3}\ \text{g mg}^{-1} \times 10^4\ \text{cm}^2\ \text{m}^{-2}$$

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

Equation 2.31

$$IR = C_s\ TF\ n\ AF\ ABS_d\ A_{skin} \times \frac{1}{10^3}\ \text{g mg}^{-1} \times 10^4\ \text{cm}^2\ \text{m}^{-2}$$

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

Equation 2.32

$$IR = C_s \left(\frac{1}{PEF}\right) V_{inh} \left(\frac{T_{site}}{24}\right) \times 10^3 \text{ g kg}^{-1}$$

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

Equation 2.33

$$IR = \left[C_s \left(\frac{1}{PEF}\right) \times 10^3 \text{ g kg}^{-1} + \left(C_s \, TF \, DL\right)\right] V_{inh} \left(\frac{T_{site}}{24}\right)$$

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

Table 2.22 Commercial land use exposure parameters

Exposure parameters for the adult female critical receptor		Value
Exposure frequency, day yr^{-1} (EF)	Direct soil and dust ingestion	230
	Skin contact, indoors	230
	Skin contact, outdoors	170
	Inhalation of dust and vapours, indoors	230
	Inhalation of dust and vapours, outdoors	170
Respiration frequency, hr day^{-1} (T_{act} and T_{pas})	Active, indoors	2.00
	Active, outdoors	0.66
	Passive, indoors	5.50
	Passive, outdoors	0.33
Soil ingestion rate, mg day^{-1} (SIR)	Soil ingestion rate	40.0
Soil–skin adherence factor, mg cm^{-2} (AF)	Indoor	14.0
	Outdoor	14.0
Exposed skin fraction, dimensionless (ϕ_{exp})	Indoor maximum exposed skin fraction	0.07
	Outdoor maximum exposed skin fraction	0.07
Exposure duration, yr (ED)		43.0
Body weight, kg (BW)	Normal PDF (mean; 5th and 50th percentile; standard deviation)	68.5; 46.4 and 68.5; 13.870
Body height, m (H)		1.623

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3 Health and Safety Executive's Approach to Exposure Modelling

3.1 Introduction

Exposure modelling at the Health and Safety Executive (HSE) is primarily performed to investigate exposure to particular substances to support exposure assessments conducted under statutory chemicals assessment schemes. In order to carry out a comprehensive review of exposure to a substance, a lot of detailed information is needed. In many cases this is not realistically achievable, and exposure assessment must be made using fewer data than is desirable. Although in many cases data may be sparse, it is also possible to estimate exposure by various techniques, including modelling. This chapter focuses on exposure to industrial chemicals, biocides and pesticides.

3.2 Exposure assessment

Substances may enter the body by being breathed in (inhalation), by passing through the skin (dermal), or swallowing (ingestion). Exposure to a particular substance should normally be understood as external exposure. This can be defined as the amount of the substance ingested, the amount in contact with the skin, and/or the amount inhaled, which is represented by the airborne concentration of the substance in the breathing zone. It does not usually refer to concentrations within the body, which are consistent with some measure of absorbed dose.

Exposure can be considered as a single event or as a series of repeated events, or as continuous exposure. As well as an estimation of the levels of exposure, either from measured or modelled data, the assessor needs to address other parameters such as duration and frequency of exposure and the size of the exposed workforce. It may also be appropriate to consider task-based exposures, particularly for acute effects.

When considering biocides, the exposed human populations are categorised by the nature of the exposure, that is, primary exposure or secondary exposure. Primary exposure to biocidal products occurs to the individual who actively applies biocidal products – the user. Secondary exposure occurs to non-users or bystanders; these individuals do not actively apply biocidal products but are indirectly exposed during or after product application by another person. Consideration is also given to the fact that the primary user group may comprise a professional at work or a non-professional, that is, the amateur or 'consumer'.

The legislative requirements for the authorisation of pesticides require that the approved use of the pesticide product will not present unacceptable risks to those consuming treated commodities, or exposed by other routes as a result of the application of the pesticide. Modelling is performed at an early assessment tier to permit the use of generic data rather than having to perform individual exposure monitoring studies for every pesticide use.

3.2.1 Assessment of worker and consumer exposure under REACH

REACH (the acronym stands for the Registration, Evaluation, Authorisation and restriction of Chemicals) is a recently implemented European Union regulation that governs the supply and use of chemicals, and its provisions apply at all levels of the supply chain including consumer use. The goal for risk assessments carried out under REACH is to identify the conditions under which substances can be used safely. Hazard data are used to identify benchmarks indicating acceptable levels of exposure called derived no-effect levels (DNEL) or derived minimal-effect levels (DMEL). An iterative exposure assessment approach is then used to identify the process operating conditions (OC) and risk management measures (RMM) that are necessary to ensure exposures during use do not exceed these benchmark values. Depending on the particular use

for a chemical it may be necessary to consider inhalation, dermal and/or oral exposures. An initial exposure assessment is performed to identify the levels of exposure that are anticipated to occur with current OC and RMM. If estimated or measured exposure levels are equal to or below the value of the DNEL/DMEL, no further assessment is required. However, if measured or estimated exposure levels are above the value of the DNEL/DMEL then it is necessary to identify what additional control measures may be necessary and estimate the exposure levels that could arise if these additional controls are implemented. Successive iterations are performed until a set of OC and RMM have been identified that have the potential to keep exposure levels below the DNEL/DMEL. This set of OC and RMM is then documented in the format of an exposure scenario. Where required, exposure scenarios are generated for each use of a chemical and companies are expected to follow the measures described in exposure scenarios when they use these chemicals. This basic process is followed for occupational and consumer exposure assessments.

In many cases measured data may not be available to inform this exposure assessment process, and it is necessary to use modelling tools to predict exposures. In recent years a lot of effort has gone into developing models that are able to take into account a range of determinants of exposure. Determinants of exposure include:

- substance-specific factors, such as volatility, particle size and chemical reactivity
- factors relating to the OC for the process, such as the type of activity, the scale, how frequently it is carried out and the process temperature
- factors relating to any RMM that may be in place, for example local exhaust ventilation (LEV) or personal protective equipment (PPE) and the effectiveness of these measures; product packaging may also be designed to limit exposure during use and should also be considered
- factors relating to the surroundings in which the task is performed, for example whether indoors or outdoors, in small or large spaces, and the level of natural ventilation present.

The introduction of new models has enabled assessors to take a tiered approach to exposure assessment. Initial Tier 1 assessments can be performed using conservative 'reasonable worst-case' estimates for the conditions of use described. If it is not possible to demonstrate adequate control of risk using Tier 1 models, the assessor can refine their exposure predictions using higher-tier models. Higher-tier models take account of a greater range of determinants of exposure, but also require more specialist knowledge to input data and interpret the exposure predictions. Most of the higher-tier tools currently available for REACH are not regarded as Tier 2 tools but rather fall somewhere between Tier 1 and Tier 2.

The exposure assessment approaches for workers and consumers are described in Chapters 14 and 15, respectively, of the chemical safety assessment guidance documents developed by the European Chemicals Agency to help companies fulfil their duties under REACH (ECHA, 2010a,b).

3.2.2 Biocides

The Biocidal Products Regulations (BPR) 2001 (SI 2001/880)[1] is the statutory instrument that implements the EU Biocidal Products Directive (98/8/EC) (BPD)[2] in Great Britain and has been amended three times since being introduced in 2001.

The Biocidal Products (Amendment) Regulations 2003 (SI 2003/429)[3] came into force on 1 April 2003. Fulfilment of the Directive means that active substances used in biocidal products must be authorised and included on a 'positive list', referred to as Annex 1. Once a substance has been placed on Annex 1, products can then be authorised at member-state level. Authorisation is an administrative act by which a member state competent authority (CA) allows a biocidal product to be marketed. In the UK the CA for biocides is the HSE. A product can be authorised once the CA is satisfied that both the human health and environmental risks are acceptable, that it is sufficiently efficacious and that there are no unacceptable effects. Assessments of active substances and products by individual member states are subject to scrutiny and agreement by all member states before authorisation is granted. To establish a consistent approach across all member states to biocide exposure assessment, the following guidance documents have been produced.

- Technical Notes for Guidance on Human Exposure to Biocidal Products (TNsG; European Commission, June 2007)
- Technical Notes for Guidance on Human Exposure to Biocidal Products (TNsG; European Commission, 2002a)
- Human Exposure to Biocidal Products – User guidance (European Commission, 2002b)

[1] http://www.opsi.gov.uk/si/si2001/20010880.htm [accessed July 2010]
[2] http://www.hse.gov.uk/biocides/glossary.htm#bpd [accessed July 2010]
[3] http://www.opsi.gov.uk/si/si2003/20030429.htm [accessed July 2010]

Complete versions of this guidance (2002a,b, 2007) and initial report of the Biocides Exposure Steering Group) are available from the European Commission website[1].

The earlier versions provide detailed insight into the models used for exposure estimation. However for all newly assessed active substances and those on the 4th Review list it is anticipated that the June 2007 guidance[2] will form the basis for exposure estimation, directing exposure assessors primarily to use the Bayesian Exposure Assessment Toolkit (BEAT) model, but allowing some flexibility to apply the approach in earlier guidance where specific data sets exist.

This guidance has consolidated the available exposure data and models on biocides and set out a unified approach for predicting human exposure to biocidal products. The overall approach for assessing human exposure to biocidal products is discussed in more detail in Section 3.4.

3.2.3 Pesticides

Exposure to pesticides can occur in a variety of ways, and several exposure scenarios are modelled to cover the different types of exposure. These scenarios can be divided into two broad categories.

- Consumption of foodstuffs that have been treated with pesticides
- Non-dietary exposure from contact with pesticides prior to, during or after application

Within these categories there are subcategories. In the non-dietary group there is the potential for dermal, inhalation and ingestion as routes of exposure; these are converted, within the model, to an overall systemic dose and summed where appropriate.

The output of the exposure modelling is normally expressed in milligrams of pesticide active substance per kilogram body weight. This is compared with a reference dose relevant to the exposure scenario being considered. The reference doses are derived[3] from no observed adverse effect levels (NOAEL) from an extensive range of animal studies mostly using the oral route of exposure. The most relevant NOAEL is divided by an uncertainty factor (most often 100) to allow for the possibility that animals used in toxicity studies might be less sensitive than humans and that there might be human subpopulations that are more sensitive than the average.

If the predicted exposure is below the reference dose, approval can be granted; if it is above then risk management decisions need to be taken.

The modelling of exposure to pesticides is covered in full in Section 3.6.

3.3 Exposure assessments of industrial chemicals for workers and consumers under REACH

The guidance documents produced by the European Chemicals Agency (ECHA) to help assessors carry out exposure assessments under REACH describe the information needed for the assessment at different tiers and how to deal with the information that is available (ECHA, 2010a,b). Where robust measured data are available that are relevant for the scenario of interest, these are given preference to data derived from modelling approaches. As far as possible, exposure estimations should take account of the control measures that have been implemented. Where suitable measured data are not available, the guidance recommends the use of modelling tools. A number of modelling tools are recommended and described in the REACH guidance documents for estimating exposure at both the Tier 1 and higher-tier levels. These models vary in their complexity and purpose. Tier 1 models are generally conservative and may well generate exposure estimates that are well above the exposure levels that occur in practice. Higher-tier estimations are much more specific, but require more detail about the circumstances of exposure and greater degree of specialist knowledge to use. Several of these models have been developed specifically for REACH and in some cases have only recently been released. As a consequence, case studies are not available to include in this document. The following description of the models that will be used to assess occupational and consumer exposure to chemicals under REACH is based on the information provided in the guidance documents published by ECHA.

3.3.1 Occupational exposure estimation

Tier 1 tools

The currently available Tier 1 tools are simple to use and inherently conservative. It is recommended that they are used to provide an initial screen allowing a defined range of OC and RMM to be quickly identified and evaluated.

[1] http://ecb.jrc.ec.europa.eu/biocides/ [accessed July 2010]

[2] Human Exposure to Biocidal Products - Technical Notes for Guidance June 2007, available at: http://ecb.jrc.ec.europa.eu/DOCUMENTS/Biocides/TECHNICAL_NOTES_FOR_GUIDANCE/TNsG_ON_HUMAN_EXPOSURE/TNsG%20-Human-Exposure-2007.pdf [accessed July 2010]

[3] For more details see IGHRC (2003); WHO (1990)

ECETOC TRA tool

The ECETOC targeted risk assessment (TRA) tool can be used to estimate inhalation and dermal exposure to workers. It is based on the EASE model, which is an empirical knowledge-based model developed by HSE (Cherrie *et al.*, 2003), but with modifications which allow a more precise, structured and simplified approach. It aims to provide conservative predictions that will allow users to demonstrate minimal risk when exposure estimates are compared with DNEL.

The ECETOC TRA uses the process categories (PROC, as presented in REACH Guidance Chapter R12, Appendix R12-3; ECHA 2010c) as a basic starting point for the exposure estimation. Process categories provide a harmonised system for users to categorise chemicals by sector of use. Each PROC is linked to estimates of inhalation and dermal exposure. These estimates are then modified on the basis of the OC and RMM that are in place. The exposure modifiers also include duration of activity, percentage of substance used (if in preparation), and the impact of working outdoors.

The following input parameters are required.

- Molecular weight (needed for recalculation from ppm to mg/kg bw/day)
- Physical state of the substance (solid or not)
- Vapour pressure (liquids/gases) or dustiness (solids)
- PROC
- Whether the activity is industrial or professional
- Whether the activity takes place indoors or outdoors
- Presence of LEV (only for indoor activities)
- Duration of the activity (in classes)
- Type of respiratory protection used
- Whether the substance is used in a preparation
- Concentration range of the substance in the preparation (in classes; only if used in a preparation)

For inhalation exposure, the model assumes that the concentration of a substance in the workplace atmosphere can be predicted by analogy with similar situations where the exposure concentration has been measured. Three parameters are included in the model: physical state, pattern of use and pattern of control. The estimated exposure is expressed in ppm or mg m^{-3}. The predicted values represent external concentrations; ECETOC-TRA worker model does not provide information on systemic exposure, hence it does not require default assumptions about body weight or respiration rates.

The estimated dermal applied dose for each scenario in ECETOC-TRA is determined by multiplying the EASE output with the assumed dermal contact area (varying with scenario). The same parameters as that of the inhalation model are included: physical state, pattern of use and pattern of control. The estimated dermal exposure is expressed in µg cm^{-2}. It is assumed that no personal protection is used and that dermal absorption/permeation is 100%. Depending on the contact area, the external, local exposure can be transformed into systemic exposure.

EMKG-Expo tool

An alternative model that can also be used to generate Tier 1 estimates of workplace inhalation exposure is the EMKG-Expo tool developed by Germany. It is a generic tool that can be used to filter out low-risk workplace situations, and may be useful in selecting appropriate control measures.

The following input parameters are required.

- Type of substance: solid or liquid
- Dustiness or volatility (boiling point/vapour pressure)
- Operational conditions (temperature, amount of substance or product used per task)
- Implemented RMM (control strategy)
- Exposure period (<15 min or >15 min)

For solids, the principal determinant of exposure is dustiness. For liquids, volatility is the key determinant. The scale of use/batch or operation (small, g ml^{-1}; medium, kg L^{-1}; or large, tonnes m^{-3}) is regarded as the most important operational factor to be considered. The control strategy is defined, with general control solutions that have the potential to reduce exposure underpinned by a series of control guidance sheets which provide practical examples of possible control approaches for common industrial tasks such as weighing and filling. The tool predicts a lower and an upper value for the exposure range (in mg m^{-3} for solids and ppm for vapours). The upper value of the exposure range is used for risk characterisation (i.e. the comparison with the DNEL value). The tool assumes that exposures occur over a full shift. If the activity is carried out for less than 15 minutes per day, the next lower exposure range can be used.

Higher–tier tools

Higher-tier assessment is conducted if an exposure assessment at Tier 1 indicates that the exposure level

is not acceptable; that is, protection is not adequate. Higher-tier assessments are generally much more detailed and specific, and can be done by any suitable method that is valid and sufficiently accurate. Several new approaches and tools are under development by industry and consortia of European institutions. Three of these approaches are recommended in the REACH guidance document for use in higher-tier assessment of occupational exposure. These are the Advanced REACH Tool, the Stoffenmanager 4.0 Tool and RISKOFDERM.

Advanced REACH Tool

The Advanced REACH Tool (ART) is the only Tier 2 model available for occupational exposure estimation at present. It is intended for use by experts and combines both mechanistically modelled estimates of exposure and any relevant measurements of exposure using a Bayesian statistical process to produce exposure estimates for the inhalation route for specific scenarios. The approach provides estimates of the whole distribution of exposure variability and uncertainty, allowing the user to produce a variety of realistic and reasonable worst-case exposure estimates depending upon the requirements of the particular risk assessment. This approach allows ART to incorporate any new data that become available during the risk assessment process, or in future.

ART can be used for assessing exposure to liquids and solids that are used in manual, semi or fully automated processes. It is also suitable for liquids and solids that are formed during processes such as fracturing of solid objects, abrasive blasting, impaction on and handling of contaminated objects. However, it cannot be used where substances are formed through reaction processes (e.g. exhaust fumes, rubber fumes). ART is particularly useful for assessing situations where exposure is determined to a relatively large extent by OC and RMM that are outside the scope of other models (e.g. automation, remote control, separation, influence of specific types of LEV, fugitive emissions) and when measured data are available that can support exposure assessment.

Inputs to ART are arranged in sets of so-called 'principal modifying factors' (MF) such as intrinsic emission rates, efficacy of local controls and methods of handling or processing of chemicals. The user of the tool is guided through these inputs.

For calculation of exposure with the mechanistic model the following inputs are needed.

- Duration of activities (each gets a separate assessment) within the shift
- Type of material used (powdered, granular or pelletised material; solid objects; liquids)
  - For powdered, granular or pelletised material:
    - dustiness (measured) or dustiness category
    - moisture content of the material
  - For solid objects:
    - material of the solid object
    - moisture content of the material
  - For liquids:
    - temperature of liquid in process (or relative to room temperature)
    - vapour pressure of the liquid
    - boiling point of the liquid
    - viscosity of the liquid
    - activity coefficient of the substance in the liquid
- For all materials: molar or weight fraction of the substance in the material
- Primary emission source in the breathing zone of the worker (yes/no)
  - if yes, secondary sources outside the breathing zone also need to be assessed

For both primary and secondary emission sources (separately) the following information has to be provided.

- Activity class of the activity:
  - in some cases activity subclasses are also defined
  - for some activity classes further questions are asked, such as spray direction (for spraying) and drop height (for dropping of material, e.g. in transfer)
  - for several activity classes a parameter representing the scale of the activity needs to be provided (in classes), e.g. use rate or surface area

For primary sources (both within and outside the breathing zone) the following information on RMM is required.

- Any control measures close to the source, with the following choices and sub-options:
  - suppression techniques (only for powdered, granular or palletised material)
  - containment without extraction
  - LEV – three options, each with two to three sub-options available

- Measures to limit surface contamination and fugitive emissions:
  - enclosure of process
  - evidently effective housekeeping
  - general housekeeping
- Conditions and measures of dispersion:
  - working indoors, outdoors or in a spray room
  - for indoors, room size and ventilation rate
  - for outdoors, placement of source relative to buildings and of worker relative to source

For primary sources outside the breathing zone only the following RMM need to be evaluated.

- Emission source segregated from the worker (several options)
- Worker separated from the emission source by a personal enclosure (several options)

For secondary sources (outside the breathing zone) the question regarding emission sources segregated from the worker also applies.

In addition to the above-mentioned technical parameters that are required to perform calculations, some administrative data on, for example, the name of the substance and the name of the assessment are also requested.

The output provides a choice of results.

- Full-shift or long-term exposure, where the long-term result takes into account typical variation within and between workers' groups
- 50th, 75th, 90th and 99th percent of exposure distribution
- 90%, 95% or 99% confidence interval around the chosen percentile

It is intended that future updates will include an exposure database from which analogous data can be derived, and with the possibility to assess short-term exposure levels.

The Stoffenmanager tool

The Stoffenmanager tool[1] was originally a web-based risk prioritising tool developed for use by small and medium-sized enterprises. Version 4.0 includes a quantitative model for estimating inhalation exposures to vapours, aerosols of low volatility and inhalable dusts.

The model is underpinned and validated by an exposure database containing around 1000 measurements. Also, the time-weighted average can be calculated for one or several combined tasks with duration of less than eight hours.

The following parameters are required to generate a quantitative exposure prediction.

- Physical state of the substance (solid or liquid)
- Whether there are activities involving articles (i.e. solid objects) that may cause emission of dust
- Vapour pressure of liquids (used directly) or dustiness (solid articles, firm granules or flakes, granules or flakes, coarse dust, fine dust, extremely dusty products)
- Type of dust emitted from solid objects (presently only stone or wood)
- Percentage of the substance(s) in the product
- Level of dilution of liquid products (undiluted = 100%)
- Handling category
- Local controls (including LEV and containment)
- Distance of the worker to the source (within 1 m or not)
- Presence of secondary emission sources:
  - other workers using the same substance simultaneously
  - a period of drying or hardening after the activity (with prolonged emission of vapours)
- Room volume
- General ventilation
- Immission control measures (such as control rooms)
- PPE used
- Whether or not the work area is regularly cleaned
- Whether machinery and equipment are regularly inspected and kept in good order

For calculating time-weighted averages, separate assessments per activity should first be made. These are then combined using the duration of each activity to calculate time-weighted averages. Stoffenmanager predicts a median task-based exposure level in mg m^{-3}. Various percentiles for the exposure distribution are also calculated for the given input values. These are based on calibration, with substantial measurement series covering exposure to vapours, liquid aerosols and inhalable dust. If conservative values are used for all inputs, the 75th percentile of the output distribution is considered as the reasonable worst case. If less-conservative values are used, the 90th percentile of

[1] www.Stoffenmanager.nl [accessed July 2010]

the output distribution is selected as a reasonable worst case.

RISKOFDERM

The RISKOFDERM dermal exposure model is a spreadsheet-based model for estimating potential dermal exposure, that is, the total amount of a substance coming into contact with the protective clothing, work clothing and exposed skin. Each task involving dermal exposure is allocated to one of six process categories, also referred to as dermal exposure operations (DEO) units. The model then uses equations that have been obtained from statistical analyses of relatively large sets of measured data to generate quantitative exposure predictions for these processes. RISKOFDERM does not take into account any protective effect of clothing or gloves.

Once the relevant process has been selected, the following parameters are required.

- Type of skin contact
- Frequency of skin contact
- Type of product handled
- Viscosity of the product
- Volatility of the product
- Dustiness of the product
- Use rate of the product
- Formation of aerosols
- Manual or automated tasks
- Direction of application
- Tools used
- Quality of ventilation
- Direction of airflow
- Segregation of worker from source
- Distance of worker from source

In all cases, the duration of exposure is also needed.

The basic estimate made by RISKOFDERM is the potential exposure per minute (for hands and/or the remainder of the body). Total exposure over a longer period is calculated by entering the duration of the activity leading to the exposure. Full-shift estimates can be made by combining the results of separate estimates for different tasks. It is noted that simple summation of exposures from each task may overestimate exposure, since this does not take account of any decontamination of the skin that may occur between tasks either by deliberate washing or from incidental transfer to other surfaces. The facility to address this issue through the use of probabilistic methods to aggregate exposures is available in the web-based version of RISKOFDERM.

3.3.2 Consumer exposure estimation

Assessment of consumer exposure deals with consumer products that can be purchased from retail outlets by members of the general public. These products may be a single substance, a preparation (mixture of substances), or an article. Exposure to substances may arise from the direct use of the product, or indirectly by a bystander near where it is being used or after it has been used. The migration characteristics of the substance in the matrix, its solubility and the amounts typically used, are also taken into account in estimating the likely exposure. The way in which consumers are exposed to substances can generally be characterised by:

- the different routes of exposure, separately or in combination
- the different phases of activity in handling the consumer product
- whether the exposure is acute or repeated.

Consumer exposure estimation should normally address the intended uses of the products containing the substance of interest, and other reasonably foreseeable uses. Deliberate misuse (abuse) should not be included. However, it is recognised that in some cases the difference between 'other foreseeable uses' and abuse will be small.

Inhalation exposure may occur in the event of substances reaching the breathing zone of consumers, either during use or as a result of volatilisation after the product has been used, or due to emissions from articles. It is expressed as the concentration of the substance in the breathing zone atmosphere, presented as an average concentration over a reference time period (e.g. per day) or, if it is of intermittent short duration, per event. Some consumer products are used as sprays in the form of aerosols; in this case, the exposure to the substance is related to the droplets (i.e. particle size) which need to be considered specifically in a higher-tier exposure model. Inhalation exposure is expressed in terms of external exposure, as mg m^{-3}.

Dermal exposure is an estimate of the amount of substance contacting the exposed surfaces of the skin, and is given as the sum of the exposure estimates for the various parts of the exposed body surface. It can occur from splashes on the skin, from direct hand or body contact with the product containing the substance, from deposition on exposed skin of particles or aerosol residues on clothing after laundering or dry cleaning. Factors that can influence

dermal exposure include the amount and concentration of the substance, the area of skin exposure and the duration and frequency of exposure. Dermal exposure is expressed in terms of the amount of substance per unit surface area of the skin exposed (mg cm^{-2}) or as external dose (mg/kg bw/day).

Substances occurring in preparations or articles that can be ingested can cause oral exposure. Exposure may occur as a consequence of migration due to sucking, chewing or licking of toys, children's books or textiles. This is of particular relevance to children due to their hand to mouth and/or mouthing behaviour. Oral exposure is expressed as the amount of substance ingested per kg body weight, and is normally presented as an average daily external dose (mg/kg bw/day).

In some instances, the assessment of other routes of exposure may also need to be considered, such as via the eyes (by splashing) or intradermal exposure, which occurs when the integrity of the skin is disrupted by the use of consumer products, for example piercings.

Four phases of activity are usually considered in consumer exposure.

- Preparation for use by the user, which includes tasks like handling and dilution of concentrates
- Use or application by the user, including use of articles during their service life
- Post-use or post-application, leading to exposure of the user (e.g. exposure to paints after use)
- Removal or cleaning, leading to exposure of a user who may be different to the one in the first phase; this includes activities such as emptying and cleaning equipment and stripping surface coating

Each phase of activity may require separate exposure estimation; in practice, however, the resulting exposure scenario for the different products would include some or all of these phases.

Consumer exposure can be due to single or repeated uses of a substance. A single use of a consumer product or article can lead to acute exposure, but in some cases to long-term exposure where residues of the product or article are released over a longer time period. Daily, weekly and monthly consumer exposures are considered as repeated exposures. Chronic exposure occurs not only from repeated use of a substance but also from the release characteristics of a substance from consumer articles during service life. Thus, depending on the type of substance, the consumer product or article type, its properties and the duration and frequency of use, exposure can be characterised as acute or chronic exposure (either intermittent or continuous).

The three major routes, inhalation, dermal and oral, are considered in consumer exposure estimation, with calculations for each route conducted separately. Initially, a Tier 1 exposure estimate can be used to derive a 'worst case'; subsequent higher-tier estimates can be used to further refine or characterise the exposure.

Where a consumer may be exposed to a substance in a particular consumer product or article by more than one route, the contribution of each route to the total exposure should be added together.

Tier 1 algorithms

A series of algorithms is provided in the guidance document for consumer exposure assessment for use in assessing exposure by the inhalation, dermal and oral routes (ECHA, 2010b).

Inhalation exposure

In a Tier 1 assessment it is assumed that all the substance is released as a gas, vapour or airborne particulate into a standard room. This may be due to direct release or by evaporation from a liquid or solid matrix. The parameters shown in Table 3.1 may be required.

In the case where the respirable fraction is not known, the amount of product used (Q_{prod}) and fraction of the substance in the product (Fc_{prod}) are used to calculate the concentration of the substance in the room air.

It is assumed that the event duration is 24 hours, that 100% of the substance in the consumer product is released at once into the room, and there is no ventilation. The concentration in air after using an amount Q_{prod} of the product is calculated as shown in Equation 3.1.

Equation 3.1

$$C_{inh} = \frac{Q_{prod} \times Fc_{prod}}{V_{room}} \times 10^3$$

This equation can also be used to assess short-term local exposure by reducing the value for V_{room} (e.g. to 2 m^3) to represent the breathing zone of the user.

Where the inhalable and/or respirable fraction is known, it is possible to estimate the inhaled dose (D_{inh}), as in Equation 3.2.

Equation 3.2

$$D_{inh} = \frac{F_{resp} \times C_{inh} \times IH_{air} \times T_{contact}}{BW} \times n$$

Table 3.1 Parameters used to assess inhalation exposure

	Description	Unit
Input parameter		
Q_{prod}	Amount of product used	g
Fc_{prod}	Weight fraction of substance in product	g g_{prod}^{-1}
V_{room}	Room size (default 20 m^3)	m^3
F_{resp}	Respirable fraction of inhaled substance (default, 1)	–
IH_{air}	Ventilation rate of person	m^3 d^{-1}
$T_{contact}$	Duration of contact per event (default, 1 day)	d
BW	Body weight	kg
n	Mean number of events per day	d^{-1}
Output parameter		
C_{inh}	Concentration of substance in air in room	mg m^{-3}
D_{inh}	Inhalatory dose (intake) of substance per day and body weight	mg kg_{bw}^{-1} d^{-1}

Table 3.2 Parameters used to assess dermal exposure as a result of direct contact

	Description	Unit
Input parameter		
C_{prod}	Concentration of substance in product before dilution	g cm^{-3}
D	Dilution factor (if not diluted, $D = 1$)	–
RHO_{prod}	Density of product before dilution	g cm^{-3}
Q_{prod}	Amount of product used	g
Fc_{prod}	Weight fraction of substance in product	g g_{prod}^{-1}
V_{prod}	Volume of product used before dilution	cm^3
V_{appl}	Volume of diluted product actually contacting the skin	cm^3
TH_{der}	Thickness of product layer on skin (default 0.01 cm)	cm
A_{skin}	Surface area of the exposed skin	cm^2
BW	Body weight	kg
n	Mean number of events per day	d^{-1}
Output parameter		
C_{der}	Dermal concentration of substance on skin	mg cm^{-3}
L_{der}	Amount of substance on skin area per event	mg cm^{-2}
D_{der}	Amount of substance (external dose) that can potentially be taken up per body weight	mg kg_{bw}^{-1} d^{-1}
Further applications		
V^*_{appl}	Volume of diluted product remaining on the skin	cm^3
Fc_{der}	Fraction of the applied product remaining on the skin	–

Since the non-respirable fraction can be swallowed, it may also be necessary to consider oral exposure (see equations 3.10 and 3.11, below).

Higher-tier models are required to assess exposure where substances are released more slowly from a solid or liquid matrix.

Dermal exposure

Dermal exposure may occur in one of two ways. In the first situation, the substance is contained in a preparation such as paint, and exposure occurs a result of direct contact with the preparation either by immersion or splashing. In the second situation, the substance is present in an article, such as residual dyes in clothing, and exposure occurs as a result of migration from the article. The parameters that may be required to assess exposure from direct contact are shown in Table 3.2.

The Instant Application Model assumes that all the substance in a preparation is directly applied to the skin. The calculation requires information on the fraction of the compound present in the total product (F_{prod}), the amount of the product applied to the skin (Q_{prod}) and the surface area of the exposed skin (A_{skin}). Exposure expressed as dermal load (L_{der}) is calculated as the amount of product per surface area of skin using Equation 3.3.

Equation 3.3

$$L_{der} = \frac{Q_{prod} \times Fc_{prod}}{A_{skin}} \times 10^3$$

The external dose D_{der} is given by Equation 3.4.

Equation 3.4

$$D_{der} = \frac{Q_{prod} \times Fc_{prod} \times n}{BW} \times 10^3$$

In scenarios where the substance is contained in a liquid into which parts of the body such as the hands may be dipped, the equation is based not on the weight, but on the concentration of the substance in the liquid. First, the concentration C_{der} of the substance in contact with skin is calculated. Three analogous calculations are available depending on the information available, as shown in Equation 3.5.

Equation 3.5

$$C_{der} = \frac{C_{prod} \times 10^3}{D} = \frac{RHO_{prod} \times Fc_{prod} \times 10^3}{D} = \frac{C_{prod} \times Fc_{prod} \times 10^3}{V_{prod} \times D}$$

The total dermal load L_{der} is then calculated by Equation 3.6.

Equation 3.6

$$L_{der} = C_{der} \times TH_{der}$$

The dermal dose is derived as shown in Equation 3.7.

Equation 3.7

$$D_{der} = \frac{L_{der} \times A_{skin} \times n}{BW}$$

The above dermal equations apply also to:

- a non-volatile substance in a medium used without further dilution; in this case the dilution factor (D) is set to 1
- a non-volatile substance contained in an undiluted medium removed from the skin by, for example, wiping or rinsing and drying (e.g. liquid soap); recalculate the V^*_{appl} 'real' volume of application based on volume of application (V_{appl}) as $V^*_{appl} = V_{appl} \times Fc_{der}$ where Fc_{der} is the fraction of the product remaining on the skin
- a non-volatile substance in a volatile medium; the concentration C_{der} (Equation 3.5) is only valid at the very beginning of exposure, however this concentration can still be used to calculate L_{der} (see Equation 3.8), because the substance is non-volatile.

The second situation involves exposure to a non-volatile substance migrating from an article, for example, skin contact with substances in textiles. In this case the exposure calculation involves estimating the amount of substance which will migrate from the area of the article in contact with the skin during the period of contact. The parameters used for this model are shown in Table 3.3.

For migrating substances, only a fraction of the total amount of substance is able to reach the skin. It is therefore important to check that the estimated daily exposure does not exceed the theoretical maximum release. This can be derived from the amount of product used (g), the concentration of the substance in the product, and the use frequency (d^{-1}). The dermal load arising due to migration is calculated as shown in Equation 3.8.

Table 3.3 Parameters used to assess dermal exposure as a result of migration out of an article

	Description	Unit
Input parameter		
Q_{prod}	Amount of product used	g
Fc_{prod}	Weight fraction of substance in product	g g_{prod}^{-1}
Fc_{migr}	Rate (fraction) of substance migrating to skin per unit time	g g^{-1} t^{-1}
$F_{contact}$	Fraction of contact area for skin, to account for the fact that the product is only partially in contact with the skin (default = 1)	cm^2 cm^{-2}
$T_{contact}$	Contact duration between article and skin	d
SD_{prod}	Surface density (mass per unit area)	mg cm^{-2}
A_{skin}	Surface area of the exposed skin	cm^2
C_{der}	Dermal concentration of substance on skin	mg cm^{-2}
BW	Body weight	kg
n	Mean number of events per day	d^{-1}
Output parameter		
L_{der}	Dermal load on the skin that is expected due to migration	mg cm^{-2}
D_{der}	Amount of substance (external dose) that can potentially be taken up, by body weight	mg kg_{bw}^{-1} d^{-1}

Equation 3.8

$$L_{der} = \frac{Q_{prod} \times Fc_{prod} \times Fc_{migr} \times F_{contact} \times T_{contact} \times 10^3}{A_{skin}}$$

If information on the surface density (Sd_{prod}) of the article is available, Equation 3.9 is used.

Equation 3.9

$$L_{der} = Sd_{prod} \times Fc_{prod} \times Fc_{migr} \times F_{contact} \times T_{contact}$$

The external dermal dose in mg kg^{-1} body weight is then calculated using Equation 3.7.

$$D_{der} = \frac{L_{der} \times A_{skin} \times n}{BW}$$

Equation 3.10

$$C_{oral} = \frac{C_{prod} \times 10^3}{D} = \frac{RHO_{prod} \times Fc_{prod} \times 10^3}{D} = \frac{C_{prod} \times Fc_{prod} \times 10^3}{V_{prod} \times D}$$

The oral dose is given by Equation 3.11.

Equation 3.11

$$D_{oral} = \frac{F_{oral} \times V_{appl} \times C_{oral} \times n \times 10^3}{BW} = \frac{Q_{prod} \times Fc_{prod} \times 10^3}{BW}$$

If an undiluted product is swallowed, $D = 1$.

Table 3.4 Parameters used to assess oral exposure due to unintentional swallowing

	Description	Unit
Input parameter		
C_{prod}	Concentration of substance in product before dilution	g cm^{-3}
D	Dilution factor	–
RHO_{prod}	Density of product before dilution	g cm^{-3}
Q_{prod}	Amount of product before dilution	g
Fc_{prod}	Weight fraction of substance in product before dilution	g g$_{prod}^{-1}$
V_{prod}	Volume of product before dilution	cm^3
V_{appl}	Volume of diluted product per event in contact with mouth	cm^3
F_{oral}	Fraction of V_{appl} that is ingested (default = 1)	–
BW	Body weight	kg
n	Mean number of events per day	d^{-1}
Output parameter		
C_{oral}	Concentration in ingested product	mg m^{-3}
D_{oral}	Intake per day and body weight	mg kg$_{bw}^{-1}$ d^{-1}

Oral exposure

Oral exposure may occur as a result of unintentional swallowing of a product during normal use, or as a result of migration from an article such as a pen, cutlery or textile that is placed in the mouth. In estimating oral exposure as a result of unintentional swallowing the parameters shown in Table 3.4 may be considered.

Where unintentional swallowing occurs of a substance in a product during normal use, the concentration in the product as swallowed is calculated from Equation 3.10.

These equations can also be used to estimate exposure arising from ingestion of the non-respirable fraction of inhaled airborne particulates.

Algorithms to estimate oral exposures due to migration from an article are not given in the guidance document.

Tier 1 modelling tools

ECETOC TRA consumer tool

The ECETOC TRA consumer tool allows calculation of consumer exposures to substances that are present in preparations and articles used by consumers. It establishes default settings for 46 specific product and article types relevant to consumer use. The tool calculates exposure via inhalation, dermal and oral routes separately, and also provides a summation of all the relevant exposure routes. It is also possible to take account of exposure to non-volatile substances which have been released from products by migration or abrasion and are present in house dust. The algorithms used within the ECETOC TRA consumer model are based on the equations described above for consumer exposure assessment. One algorithm per exposure route (inhalation, dermal, oral) is used to calculate the exposure for all consumer product and article categories.

For all three algorithms, the user of the TRA tool has to select a product or article category and subcategory. It is necessary to have information on the volatility of the substance to assess inhalation exposure. The assessor can use either default values for the fraction of substance in the consumer product or article, or can input specific information if this is available. The default values suggested by the tool for dermal contact surface area, the 'mouthed' surface area and the amount of product used per application can also be adjusted if the information is available.

Inhalation exposure

The TRA calculates the inhalation exposure as concentration in room air (mg m^{-3}) over a day, resulting from one or more events of product or article application, or as dose (amount per kg body weight) inhaled over the duration of the event. It is assumed that substance transfer to air is instantaneous and the released substance distributes in the room volume uniformly. No ventilation or other factors that potentially change the concentration over time are taken into account.

The algorithm to calculate airborne concentration is given by Equation 3.12.

- For substances with a vapour pressure <10 Pa in non-spray application only a fraction of the substance in the products or article is assumed to be transferred to air. The fraction is based on vapour pressure bands.
- For substances with vapour pressures >10 Pa it is assumed that the substance is completely released into the air instantly. A transfer fraction of 1 is applied.

Equation 3.12

$$C_{inh} = \frac{PI \times A \times FQ \times F \times 10^3}{V}$$

Where: C_{inh} is the concentration in room air over a day, mg m^{-3}
PI is the product ingredient fraction by weight, g g^{-1}
A is the amount of product used per application, g $event^{-1}$
FQ is frequency of use, events d^{-1}
F is the fraction released to air, g g^{-1}
V is room volume, m^3

The algorithm to calculate inhaled dose is given by Equation 3.13.

Equation 3.13

$$D_{inh} = \frac{PI \times A \times FQ \times F \times ET \times IR \times 10^3}{V \times BW}$$

Where: D_{inh} is the inhaled dose, mg kg^{-1} d^{-1}
PI is the product ingredient fraction by weight, g g^{-1}
A is the amount of product used per application, g $event^{-1}$
FQ is frequency of use events, d^{-1}
F is the fraction released to air, g g^{-1}
ET is the exposure time, hr
IR is the inhalation rate, m^3 hr^{-1}
V is room volume, m^3
BW is body weight, kg

- For substances with vapour pressures of 1–10 Pa it is assumed that 10% will be transferred to air.
- For substances with vapour pressures of 0.1–1 Pa it is assumed that 1% will be transferred to air.
- For substances with vapour pressures <0.1 Pa it is assumed that 0.1% will be transferred to air.
- For non-volatile substances (vapour pressure $<10^{-4}$ Pa) the assumption that 0.1% will transfer to air is considered to cover exposure to the substance in house dust by the oral and dermal routes.

Dermal exposure

The algorithm for the calculation of the dermal dose is given by Equation 3.14.

Equation 3.14

$$D_{der} = \frac{PI \times CA \times FQ \times TL \times D \times 10^3}{BW}$$

Where: D_{der} is the dermal dose, mg kg^{-1} d^{-1}
PI is the product ingredient fraction by weight, g g^{-1}
CA is the contact area, cm^2
FQ is frequency of use, events d^{-1}
TL is the thickness of layer, cm
D is the density, g cm^{-3}
BW is body weight, kg

It assumes that there is 100% transfer of substance from the product or article layer in contact with the skin (default values of 0.01 and 0.001 cm are used, respectively), that the transfer is instantaneous, and that dermal absorption is 100%. It does not take into account duration of exposure. Values for the skin contact area are linked to product and article subcategories depending on the areas of the body that might be exposed. Eight categories are identified and default values are provided within the model for adults and children. If the defaults for the fraction of substance in the product or article and the skin contact area are not suitable for the assessment it is possible for the user to provide specific data.

Oral exposure

REACH does not deal with accidents or assessment of consumer exposure to food, food-related and pharmaceutical products, therefore assessment of consumer oral exposure under REACH is limited to situations where:

- exposure occurs as a result of unintentional swallowing (e.g. ingestion through hand–mouth contact)
- articles are mouthed by small children.

The algorithm used is shown in Equation 3.15.

Equation 3.15

$$D_{oral} = \frac{PI \times V \times FQ \times D \times 10^3}{BW}$$

Where: D_{oral} is the ingested dose, mg kg^{-1} d^{-1}
PI is the product ingredient fraction by weight, g g^{-1}
V is the volume of product swallowed, cm^3
FQ is frequency of use, events d^{-1}
D is the density, g cm^{-3}
BW is body weight, kg

The ECETOC TRA tool will estimate exposure due to hand-to-mouth contact for product categories where this is relevant. The volume of product swallowed is related to the oral contact area (CA), this is a default area depending on the part of the hand that may be in contact with the mouth, and the thickness of product layer (TL) on that part of the hand (default 0.01 cm). It is assumed that 100% of substance present on the hand is transferred and available for ingestion.

It is also possible to calculate exposure due to mouthing for some article categories. In this case, the volume of product swallowed is calculated based on the article area in contact with the mouth (default 10 cm^2) and the thickness of article layer assumed to be in contact during mouthing (default 0.01 or 0.001 cm). It is assumed that 100% of the substance present in the contact layer is ingested. The volume of product swallowed is calculated by using Equation 3.16.

Equation 3.16

$$V \text{ (volume product swallowed)} = CA \times TL$$

Based on the substance amount swallowed during the mouthing or ingestion events during the day, a systemic exposure dose for a child is calculated.

Higher–tier modelling tools

Two modelling tools for higher-tier assessments are discussed in the guidance document: a refined version of the ECETOC TRA tool and ConsExpo. However, assessors are not tied to these models and if other suitable models are available such as the E-Fast model developed by the US Environmental Protection Agency (EPA), or the GExFRAME system provided by the Joint Research Centre in the EU, these may be used providing the assessor documents their reasons for choosing a particular model.

E-Fast (exposure and fate assessment screening tool)[1] has been developed by the US EPA to estimate chemical concentrations in water to which aquatic life may be exposed, as well as generate human inhalation, drinking water ingestion and fish ingestion exposure resulting from chemical releases to air, land and water. GExFrame (GlobalExpoFrame)[2] is a web-based software system that houses scientific data and models, particularly those relevant to estimating exposures to chemicals from consumer products.

ECETOC TRA consumer tool

Assessments produced using the ECETOC TRA tool can be refined by revising some of the default parameters used for Tier 1 assessments to give more realistic exposure estimates. However, expert judgement is required so these refinements can only be conducted by people with experience in consumer exposure assessment. In several scenarios, Tier 1 assessments using the most conservative assumptions (small room size and high use volume) result in combinations of input values that are mismatched. As an example, a Tier 1 assessment may be performed for the use of a lubricant with the assumption that up to 5000 g product per day may be used in a room with a default size of 20 m^3. While the amount of product used may be representative for lubrication of a large motor, it is more likely that this would take place in a large garage or outdoors rather than a default room. In such cases, the assessor may wish to change the values to reflect a more realistic assumption.

[1] http://www.epa.gov/oppt/exposure/pubs/efastdl.htm [accessed July 2010]
[2] http://gexframe.jrc.ec.europa.eu/Default.aspx [accessed July 2010]

Where parameters are modified the assessor should provide justification. It is not possible to adjust all parameters; some default parameters such as fraction released, conversion factor and body weight are locked and the user would need to perform manual calculations outside of the tool.

ConsExpo (Version 4.1)

The ConsExpo (Version 4.1) computer tool[1] is a well-known higher-tier tool for expert consumer exposure assessment. It comprises a set of coherent, general models that enables an estimation of the exposure to substances from various consumer products via the dermal, inhalation and oral routes and their uptake by humans. Data about the application of products and data from mathematical models are used to build up the ConsExpo program. The most appropriate exposure scenario and uptake model is chosen for each route to calculate the exposure and uptake for humans. It draws a set of random numbers from the specified distributions (uniform, normal, lognormal, triangular) for distributed parameters and calculates the endpoint of choice with this set. For non-distributed parameters, the specified point value is taken. Exposure and dose distributions reflect stochastic parameters and these distributions can be depicted and the percentiles quantified. The program can also provide sensitivity analyses for each parameter, where mean exposures or doses as function of the value of a selected stochastic parameter are depicted and analysed.

Inhalation exposure

The concentration of a chemical in room air depends on the amount of chemical present in the room, the room size, ventilation, vapour pressure of the compound and the rate at which the substance is released into the air. A refined estimation should also consider time. Modelling exposure therefore requires data that describe the duration of use and the duration of primary and secondary exposure. Three different higher-tier models are available in ConsExpo. The choice of model depends on the information available on physicochemical properties of the compound and the use of the product. The three models are as follows.

- The Constant Rate Model, which describes the release of a substance with a constant rate of release over a certain period of time. In addition to the parameters used in the Tier 1 inhalation model, the Constant Rate Model also uses the emission duration, that is, the time during which the compound is released.
- The Evaporation Model, which describes the release of a substance from the surface of a product by evaporation, and can be used if information on the application duration, the release area and the release rate of the compound from the product is available. The release rate is estimated from the temperature, the molecular weight, vapour pressure and the mass transfer rate (the velocity by which a compound is transferred between the product and the air).
- The Spray Model, which describes the indoor inhalation exposure to slowly evaporating or non-volatile compounds in droplets that are released from a spray can. Inhalation in this case is influenced by factors including the size of the droplets, the breathing pattern and human physiology. Only the droplets that penetrate the alveolar region reach the lung–blood barrier and give rise to inhalation exposure. General exposure parameters needed for this model are spray duration, exposure duration, room volume, room height, ventilation rate and spray direction. The specific spray parameters are the mass generation rate, the airborne fraction, the weight fraction of non-volatiles, the mass density of the total non-volatile substances, the weight fraction of the substance in the preparation and the initial particle distribution.

Dermal exposure

A higher-tier assessment of dermal exposure takes into account the extractability of substances from articles such as textiles. For migrating substances it is assumed that only the part of the total amount available that is in contact with the skin is able to penetrate the skin. Three higher-tier models are available.

- The Constant Rate Model is similar to the Tier 1 Instant Application Model. It assumes that all compound in the product is directly applied to the skin. It calculates the amount of product per surface area of skin or per kg of body weight over a period of time. If the release duration and the rate at which the product is applied to the skin are known, it is possible to refine an assessment based on the assumption of instant application using this model.
- The Rubbing-off Model describes a secondary exposure in which a surface (e.g. a table top) is treated with a product and dermal exposure arises from contact with the treated surface. The additional parameters used in this model are the transfer coefficient (treated surface area in contact with the skin over time), the dislodgeable amount, the contact time and the rubbed surface.
- The Diffusion Model describes the diffusion of substance out of a product and into skin following direct application to the skin. It can be used when

[1] Downloadable from www.consexpo.nl [accessed July 2010]

the diffusion coefficient of the compound in the product is known or can be estimated. The parameters required to use this model are the thickness of the layer of product applied and the exposure time.

Oral exposure

One model, the Constant Rate Model, is available to refine assessments of oral exposure. It describes a scenario in which the substance is ingested over a certain period of time, for example in the secondary exposure resulting from dermal exposure on the hands and subsequent hand-to-mouth contact. To use this model the ingestion rate and exposure time are required.

3.4 Exposure assessment: Biocides

The Health and Safety Executive is the competent authority for assessment of biocides in the UK. At a Community level, substances are assessed to prove an acceptable use exists, resulting in an Annex 1 listing. HSE participates in the European-wide review process for existing biocidal substances, where specific substances are allocated to the UK. HSE also acts as rapporteur for new substances (i.e. those that had not been notified prior to 14 May 2000) – in this case applicants can approach any of the competent authorities in the EU to perform the role of rapporteur for their new substance. A third role for HSE as the competent authority in the UK is to authorise products, once active substances have achieved Annex 1 listing. A full explanation of the roles and responsibilities of HSE and others in the biocides processes is available from the HSE website[1].

The processes for estimation of exposure to biocides and associated products have been determined by the findings of the Biocides Exposure Steering Group. Biocides are categorised within 21 product types, covering a wide range of uses such as insecticides, disinfectants, slimicides, antifouling paints, timber-treatment products and in-can preservatives. The latest report: *Human Exposure to Biocidal Products – Technical Notes for Guidance* was endorsed by the member states competent authorities for the implementation of Directive 98/8/EC concerning placing of biocidal products on the market (19–21 June 2007).

The guidance demands a tiered approach to exposure assessment, which is briefly described below.

[1] http://www.hse.gov.uk/biocides/index.htm [accessed July 2010]

The tiered approach to exposure assessment

Exposure estimates are intended to be used as a screening tool. Real exposure data from real workplaces have been collected to populate a range of exposure models. Many of these models have been developed for use in assessment of pesticide and biocide products in Europe and the USA. The underlying data have been used in a generic sense so they can be applied to many formulations and situations. Exposure to water-based in-use products are particularly well described, and much is known about the challenge to the user for a wide range of tasks.

Tier 1 assessment

Tier 1 estimates are designed to produce highly conservative values taken from the high end of distributions of measured exposure and the other parameters that affect the final outcome of the assessment process (e.g. longest duration of task, highest frequency of task, no effective use of PPE). If the predicted exposures that result from this processing are deemed acceptable, when compared with toxicological endpoints relevant to human exposure, then there is probably no need to introduce any refinement to the exposure estimation process.

Tier 2 assessment

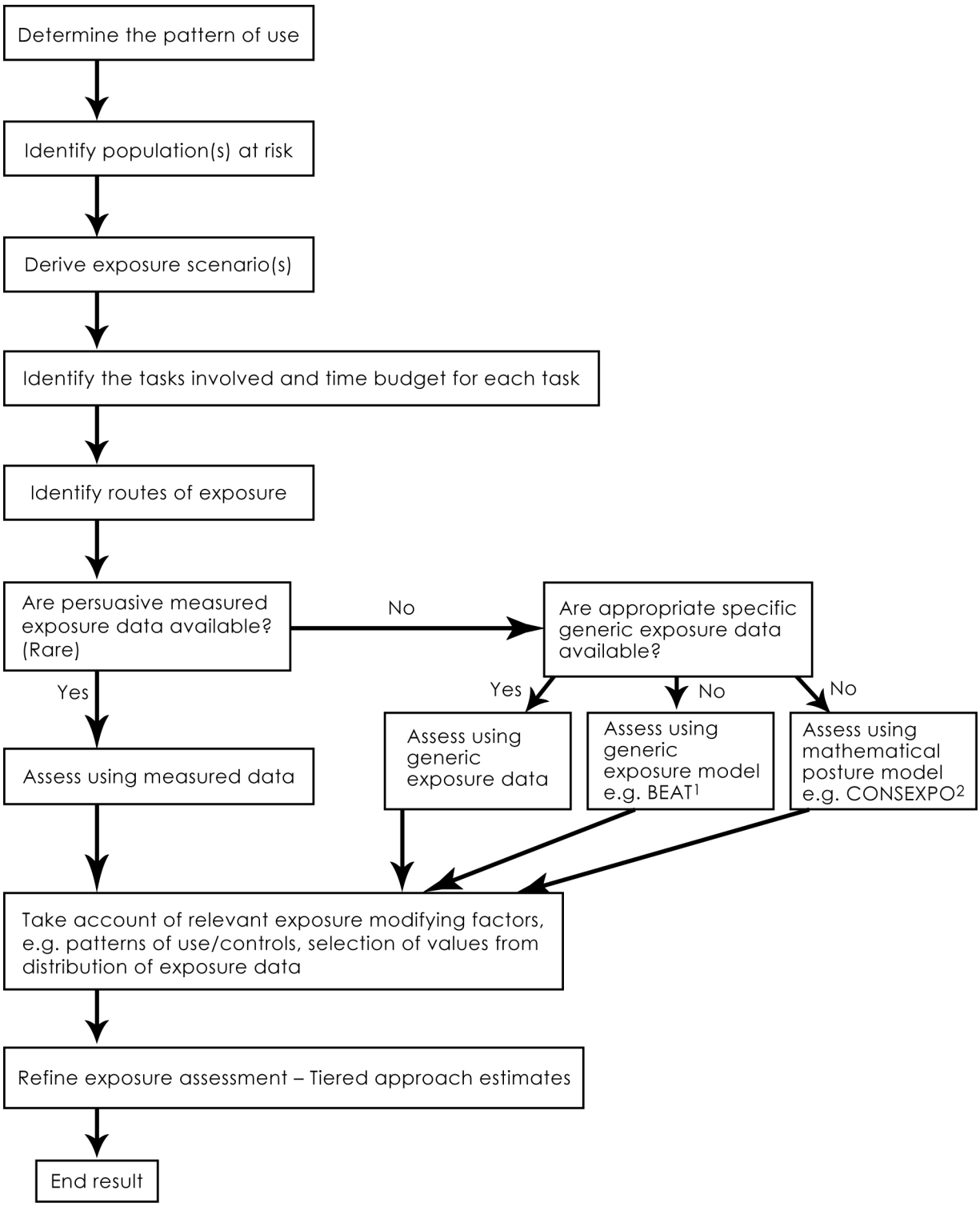
If the exposures resulting from a Tier 1 assessment are deemed too high, there is a need to re-estimate the exposure using a more refined data set. This refinement can be achieved through addressing process controls, taking account of reduction in exposure through use of PPE, or using more realistic information on patterns of use. The outcome of Tier 2 assessment is often an order of magnitude, or more, lower than the Tier 1 assessment.

Exposure studies

Ultimately, and only if the Tier 2 assessment is unable to deliver a clear and acceptable margin of safety when compared with relevant toxicological endpoints, there remains the possibility of demonstrating acceptable levels of exposure through specific exposure studies. These studies need to be big enough, well-enough designed, well described, and of good-enough quality to demonstrate that the distribution of exposure falls well within the range of modelled estimates. A single simple study is unlikely to provide the necessary reassurance to those assessing the risk.

Human exposure assessment to biocides demands that a representative range of scenarios is established, covering industrial, professional and non-professional use. Assessment should also consider secondary exposures resulting from inadvertent contact or environmentally mediated exposures, such as through the food chain. The exposure assessment process

Figure 3.1 Scheme for estimation of human exposure (primary and secondary) to biocides



[1] Bayesian Exposure Assessment Tool; [2] CONSumer EXPOsure models

requires knowledge of the pattern of use, identification of the exposed population, establishment of exposure pathways and quantification. Depending on specific properties of the active substance and formulations it may be necessary to assess exposures relevant to local or systemic effects. A schematic overview of the process is given in Figure 3.1.

3.4.1 Patterns of use

Pattern of use information underpins human biocide exposure assessment and ultimately is the main determinant of the magnitude of predicted exposure. These data are used with information about the product (physical state, concentration, vapour

pressure). Information relevant to pattern of use may include:

- the concentration of active substance in the product (physical state and concentration)
- where and how the product will be used (concentration, location, method of application)
- who uses the product (industrial, professional, non-professional)
- frequency and duration of task
- controls and use of PPE.

Product-specific information on patterns of use for many biocidal products types is limited. The Technical Notes for Guidance[1] provide information to exposure assessors relevant to patterns of use.

Exposure scenarios identify modes of contact between a person and a biocide. Further information is available in the Technical Notes for Guidance. For each scenario there is often a set of specific parameters that characterise the biocidal product's uses and control measures – the assessor adopts these parameters in exposure calculations unless specific arguments are available to refine the modelling process. There is usually more than one scenario for each product to allow for variations in its use and the several routes by which exposure could occur. Also a company may apply for approval to market more than one product containing a particular biocidal active substance. There are often several primary and secondary exposure scenarios to consider for each biocide. To be of use, an exposure scenario must be well documented, realistic and, in the absence of good data, generate a reasonable worst-case (RWC) estimate. Most of the information required to construct exposure scenarios is derived from the company submission or from pre-existing information within the Technical Notes for Guidance, for example information about the physical state and in-use concentration of the product, where and how it would be used and by whom (professionals, amateurs or both). Guidance directs the assessor to supplementary information on specific tasks for certain exposure scenarios, for example the number of batches that an industrial timber treatment plant may produce per day. Secondary exposure scenarios depend on the type of product and its intended use.

3.4.2 Primary exposure scenarios

'Primary exposure' relates to the user of the biocidal product. The exposure scenario is constructed from a series of tasks; three distinct phases of use have been identified.

- Mixing and loading
- Application
- Post-application (such as cleaning equipment)

3.4.3 Secondary exposure scenarios

Secondary exposure relates to bystanders and post-application exposure. Secondary exposure can be relevant in industrial, professional and non-professional settings. A user applying the product could experience both primary and secondary exposure; a non-user would only experience secondary exposure. A feature of secondary exposure is that the exposed person may not be aware it has occurred.

Both short-term and long-term exposure potential is considered by all relevant routes. There are no well-defined tasks for secondary exposure and the assessor may need to develop specific scenarios or be informed by precedent. Patterns of use are derived to address RWC scenarios. What may be an appropriate scenario to address secondary exposure arising from use of an antifouling paint may not be appropriate to address a timber treatment product or an in-can preservative used in indoor water-based paints. On occasions a 'reverse reference scenario' (see Glossary) can be a useful way to demonstrate acceptable risk. An example may be to consider how much food needs to be eaten to exceed the acceptable margin of exposure– it may indicate the need to eat 10 kg of apples!

3.4.4 Evaluating exposure scenarios

After establishing the relevant exposure scenario(s), component tasks and time spent are identified. Analysis of the activities involved in each task leads to the selection of an appropriate model and indicative exposure data for equivalent activities that can be used to predict for the proposed use. To calculate exposure, data are required. In an ideal world real exposure data would be used, but for new active substances used in unfamiliar ways this is largely impractical. Exposure studies rarely provide enough reassurance that they cover the possible exposure distribution and may often fail the test of quality or relevance to the full range of in-use scenarios. Where specific data are unavailable or inadequate (which is most of the time), exposures are modelled using generic data or mathematical models. Reasoned arguments may be developed for selection of appropriate defaults or for exclusion of particular data points. The UK preference has been to use database models where the source of the data is well understood.

[1] European Commission, June 2007 http://ecb.jrc.ec.europa.eu/biocides [accessed July 2010]

3.4.5 Estimating exposure through use of models

Exposure studies have been carried out with the specific purpose of generating generic data that can be used for a wide range of exposure assessment purposes. The generic data have often used biocidal active substances as the primary analyte. However, in reality any non-volatile component of an in-use formulation could be used to provide a generic metric of amount of in-use product that can be adapted to a wide range of use scenarios. For instance, painting tasks can generate an aerosol leading to inhalation and skin deposition. Exposure can be described as quantity of paint rather than as a concentration of a specific component – this approach allows many data sources to be mined to help strengthen the generic exposure data set and reassure assessors that the full distribution of possible results has been captured and defined. The EU-funded RISKOFDERM project delivered a significant quantity of exposure data for modelling purposes, supplementing the major source of data generated earlier through funding by the HSE in the UK.

It is more important for the exposure assessment process to be accurate than precise. Spurious precision leads to a false sense of accuracy in the outcome. The database models are believed to be an accurate predictor of the distribution of exposure (challenge) to the skin and via inhalation. The further step to predict realistic systemic dose is less well understood, though in some cases biological monitoring has provided insight into systemic dose arising from processes such as industrial timber treatment. At each stage the exposure assessment process is conservative.

The available generic data, considered adequate for the majority of scenarios encountered during assessment of human exposure to biocides, are described in the Technical Notes for Guidance and summarised in the User Guidance (European Commission, 2007 and 2002a;b). In these documents a series of models have been proposed. Default values to be adopted for exposure and risk assessment are taken from generic data for specific tasks. The models present default values to be selected and used from indicative points on the exposure distribution, such as the 50th percentile 75th percentile and 95th percentile values.

Published generic models are available for:

- mixing and loading or handling concentrated products (seven models)
- spraying in-use products (11 models)
- handling (timber, treated fish nets, glued wood, mineral fibre, embalming; four models)
- dipping (five models)
- surface disinfection (three models)
- subsoil treatment (two models)
- dust and soil adhesion (three models)
- fogging and misting (three models)
- metalworking fluids (three models)
- pyrotechnic aerosol settlement (one model)
- PPE penetration and deposition (one model)
- consumer spraying (three models)
- consumer painting (four models).

The above-listed models are based on collections of relevant studies that are representative for particular biocidal use areas. Generic exposure data have been used to develop a computer-based model, the Bayesian Exposure Assessment Toolkit (BEAT). BEAT is a Bayesian task-based exposure model for assessing dermal and inhalation exposure in a wide variety of scenarios and was developed specifically for assessment of biocidal products. BEAT is applicable beyond biocides and can be used to assess any task-based operation that is considered to be close enough to the descriptions contained within it. BEAT can be accessed through the HSE website[1].

BEAT provides the user with the flexibility to select specific data sets, or mix data sets to provide an amended exposure estimate for similar but different scenarios – the user has to apply some professional judgement in selection of data sets. The European process for listing of biocidal active substances ensures any selection process is scrutinised by exposure experts across the Community and the final selection may be a compromise position agreed between experts – it should then set a precedent.

As an example, if the scenario under consideration was spray application of an aerosol insecticide product, the BEAT database would be examined for appropriate data sets on tasks involving spray application. A judgement would then be made by the assessor about which of the described tasks in the BEAT database were most relevant. In this example, exposure data from use of handheld trigger sprays and aerosols may be relevant, but spraying from a low-pressure knapsack sprayer would not.

The BEAT database contains supporting information on each data point and can be updated as new data become available. BEAT applies a distribution of

[1] http://xnet.hsl.gov.uk/download/ [accessed July 2010]

exposure to the selected data and can provide outputs from a number of points on that distribution to inform typical, worst case, chronic or acute exposure assessments. BEAT also provides information on uncertainty associated with the modelling process.

The outputs from BEAT are often slightly different from the manual selection of points from a distribution, and this is particularly evident at the high end of the distribution where BEAT has applied a distribution curve to the data set and may predict higher values for exposure.

UK Predictive Operator Exposure Model (UK POEM), described in Section 3.6.2 on assessment of plant protection products, is sometimes used as a supplementary means to assess biocides. The data sets within BEAT and POEM, although presented differently, demonstrate reasonable agreement. For dermal exposures, BEAT values are generally presented as mg deposition of in-use product per minute of task. For POEM, values are presented as mg of exposure to active substance per kg of active substance handled. This reflects the different context of use of plant protection products and biocides.

Consumer exposures

Specific database models exist for determination of exposures in many scenarios relevant to consumers. Typical tasks such as spraying, painting, touching treated surfaces and wiping surfaces are all well described in the Technical Notes for Guidance. Exposure estimates may also be developed through application of very simple tools, such as the US EPA Film Thickness Model that predicts a typical hand retains 5 ml of fluid after immersion. At other times very simple crude estimates of exposure are developed based on realistic worst-case assumptions – if that leads to acceptable exposure no further refinement is deemed necessary.

The software model ConsExpo is available to estimate exposure of consumers to products in the absence of other simpler methods. It is the expected tool for exposure assessment for biocides. The underlying architecture of ConsExpo is not clear for all to understand and some of the algorithms are complex. ConsExpo has been developed by RIVM (Netherlands National Institute for Public Health and the Environment, or *Rijksinstituut voor Volksgezondheid en Milieu* in Dutch). The model is more useful for assessing exposure via the inhalation route and less so via the dermal route – although it does incorporate some of the data sets developed in the UK and through RISKOFDERM.

ConsExpo contains a set of general models that enables an estimation of the exposure to substances from various consumer products via the dermal, inhalation and oral routes. ConsExpo provides an estimate of systemic dose. The most appropriate exposure scenario and uptake model is selected for each route to calculate the exposure and uptake for humans. Highly detailed factsheets have been published by RIVM to help the user understand and apply the model and select sensible default parameters for input. These factsheets contain much default information on patterns of use of consumer products. Currently, the factsheets cover general issues, paint, cosmetics, children's toys, disinfectants, cleaning and pest-control products. The factsheets are added to or amended as results from new research become available. The model, all associated guidance and the fact sheets can be accessed via the RIVM website[1].

Mathematical models

In the absence of product-specific or generic exposure data for a particular biocidal use or scenario, mathematical models for assessing human exposure to biocidal products may on rare occasions be adopted. An example of a mathematical model is the US EPA SWIMODEL[2], which is used specifically to assess human exposure to biocidal agents used in swimming pools and spas. A wide range of user-defined and physicochemical parameters can be used with this model, although pre-existing default assessments are available for some common additives to pool water.

Mathematical models are often not well validated and act as a Tier 1 screening tool presenting very conservative predictions. A range of mathematical models, many generated by the US EPA, are previewed in the EU Biocides Technical Notes for Guidance (2007).

The Technical Notes for Guidance alert the exposure assessor to a number of mathematical models. The UK HSE has little experience of these models and would seek some assurance of validity before use within a UK or European context.

3.4.6 Estimating systemic dose

Most models used to assess exposure to biocidal active ingredients deliver an estimate of challenge to the skin surface or a concentration related to inhalation exposure. The potential dermal exposure (i.e. what lands on the outer surfaces of workwear) is transformed to a value for actual dermal exposure through appropriate reductions associated with the penetration of the protective barrier (clothing, gloves,

[1] http://www.rivm.nl/en/healthanddisease/productsafety/ConsExpo.jsp [accessed July 2010]

[2] Swimmer Exposure Assessment Model (Version 3). US Environmental Protection Agency, Office of Pesticides Programmes. http://www.epa.gov/oppad001/swimodel.htm [accessed July 2010]

protective footwear). Values for protection afforded by protective clothing have been assigned by the EU Biocides Human Exposure Expert Group (HEEG) based on evaluation of the evidence gleaned from exposure studies where amounts of chemical have been estimated both on and under protective workwear.

At a Tier 1 level no provision is made for protection afforded by clothing, so 100% clothing penetration is assumed. At Tier 2, typical default values for clothing protection are 75%, 80%, 90%, 95% and 99%, depending on the challenge and specific areas of use or product type being assessed – different challenges produce a different profile of clothing penetration. Many of the derived exposure models have information on the distribution of in-glove and in-shoe exposure.

Once actual dermal exposure and exposure to aerosol or vapour arising from in-use product has been predicted it is possible to estimate the systemic dose. At a Tier 1 level, a default skin absorption value is usually proposed at 100%. A Tier 2 assessment uses a refined value derived from animal, *in vitro* or human study. Absorption via inhalation is invariably considered to be 100% of the inhaled dose unless there are data which allow a more accurate estimation of absorption.

Inhalation

When converting the airborne concentration for the active ingredient into a systemic inhaled dose, for an adult it is usual to assume a breathing rate of 1.25 m^3 hr^{-1} (equating to a moderate level of activity) and that 100% of the inhaled material is absorbed. The breathing-rate value is one that is widely used within the EU for risk assessments for workers. If an assessor considers that a different value is more appropriate then the alternative value can be used providing this can be scientifically justified.

3.5 Case study

Some examples of exposure assessments for biocidal products have been included in the Human Exposure to Biocidal Products – User Guidance (European Commission, 2002b). To illustrate the assessment process for a biocidal product, the example of a wood preservative is presented. Table 3.5 describes exposure scenarios for wood preservatives and provides pattern-of-use and default values that may be applied in exposure assessments. One primary exposure scenario and one secondary exposure scenario are described.

3.5.1 Primary exposure: Low– to medium–pressure spraying of a wood preservative product

Solvent-based or water-based products are supplied as concentrates for dilution on site, or ready for use. Professional products are normally obtained from wholesalers in containers up to 25 litres. Retail outlets supply non-professional products in 1 to 10 litre cans.

Before a wood preservative product is used there is usually some preparation of the site to be treated. It is therefore assumed that a professional using a timber treatment product is exposed no more than twice per day and no more than a few times per week. Exposure to an individual product on a regular basis is foreseeable only where there is a need for extensive remedial treatment during a single project. The duration of spraying for each treatment ranges from six to 100 minutes: median 40 minutes (default data in Table 3.5). It is anticipated that a non-professional could spend 40 minutes spraying, one or two times per year. Generic exposure data are available for both professional and non-professional *in situ* treatment of timber with wood preservatives using a hand-held sprayer, and these have been used in the following exposure assessments (Table 3.6).

This is a Tier 1 assessment: it assumes there is no protection from clothing and that 100% of the active substance in contact with the skin is absorbed. Refinements in subsequent tiers may be made by taking into consideration the protection to skin afforded by clothing, and by substituting experimental dermal penetration data for the default assumption that all the active substance in contact with the skin is absorbed. In the case of clothing, it is assumed that a professional would wear cotton coveralls. As a default it is assumed that cotton coveralls allow 10% penetration (i.e. 90% of the material that lands on the coveralls does not reach the skin). It is assumed that non-professionals may wear shorts and shirt and that 50% of the material landing on this clothing might penetrate through to the skin.

3.5.2 Secondary exposure: Sanding treated wood

Scenario: Adult (non-professional) using a power sander on wooden posts (4 × 4 × 250 cm) for one hour. The posts have been previously treated with wood preservative solution; the effective retention of the wood preservative on the timber is 0.11 mg active substance cm^{-2}.

Table 3.5 Exposure scenarios for wood preservatives and default values for pattern of use in exposure assessments

Primary exposure	Process or task	Use pattern	Secondary exposure
Professional user Pre-treatment of imber in industrial premises	Vacuum pressure	Default (median) = 3 cycles day^{-1} (180 minutes cycle^{-1}) Wood absorbed 150 litres of preservative m^{-3}	**Short term** adult cutting and sanding treated wood (consumers) infant chewing preserved timber offcuts
	Double vacuum pressure	Default (median) = 6 cycles day^{-1} (60 minutes cycle^{-1})	**Long term** adult cleaning work clothes at home
	Deluge	120 minutes	adult cutting and sanding treated wood (professional)
	Dipping	Default (median) = 30 minutes batch^{-1}	adult/infant inhaling volatilised residues indoors children playing on preserved timber structures infant playing on preserved timber structure and making hand-to-mouth contact
Professional user Remedial (curative) timber treatment *in situ*	Mixing and loading	3 operations day^{-1}	**Short term**
	Spraying	Range = 6–100 minutes application^{-1} (2 applications day^{-1}) Default (median) = 40 minutes application^{-1}	not relevant **Long term** adult/infant inhaling volatilised residues
	Spreading paste	30 minutes (application rate = 1 kg m^{-2})	
Non-professional Remedial (curative) timber treatment *in situ*	Spraying	40 minutes day^{-1} (1 to 2 times year^{-1})	
	Brushing	Range = 76–241 minutes day^{-1} (1–2 days year^{-1}) Default (median) = 155 minutes day^{-1}	

Inhalation exposure

Inhalation exposure to the active biocidal substance will occur as a result of inhaling sawdust from treated timber.

The treated article is a wooden post of dimensions 4 cm × 4 cm × 250 cm (surface area = 4032 cm^2, volume = 4000 cm^3). Assuming the active substance (a.s.) is fixed in the outer 1 cm layer of the post, the volume of the wooden post containing the wood preservative is:

vol. of post – vol. of untreated inner core of post
= 4 × 4 × 250 – 2 × 2 × 248 = 3008 cm^3

If the effective retention of the wood preservative on the timber is 0.11 mg a.s. cm^{-2}, the concentration of active substance in the volume of timber comprising the outer 1 cm layer is:

a.s. on surface × surface area of wooden post ÷ volume of treated wood in the post
= 0.11 × 4032 ÷ 3008 = 0.1475 mg a.s. cm^{-3}

The concentration of active substance in the wood dust is also 0.1475 mg a.s. cm^{-3}.

An inhalation rate of 1.25 m^3 hr^{-1} is assumed for the adult worker. If this person was to inhale wood dust at 5 mg m^{-3} wood dust (workplace exposure limit for wood dust) for one hour, the inhalation exposure would be:

5 mg m^{-3} × 1.25 m^3 = 6.25 mg of wood dust

Assuming the density of the wood is 400 mg cm^{-3} then 6.25 mg of wood dust is equivalent to:

6.25 ÷ 400 = 0.0156 cm^3 of wood dust

As the concentration of active substance in the wood dust is 0.1475 mg a.s. cm^{-3}, inhalation exposure to the active substance is:

0.1475 mg a.s. cm^{-3} × 0.0156 cm^3 = 0.0023 mg

Dermal exposure (hands)

The effective retention of the wood preservative on the timber is 0.11 mg a.s. cm^{-2}. The surface area of both palms of hands is 420 cm^2 (US EPA, 1997) and it is assumed that, during prolonged and repeated contact with the treated timber, 20% of the hand is contaminated (European Commission, 2002a). Hence, dermal exposure to the active substance on treated wood is:

0.11 mg a.s. cm^{-2} × 420 cm^2 ÷ 20/100 = 9.24 mg

Table 3.6 Primary exposure for professional and non–professional users spraying remedial (curative) wood preservatives using a water–based product containing 2% active substance

Product	Units of measurement	Exposure to a professional user	Exposure to a non-professional user
Active substance	%	2	2
Potential body exposure			
Clothing type		For Tier 1, assume no protection	For Tier 1, assume no protection
Indicative value[1]	mg min^{-1}	222	120
Duration	min	40	40
Potential dermal deposit	mg	8880	4800
Clothing penetration	%	100	100
Actual dermal deposit [*product*]	mg	8880	4800
Hand exposure			
Gloves worn[2]		yes	no
Indicative value[1]	mg min^{-1}	7.8	176
Duration	min	40	40
Actual hand deposit [*product*]	mg	312	7040
Total dermal exposure			
Product	mg	9192	11840
Active substance	mg	184	237
Skin penetration	%	100	100
Total systemic exposure to the active substance via the skin	***mg***	***184***	***237***
Exposure by inhalation			
Indicative value	mg m^{-3}	76	115
Duration	min	40	40
Inhalation rate	m^3 min^{-1}	0.021	0.021
Inhaled volume	m^3	0.84	0.84
Mitigation by RPE	Protection factor	none	none
Inhaled [*product*]	mg	64	96
Active substance inhaled	mg	1.27	1.92
Total systemic exposure (dermal plus inhalation)	***mg***	***185.1***	***238.7***
Body weight	kg	60	60
Total systemic dose	***mg kg^{-1} day^{-1}***	***3.1***	***4.0***

RPE, Respiratory protective equipment

[1] Indicative data are provided by generic exposure data in the TNsG. Spraying model 2, TNsG, Part 2, p146 and consumer spraying and dusting model 3, TNsG part 2, p 197.

[2] The indicative data for professional spraying are for the amount of product on hands inside gloves, hence the reduction in exposure from wearing gloves is already taken into account.

3.6 Exposure assessment of pesticides

3.6.1 Introduction

The Chemicals Regulation Directorate (CRD), based within HSE, in common with many other pesticide regulatory authorities around the world performs exposure modelling as part of the overall risk assessment process for pesticides. The legislative requirements for the authorisation of pesticides are that the approved use of the pesticide product will not present unacceptable risks to those consuming treated commodities or exposed by other routes as a result of the application of the pesticide.

Modelling is performed at an early assessment tier to permit the use of generic data rather than having to perform individual exposure-monitoring studies for every pesticide use.

Exposure assessment

As exposure to pesticides can occur in a variety of ways, a number of exposure scenarios are modelled to cover the different types of exposure, and these can be divided into two broad categories.

- Consumption of foodstuffs that have been treated with pesticides
- Non-dietary exposure from contact with pesticides prior to, during, or after application

Within these categories there are subcategories, which are described in detail below. Within the non-dietary group there is the potential for dermal, inhalation and ingestion routes of exposure; these are converted, within the model, to an overall systemic dose and summed where appropriate.

The output of the exposure modelling is normally expressed in mg (of pesticide active substance) kg^{-1} bw. This is compared with a reference dose relevant to the exposure scenario being considered. The reference doses are derived (for more details see IGHRC, 2003; WHO, 1990) from no observed adverse effect levels (NOAEL) from an extensive range of animal studies mostly using the oral route of exposure. The most relevant NOAEL is divided by an uncertainty factor (most often 100) to allow for the possibility that animals used in toxicity studies might be less sensitive than humans and that there might be human subpopulations that are more sensitive than the average.

If the predicted exposure is below the reference dose, approval can be granted; if it is above then risk management decisions need to be taken.

3.6.2 Exposure modelling for consumption of foodstuffs

There are two types of dietary exposure that are modelled, one is based on a single-day ('short-term') exposure to reflect high-end peak intakes, and the other is for a lifetime exposure, reflecting high-end long-term intakes. There are a number of aspects common to both models.

Currently, ten consumer subgroups are modelled. The ten groups are:

- adult (19–64 years)
- infant
- toddler
- 4–6 year-old child
- 7–10 year-old child
- 11–14 year-old child
- 15–18 year-old child
- vegetarian (15 years and above)
- elderly (64 years and above, own home)
- elderly (residential).

The food consumption patterns of these consumer groups were determined in a number of dietary and nutritional surveys performed over the past 20 years. The Food Standards Agency leads on these surveys, and more details can be found in Section 4.2 (data sources) and Section 4.3.

The upper 97.5th centile value is used from the food consumption database. For the short-term intake it is the 97.5th centile of the daily consumption values. For the long term it is the 97.5th centile of the daily average over the short period of the survey (typically 4 to 7 days; see sections 4.2 and 4.3). This is based on the proportion of the sample identified as consumers, that is, non-consumers are excluded from the determination of the 97.5th centile value.

Within the data package required to support licensing of a pesticide, studies (supervised residue trials) must be included that determine the amount of pesticide active substance (and relevant metabolites) left in foodstuffs after application(s) of the pesticide. Trials are normally performed according to the critical good agricultural practice (GAP) using the maximum recommended dose and the shortest interval between application and harvest. These studies tend to overestimate the residue levels present when the commodity is consumed. There are very few examples of pesticides that produce a more toxic residue after environmental degradation, but where it does occur this is taken into account in the assessment. In addition there is an assumption that 100% of the crop consumed is treated.

For major crops (e.g. potatoes and wheat) there is a minimum of eight trials, with four required for minor crops (e.g. berries)[1]. These studies provide a wide range of data, including three key values used in consumer exposure modelling.

- The supervised trial median residue (STMR)
- The highest residue (HR) found in the supervised trials
- The maximum residue level (MRL), which is derived statistically and is above the HR; the MRL is the statutory limit.

There are also post-marketing surveillance schemes where levels of pesticide residues in commodities in the food chain are determined[2]. Exposure modelling linked to surveillance schemes uses the actual values found rather than those from the supervised trials.

The CRD uses a tiered approach to exposure modelling, with conservative default values replaced by actual data when these are available. For example, if a commodity is always cooked before consumption then the change in residue on cooking can be taken

[1] Some extrapolation between similar crops is permitted.
[2] See http://www.pesticides.gov.uk/prc_home.asp [accessed July 2010]

into account by applying a 'processing factor'. An initial default assumption adopted by CRD is that commodities are not peeled before consumption.

The consumer intake models for single-day and lifetime exposures run on Microsoft Excel spreadsheets[1]. The input variables are the pesticide name, the commodity(s); the residue level for the raw agricultural commodity and any processing factor. The model combines these with the consumption data to generate the estimated daily exposure in a manner similar to that described in sections 4.3.1 and 4.3.2. Currently the output uses a point estimate approach, but probabilistic approaches are being developed.

Single–day exposure

This relatively recent concept was first used extensively in the mid 1990s. The estimated exposure, called a national estimate of short-term intake (NESTI) is compared with the acute reference dose (ARfD) for each chemical. The residue level used is the highest residue (HR) found in the relevant supervised trial, or the actual value from surveillance schemes (there is debate about whether to use the HR or MRL, but the current international approach is to use the HR). For many commodities, the residue analyses are performed on composite samples, typically a minimum of 1 kg, containing a number of individual items. It is likely that the residue in a composite sample of some commodities will not be evenly distributed across all the items in the sample. To account for this a variability factor (v) is applied. The default variability factor applied depends on parameters including unit weight of the commodity and its relation to the amount consumed, and whether the commodity is mixed well during processing[2].

Generally the default value of the variability factor v is:

- for large commodities (unit weights >250 g, e.g. melons), $v = 5$
- for medium commodities treated using soil-applied granular pesticides (unit weights usually of 25–250 g, e.g. beetroot, potatoes and carrots), $v = 10$
- for medium commodities treated using non-granular, foliar-applied pesticides (unit weights usually of 25–250 g, e.g. apples, pears and citrus fruit), $v = 7$
- for small commodities (unit weights <25 g), v does not apply since the composite residue data reflect the residue level in the food commodity as consumed, e.g. cherries and oilseed rape.

Where a supervised trial includes data on variability these can be used to replace the defaults. This is a developing area and there is a proposal at the international level that a single variability factor of 3 can be used if a value other than 1 is considered appropriate.

The NESTI equation (Equation 3.17) comprises two main terms. The first calculates the dietary intake for the first commodity unit consumed in a day and assumes it contains a very high residue by applying the variability factor to this term. The second term calculates the dietary intake for the other commodity units within the remaining daily consumption. NESTI calculations are performed for all ten consumer subgroups described earlier.

Equation 3.17

$$NESTI = \frac{\left(U \times HR.P \times \nu\right) + \left(\left\{F - U\right\} \times HR.P\right)}{mean\ body\ weight}$$

Where: *NESTI* is the national estimate of short-term intake for each commodity for a single-day exposure, in mg kg^{-1} bw
U is the weight (in kg) of the first commodity unit, obtained from surveys of typical commodity weights (USDA 2010; Gebhardt & Thomas, 2002; MAFF, 1993). Where *U* is greater than *F* only a consumption value up to *F* can be used, and so *F* is applied in the first part of the equation instead of *U*.
F is the full portion, 97.5th centile, consumption data (in kg) for all forms of the commodity obtained from the FSA survey data (converted to raw commodity from recipe data if necessary). Where the full portion consumption data is less than or equal to the mass of one commodity unit, or the product consumed is well mixed during processing, then the second term of the equation drops out.
v is the variability factor, from 0 to 10 depending on commodity
HR.P is the highest residue level detected (incorporating processing steps other than peeling), in mg kg^{-1}. Where data are available on the residues in the edible portion, or where processing data are available, they should be used rather than HR. HR.P can be higher than HR if there is a concentrating step, e.g. in production of tomato puree.
mean body weight is taken from the relevant consumption survey, kg

Lifetime exposures

The exposure estimate is compared with the acceptable daily intake (ADI). The residue level used is normally the supervised trial median residue (STMR). The spreadsheet can be used for calculating

[1] Further information can be found at: http://www.fao.org/WAICENT/FAOINFO/AGRICULT/AGP/AGPP/Pesticid/JMPR/Download/faom2002.doc [accessed July 2010]

[2] With more data now available on the relationship between residues in composite samples and individual items, there are proposals to revise the default variability factors: see page 17 of: http://www.fao.org/ag/AGP/AGPP/Pesticid/JMPR/DOWNLOADS/2005_rep/report2005jmpr.doc [accessed July 2010]

both individual commodity national estimates of dietary intakes (NEDI) and total dietary intake (*total* NEDI) using the Rees–Day model (discussed in more detail below). These are a first estimate of long-term pesticide intake or as a primary screen of total dietary intake for pesticides. Estimations for individual commodities are normally performed only when a new pesticide with limited uses is being evaluated for the first time. The Rees–Day model sums the two highest 97.5th percentile commodity intakes and the average intakes across all the remaining commodities for each of the consumer subgroups. If residue data are limited, for example as may be the case with a pesticide that was initially approved many years ago, the theoretical maximum daily intake (TMDI) can be calculated by using a MRL value instead of using the STMR (this is a conservative assessment). The equation for a NEDI is given below (Equation 3.18).

Equation 3.18

$$NEDI = \frac{F \times STMR}{body\ weight}$$

Where: *NEDI* is the national estimate of dietary intake for each commodity of the pesticide over a lifetime, mg kg^{-1} bw
F is the full portion, 97.5th centile, consumption data for all forms of the commodity obtained from the FSA survey data (converted to raw commodity from recipe data if necessary, kg)
STMR is the supervised trial median residue level, mg kg^{-1}, calculated from the residue trials
body weight is the mean weight (kg) for the respective consumer subgroup, i.e. adults, schoolchildren, toddlers or infants

The Rees–Day model was developed because, in estimating total long-term dietary intakes, it is not appropriate to sum the individual long-term intakes from all different commodities, as this would result in a gross overestimate. Work on UK consumption data suggested that there were no adults consuming more than five food groups (widely defined) at the 97.5th percentile level, and the vast majority consumed less than two food groups at the 'high level' (97.5th percentile) consumption. Therefore, total dietary intakes (*total* NEDI) are estimated on the STMR using the following 'Rees-Day' model (Equation 3.19).

Equation 3.19

$$Estimated\ Total\ Intake = \sum \left(Two\ Highest\ Intake + Mean\ Population\ Intake\ from\ the\ rest\ of\ the\ diet \right)$$

$$Estimated\ Total\ NEDI = \sum \left(Two\ Highest\ NEDI + Mean\ Population\ Intake\ from\ the\ rest\ of\ the\ diet \right)$$

3.6.3 Exposure modelling: Non–dietary exposures

Four groups are modelled by the CRD in the non-dietary exposure scenario.

- Operators
- Workers
- Bystanders
- Residents

All four groups are normally compared with an acceptable operator exposure level (AOEL). Toxicity studies of up to 90 days' duration are normally used by CRD (or EU bodies) to derive an AOEL, although shorter or longer durations can be used to coincide with the use pattern of the pesticide product. AOEL are normally derived from oral studies, corrected for the extent of oral absorption to give a systemic value in mg kg^{-1} bw per day. Assessments are usually performed using a tiered approach, using fewer generic defaults when product-specific data are available. Exposure estimates are generated as point estimates.

Most pesticides are of low to moderate volatility (one or more orders of magnitude less than water) and for these, all exposure scenarios include potential exposures via dermal, inhalation and ingestion routes. For the small number of more highly volatile products, such as gaseous fumigants, the generic models are considered inappropriate and specific monitoring data are required before exposures can be estimated.

The first tier assessment uses a predictive model (see below); more refined assessments can be performed using additional data. The highest tier assessment would be based on specific biomonitoring studies using the pesticide product in line with the recommendations on the product label.

Operators

Operators are defined as people involved in activities relating to the application of a pesticide product. This includes such activities as mixing and/or loading the product into the application machinery, operation and repair of that machinery while it contains the pesticide product, and emptying and/or cleaning of the machinery and/or containers after use. Professional operators should be trained and are expected to take steps to minimise exposures to themselves and others.

Professional operators should have access to appropriate PPE. Amateur operators (that is, home garden users), for the purpose of exposure assessments, are assumed not to have access to PPE.

Exposures would be via dermal and/or inhalation routes[1]. A professional operator might use the same product more than once per day, or possibly for an entire working day (ca 8 hours), and might use the same or a similar product repeatedly during a growing season. Amateur operators could be exposed in similar ways to a professional, although the equipment would normally be more basic, for example a small sprayer or basic granule applicator. Amateur operators might use the same product more than once per day, and might use the same or a similar product several times during the year. However, for most products it is considered very probable that, when compared with a professional operator, an amateur operator will use far less of the product on any one day and would use it over a shorter timescale. Unlike professional operators, amateur operators are considered to be untrained and with no access to PPE. These conditions could result in amateur operators receiving proportionately higher exposures relative to the amount of product used. However, the differences between professional and amateur exposures in terms of work rate and absence of PPE are taken into account in the assessment of amateur operator exposures. Amateur operators are assumed to wear a T-shirt (leaving 10% of the trunk and arm surface exposed and allowing 20% penetration of the remaining 90%) and shorts (leaving 70% of the leg area exposed and allowing 18% penetration of the remaining 30%).

Predictive operator exposure model

Operator exposures for professional and amateur operators are routinely modelled using the Predictive Operator Exposure Model (POEM)[2]. POEM is based on a Microsoft Excel spreadsheet. POEM contains information on nine types of application technique for pesticides. Default values for work rate and duration of spraying are triggered by particular application techniques (e.g. spraying with a knapsack), but can be altered if appropriate product-specific data are available. Additional input options, which are product specific, relate to either solid or liquid formulations, the type of container the product is sold in, the dose applied, the dilution rate, level of PPE used, and dermal penetration. Based on the input information, the model calculates dermal and inhalation exposures during mixing/loading, during application, and a total predicted exposure. A sample output is shown as a case study in Section 3.7.

The data within the model are based on a number of studies where operator exposures were determined either by biomonitoring, measuring concentrations in the breathing zone or measurements of surface deposition. For each particular measurement the 75th centile value from the studies is used (the 75th percentile was chosen to include high-end regular exposure, but exclude one-off accidents).

Default values within POEM are as follows.

- A body weight of 60 kg
- Protection by gloves: 90% for organic solvent-based products, 95% for aqueous-based products, 99% for solids
- Typically 95% protection by an impermeable coverall (can vary with level of contamination)
- 100% absorption of any inhaled dose
- An initial default dermal absorption value of 100%

POEM does not cover all possible application techniques, for which case-by-case exposure estimates are performed. These use many of the defaults in POEM, but specific values can be used (see Annex to Section 3 for skin surface area and respiration rate data). Alternatively, applicable models developed by other agencies can be adapted to UK conditions, for example the US EPA Pesticide Handler Exposure Database (PHED).

Workers

Workers are defined as people who, as part of their employment, enter an area that has been treated previously with a pesticide product or who handle a crop commodity that has been treated with a pesticide product. Re-entry workers or harvesters might be exposed to a pesticide product when they enter an area (indoors or outdoors) that has been treated previously, or by handling a crop that has been treated with a pesticide product. This could be related to a number of different types of activity: inspection (e.g. for disease or readiness for harvest), thinning, pruning, weeding, harvesting or cutting, sorting, and handling crops treated prior to or during storage.

As a means of providing protection to workers, re-entry to a treated area can be prohibited for a period specified on the product label, to allow for degradation or dissipation of the residue.

There is anecdotal evidence to indicate that the clothing worn by workers and their use of gloves are

[1] Exposure via ingestion is taken account of in other groups – operators are assumed not to put things in their mouths. Certain activities do, however, increase the chance of exposure by ingestion, e.g. when unblocking nozzles.

[2] http://www.pesticides.gov.uk/uploadedfiles/Web_Assets/PSD/UK_POEM1.xls [accessed July 2010]

very variable, thus it is assumed that re-entry workers and harvesters usually have no protective equipment. Work periods can be of up to 8 hours per day. Exposures would be via dermal and/or inhalation routes. A member of the public, such as a walker who moves through an area treated with a pesticide product, can be considered to be exposed in a manner similar to a re-entry worker entering a treated crop. A default body weight of 60 kg is used for adults[1].

Worker exposure scenarios are modelled using activity-specific equations detailed below.

Maintenance and harvesting: Dermal exposure (Tier 1)

For maintenance and harvesting, dermal exposure is estimated by Equation 3.20.

Equation 3.20

$$D = DFR \times TC \times WR \times AR \times P$$

Where: D is the potential dermal exposure, µg active substance person^{-1} day^{-1}
DFR is the dislodgeable foliar residue, kg active substance ha^{-1}
TC is the transfer coefficient, cm^2 person^{-1} hour^{-1}
WR is the work rate, hours day^{-1}
AR is the application rate, kg active substance ha^{-1}
P is the penetration factor for clothing [= 1], which assumes no clothing; a correction for clothing is in the transfer coefficient

The dislodgeable foliar residue (DFR) can be considered to be the application rate (AR) divided by the leaf area index (LAI; Equation 3.21).

Equation 3.21

$$DFR = \frac{AR}{LAI}$$

Where: DFR is the dislodgeable foliar residue, kg active substance ha^{-1} or µg cm^{-2}
AR is the application rate, kg active substance ha^{-1}
LAI is the leaf area index – the ratio between the (one-sided) foliage surface and the ground surface on which it grows

An empirical approach gives a DFR value of 3 ng cm^{-2} for each kg of active substance applied per hectare. These formulae do not consider the dissipation (decay) of the active substance on the foliage. This may be introduced as a factor or as a formula if the exact nature of the dissipation over time is known. If no data are available on the degree of dissipation, the worst-case approach is to assume no dissipation at all. In that case DFR is used for calculations, that is, the residue available directly after application (when dry). In practice this would mean that if no dermal exposure measurements are available, the exposure can be calculated using the relevant application rate and/or data or assumptions on dislodgeable foliar residue, the duration of the exposure and information on transfer coefficients.

The transfer of residues from the plant surface to the clothes or skin of the worker can be regarded as more or less independent of the kind of product applied, and the level of exposure would depend on the intensity and duration of contact with the foliage. This is also determined by the nature and duration of the activity during re-entry. Therefore, it is possible to group various crop habitats and re-entry activities. The EUROPOEM Re-entry Group (van Hemmen, 2002) has recommended the following indicative transfer coefficient (TC) values for potential dermal exposure in four different harvesting scenarios. These TC values assume harvesting is performed with bare hands, and that dermal exposure to the body is reduced ten fold by clothing worn by the worker.

For other re-entry scenarios, TC data may be extrapolated where the scenarios are considered to be comparable, that is the intensity and duration of contact with the foliage. The TC values in Table 3.7 may be used in the first tier of the exposure assessment. For higher tiers, specific TC values may be derived from experimental studies.

Table 3.7 Transfer coefficients for potential dermal exposure for four different harvesting scenarios (EUROPOEM Re-entry Group)

Crop	Nature of task	Transfer coefficient (cm^2 hr^{-1})
Vegetable	Reach, pick	2500
Fruit (from trees)	Search, reach, pick	4500
Berry	Reach, pick	3000
Ornamental	Cut, sort, bundle, carry	5000

Maintenance and harvesting: Inhalation (Tier 1)

Maintenance and harvesting inhalation exposure is estimated by Equation 3.22.

Equation 3.22

amount inhaled = amount applied × task specific factor

Where: *amount inhaled* is the amount of active substance inhaled, mg active substance inhaled hr^{-1}
amount applied is the amount of active substance applied, kg active substance applied ha^{-1}
task-specific factor is a factor to take account of variations in activities such as cutting ornamentals or re-entering greenhouses (see below)

[1] When considering entry to a crop, modelling worker exposure based on an assumption of a full-day exposure also covers incidental exposure of children and others arising from shorter duration activities. For some scenarios, e.g. exposure to lawn treatments, child-specific assessments are done.

Although in many cases inhalation exposure would be less significant for the exposure assessment than dermal exposure, the EUROPOEM Re-entry Group (van Hemmen, 2002) has proposed task-specific factors that may be used for the first tier of an exposure assessment relating to harvesting ornamentals and to the re-entry of greenhouses approximately 8–16 hours after treatment.

The *indicative* task-specific factors proposed for the first tier of the exposure assessment are:

- 0.1 for cutting ornamentals
- 0.01 for sorting and bundling of ornamentals
- 0.03 for re-entering greenhouses after low-volume mist application
- 0.15 for re-entering greenhouses after roof fogger application.

These task-specific factors were derived from monitoring studies or, in the case of foggers, an empirical value supported by measurements (Kirknel *et al.*, 1997).

This approach may be used for non-volatile pesticides, where levels of inhalation exposure (vapour and dust) would be expected to be low in comparison with dermal exposure. Products applied as aerosols and volatile pesticides may require further data or information. The volatility of the active substance is not used directly in these calculations.

Soil contact exposure (Tier 1)

For situations where exposure to soil-borne residues occurs in the absence of contact with treated foliage, for example when working with treated soil or compost, an estimate of potential (dermal) exposure may be derived by considering the concentration in the treated soil or medium and soil dermal adherence data.

Council Directive 91/414/EEC Annex III (set out in Commission Directive 95/36), Point 9.1.3 *Estimation of expected concentrations in soil*, requires predicted estimations of concentrations in soil. These estimations assume a soil density of 1.5 g cm^{-3} dry weight, a soil layer depth of 5 cm for applications at the soil surface or 20 cm when direct incorporation is used, and that where ground cover is present at the time of application a minimum of 50% of the applied dose reaches the soil surface, unless actual experimental data give more specific information. (In the absence of ground cover, 100% of the applied dose is assumed to reach the surface.) Other factors to be considered relate to direct and indirect application to soil, drift, run off and leaching, and include processes such as volatilisation, adsorption, hydrolysis, photolysis and aerobic and anaerobic degradation.

In some circumstances, (higher tier) field studies on dissipation in soil or residues in soil may be available.

Field studies investigating dermal exposure to soil by direct gravimetric measurements (Kissel *et al.*, 1996) suggest that an appropriate hand–soil loading (dermal adherence) for a worker would be 0.44 mg cm^{-2} (geometric mean peak value for farmers involved in hand weeding).

Dermal exposure is estimated using equations 3.23 and 3.24.

Equation 3.23

$$dermal\ exposure = C \times DA \times SAC \times T$$

Where: D is dermal exposure, mg
C is the concentration of pesticide in soil, mg kg^{-1}
DA is the dermal adherence factor, mg soil cm^{-2} skin, default of 0.44
SAC is the skin area contaminated, cm^2 [820 cm^2 for hands]
T is the transfer from soil to skin, %

Equation 3.24

$$absorbed\ dose = dermal\ exposure \times dermal\ absorption$$

Where: *absorbed dose*, mg
dermal exposure, mg
dermal absorption, % [initial default of 100%]

It is accepted that not all of the active substance in a layer of soil applied to skin may be bioavailable. However, in the absence of specific information on the transfer of the active substance from soil to the skin, conservative assumptions are used for this parameter (e.g. 100%).

Inhalation exposure can be estimated by using field data on personal exposure levels to soil dust during relevant operations. Available data from California (Nieuwenhuijsen *et al.*, 1998) indicate this would be significantly lower than exposure via other routes, with an estimate that a 60 kg person working for eight hours would be exposed to 30 ng kg^{-1} bw based on an application rate of 1 kg ha^{-1} and uniform incorporation to a depth of 5 cm.

Bystanders

Bystanders are defined as people located within or directly adjacent to the area where pesticide application or treatment is in process; whose presence is incidental and unrelated to work involving pesticides, but whose position may put them at risk of potential exposure; who take no action to avoid or control exposure, and, it is assumed, wear no protective clothing and perhaps little ordinary

clothing. Activities that could result in bystander exposure include:

- walking into a crop during application
- walking or travelling adjacent to an area being treated
- being in a garden next to a field or orchard being treated.

Exposures could be by dermal or inhalation routes, from spray drift and/or vapour, and would occur over a relatively short period of time.

There is no agreed international method for assessing bystander exposure to non-volatile pesticides. The approach developed by the Pesticide Safety Directorate to assess this type of exposure assumes that bystander exposure from spray drift at the time of application would dominate other pathways of exposure, such as exposure to volatised residues in air post application, and exposure to pesticides absorbed onto dust particulates. The method assumes that an adult individual would be eight metres directly downwind of a working sprayer (a model for children is currently under development). The estimate considers potential dermal exposure from the application (i.e. pesticide impacting on the bystander's skin and clothing), inhalation exposure and the fraction absorbed through the skin.

The estimate is based on the trials conducted in the 1980s[1] (Lloyd & Bell, 1983; Lloyd *et al.*, 1987) where representative applications were made by spraying volunteer bystanders under a range of conditions. For example, arable field crop sprayers were tested, applying spray volumes of 50–270 litres ha^{-1}, using various nozzles, over short grass (worst case for drift), and with wind speeds up to 24 km h^{-1}. Orchard sprayer trials were done, spraying 34–422 litres ha^{-1} using various nozzles, in wind speeds up to 12.2 km h^{-1}. It is worth noting that spray technology has developed since these trials were conducted. For example, the use of low-drift nozzles is now quite widespread and the values used might over-estimate drift from modern machinery.

The exposure assessments use the mean potential dermal contamination and inhalation exposures from the worst-case subsets in the two scenarios (165 litres ha^{-1} for arable and 422 litres ha^{-1} for orchard). Mean values were selected because the risk assessment assumes repeated exposure. The range of wind speeds in the two sets of trials included speeds in excess of 9.6 km h^{-1}, which is the wind speed above which the Code of Practice for the Safe Use of Pesticides on Farms and Holdings states that spraying is inadvisable. This was used because it is known that in practice growers may sometimes work in stronger winds than the Code recommends.

Internal exposures are estimated assuming no protection from clothing and no reduction in potential inhalation exposure. The dermal and inhalation exposures are summed after taking account of the likely extent of dermal absorption. Historically, bystander exposure estimates have been calculated manually; a spreadsheet-based system is currently being finalised.

Residents

Residents are defined as people who live, work or attend school or any another institution adjacent to an area that has been treated with a pesticide product; whose presence is quite incidental and unrelated to work involving pesticides but whose position may put them at risk of potential exposure; who take no action to avoid or control exposure; who wear no protective clothing and perhaps little ordinary clothing, and who might be in the location for 24 h day^{-1}.

Resident exposures could result from several scenarios related to residing adjacent to an area treated with a pesticide product, including contact with surfaces that have been subject to spray drift, for example turf, or that have been directly treated, or breathing air containing volatile active substances. Exposures to contaminated surfaces could occur daily; inhalation of volatile components could be for 24 h day^{-1}. The magnitude of resident exposure is likely to be greatest immediately following application (or venting) and then reduce over time as the residue declines or is dispersed. It is possible that residents could be adjacent to areas that are treated repeatedly.

Maximum 24-hour inhalation model: Adults and children

Two sources of data have been used as surrogate values to estimate maximum 24-hour inhalation values: Californian Air Resource Board (ARB)/Department of Pesticide Regulation (DPR) (California Environmental Protection Agency, 1996; 1998; 1999a,b,c; 2000) air monitoring reports provide detailed results from monitoring adjacent to treated fields or orchards over 72 hours following the start of an application of a limited range of pesticides. Some experimental monitoring has also been performed in Germany (Siebers *et al.*, 1999).

A tiered approach is taken regarding the selection of the surrogate data. The ARB data on chlorpyrifos have been used in the first instance. From these data a maximum 24-hour time-weighted value of 15 $\mu g\ m^{-3}$ was calculated. This value is considered to be a worst case for most compounds applied as sprays, because

[1] Lloyd & Bell, 1983 and Lloyd *et al.*, 1987 are internal documents available from CRD on request..

chlorpyrifos is a relatively volatile compound (vapour pressure 2 mPa), the treatment monitored was for a broadcast air-assisted treatment which causes more drift than ground boom applications, and the application involved two significant treatment periods on two consecutive days (the highest air levels were measured on the second day and are presumably a result of the combination of volatilisation and drift from the application). In addition, the highest value from the four samples taken at each compass point has been used to estimate the level, even though that means combining values from different locations to calculate a maximum time-weighted value that was not actually observed at any single location.

However, based on a consideration of vapour pressure alone, the use of chlorpyrifos as a surrogate may lead to underestimates of air concentrations of some volatile pesticide active substances. However, ARB monitoring data for naled and dichlorvos together, which have greater vapour pressures at 270 and 290 mPa, respectively, show lower air levels than occurred following the application of chlorpyrifos (California Environmental Protection Agency, 1996). In addition, Turnbull (1995) reported air levels of trifluralin (vapour pressure 6 mPa) up to 2.3 ng m^{-3} in 24- or 48-hour samples, reportedly taken in the vicinity of application of the compound (specific details were not given) which are also well within the levels of chlorpyrifos found by the ARB. Therefore the ARB chlorpyrifos data are likely to be appropriate for other relatively volatile compounds. If an initial tier exposure estimate using chlorpyrifos gives rise to an exceedance of the AOEL, and its vapour pressure is significantly lower than chlorpyrifos, a second tier estimate is performed using German data (Siebers *et al.*, 1999) for a compound with a more appropriate vapour pressure.

The maximum 24-hour potential inhalation value is calculated using the above surrogates for adults and toddlers and Equation 3.25.

The default assumption is that there is 100% absorption of the inhaled dose.

Children's dermal exposure model

Children may be exposed to surface residues following drift into gardens. From arable applications the worst-case level of drift fallout is assumed to be around 1% of the field rate (Rautmann *et al.*, 2001). This would be equivalent to a deposit of 0.1 µg cm^{-2}, while for broadcast air-assisted applications the level of fallout may be much higher. Allowing for a realistic orchard structure, the worst-case level of fallout (from early season applications to bare trees) in an area adjacent to the orchard may be equivalent to about 20% of the field rate. The level of deposit would

Equation 3.25

$$Max\ 24h\ PIE = Max\ 24h\ TW\ level \times \frac{LTIR}{BW}$$

Where: *Max* 24*h PIE* is maximum 24-hour time potential inhalation exposure, µg kg^{-1} bw
Max 24 h TW level is the maximum 24-hour time-weighted level, µg m^{-3}, i.e. 15 µg m^{-3} (chlorpyrifos) or 1 µg m^{-3} (parathion – rounded-up value)
LTIR is the long-term inhalation rate, m^3 day^{-1} (mean value), i.e. 15.2 m^3 day^{-1} for adult males[1] (19–65+ yrs) and 8.3 m^3 day^{-1} for children 3–5 yrs (US EPA, 1997)
BW is body weight; adults = 60 kg (standard assumption which is equivalent to the 50th percentile for UK 16–24 yrs females)[1]; children = 15 kg (average of UK 1995–7 Health Surveys for England values for males and females aged 2 and 3 yrs)

[1] Combination of lower female body weight and higher male inhalation rates gives a conservative outcome

Equation 3.26

$$SE(d) = \frac{AR \times DF \times TTR \times TC \times H \times DA}{BW}$$

Where: *SE(d)* is the systemic exposure via the dermal route, mg kg^{-1} bw
AR is the field application rate, kg ha^{-1}
DF is the drift fallout value, % [1% from ground boom applications and 10% from broadcast air-assisted applications]
TTR is the turf transferable residue [the EPA default value of 5% is used in all estimates]
TC is the transfer coefficient, cm^2 h^{-1} [the EPA value of 5200 cm^2 h^{-1} is normally used for all estimates]
H is the exposure duration for a typical day, hours [this has been assumed to be 2 hours, which matches the 75th percentile for toddlers playing on grass in the EPA Exposure Factors Handbook; US EPA (1997)]
DA is percent dermal absorption [initial default = 100%]
BW is body weight [15 kg]

decline away from the boundary to just over 5% at 10 m. A reasonable estimate of an average over the whole area from the boundary to 10 m is assumed to be 10%. This would be equivalent to a deposit of about 1 µg cm^{-2} kg^{-1} applied ha^{-1}. In practice the common presence of a windbreak or hedge around an orchard would significantly reduce the levels of drift.

Systemic exposures via the dermal route are calculated using the above drift fallout values and Equation 3.26.

Children's hand-to-mouth exposure model (ingestion)

Hand-to-mouth exposures are calculated using turf transferable residue levels in Equation 3.27.

Equation 3.27

$$SE(h) = \frac{AR \times DF \times TTR \times \left(\frac{SE}{100}\right) \times SA \times Freq \times H}{BW}$$

Where: *SE(h)* is the systemic exposure via the hand to mouth route, mg kg^{-1} bw
AR is the field application rate, kg ha^{-1}
DF is the drift fallout value, % [1% from ground boom applications and 10% from broadcast air-assisted applications]
TTR is the turf transferable residue [the EPA default value of 5% derived from transferability studies with wet hands is used in all estimates]
SE is the saliva extraction factor,% [the default value of 50% is used]
SA is the surface area of the hands [the assumption used here is that 20 cm^2 of skin area is contacted each time a child puts a hand in his or her mouth, equivalent to the palmar surface of three fingers]
Freq is the frequency of hand-to-mouth events h^{-1} [for short-term exposures the value of 20 events h^{-1} is used, this is the 90th percentile of observations that range from 0 to 70 events h^{-1}; ORD, 2002]
H is the exposure duration for a typical day, hours [assumed to be 2 hours, which matches the 75th percentile for toddlers playing on grass in the EPA Exposure Factors Handbook; US EPA (2002)]
BW is body weight, kg [15 kg]

Children's object-to-mouth exposure model (ingestion)

Object-to-mouth exposures are calculated using turf transferable residue levels and Equation 3.28.

Equation 3.28

$$SE(o) = \frac{(AR \times DF \times TTR \times IgR)}{BW}$$

Where: *SE(o)* is the systemic exposure via mouthing activity, mg kg^{-1} bw
AR is the field application rate, kg ha^{-1}
DF is the drift fallout value, % [1% from ground boom applications and 10% from broadcast air-assisted applications]
TTR is the turf transferable residue [the default value of 20% transferability for object-to-mouth assessments is used]
IgR is the ingestion rate for mouthing of grass per day [this was assumed to be equivalent to 25 cm^2 of grass day^{-1}, an upper centile value proposed by US EPA Office of Pesticide Programs; OPP, 1997]
BW is body weight, kg [15 kg]

Children's total exposure

Children's total dermal exposure was estimated as the sum of the dermal, hand-to-mouth, and object-to-mouth exposures, as in Equation 3.29.

Equation 3.29

$$Children\ Total\ Dermal\ Exposure = SE(d) + SE(h) + SE(o)$$

3.7 Case study

3.7.1 Exposure modelling: Herbicide application

The example detailed in Figure 3.2 below shows use of the Predictive Operator Exposure Model (described in Section 3.6.2) for an operator applying a product containing 125 g l^{-1} of the herbicide quinmerac using a tractor-drawn boom sprayer.

The consumer intake estimates use procedures similar to those of the Food Standards Agency, an example of which is presented in Section 4.4.

Annex: Default skin area and respiration rates used in pesticide exposure assessments

Skin areas

Table 3.8 Surface areas for regions of adult body (80th percentile male) and locations of dermal exposure dosimeters[1]

Region of body	Surface area (cm^2)	Location of dosimeters
Head and face (Face)	1300 (650)	Head (front of cap, hood)
Back of neck	110	Back (outside dosimeter)
Front of neck (includes V of chest)	150	Chest (outside dosimeter)
Back	3550	Back (inside dosimeter)
Chest/stomach	3550	Chest (inside dosimeter)
Upper arm	2910	Each upper arm
Forearm	1210	Each forearm
Upper leg	3820	Each thigh
Lower leg	2380	Each lower leg (shin)
Foot	1310	Each foot or sock
Hand	820	Absorbent glove or hand wash method used[2]

Source: Adapted by US EPA (1987) from Berkow (1931) and US EPA (1985)
Surface areas include both arms, both legs and both hands
[1] One patch on head, back, chest, each forearm, each upper arm, each thigh and each lower leg
[2] No surface area calculation is required when either the absorbent glove or the hand wash method is used

For children, data are taken from the US EPA Exposure Factors Handbook (1997) and/or the US EPA Child Specific Exposure Factors Handbook (US EPA, 2002).

Figure 3.2 An example of a Predictive Operator Exposure Model estimate, for a product containing quimerac applied using a tractor–drawn boom sprayer

Application method	Tractor-mounted/trailed boom sprayer: hydraulic nozzles			
Product	BAS 526 14 H		Active substance	quinmerac
Formulation type	water-based		a.s. concentration	125 mg/ml
Dermal absorption from product	2 %		Dermal absorption from spray	5 %
Container	10 litres 63 mm closure			
PPE during mix/loading	Gloves		PPE during application	Gloves
Dose	2 l/ha		Work rate/day	50 ha
Application volume	100 l/ha		Duration of spraying	6 h

EXPOSURE DURING MIXING AND LOADING

Container size	10	litres
Hand contamination/operation	0.05	ml
Application dose	2	litres product/ha
Work rate	50	ha/day
Number of operations	10	/day
Hand contamination	0.5	ml/day
Protective clothing	Gloves	
Transmission to skin	5	%
Dermal exposure to formulation	0.025	ml/day

DERMAL EXPOSURE DURING SPRAY APPLICATION

Application technique	Tractor-mounted/trailed boom sprayer: hydraulic nozzles			
Application volume	100	spray/ha		
Volume of surface contamination	10	ml/h		
Distribution	Hands	Trunk	Legs	
	65%	10%	25%	
Clothing	Gloves	Permeable	Permeable	
Penetration	10%	5%	15%	
Dermal exposure	0.65	0.05	0.375	ml/h
Duration of exposure	6	h		
Total dermal exposure to spray	6.45	ml/day		

ABSORBED DERMAL DOSE

	Mix/load		Application	
Dermal exposure	0.025	ml/day	6.45	ml/day
Concen. of a.s. product or spray	125	mg/ml	2.5	mg/ml
Dermal exposure to a.s.	3.125	mg/day	16.125	mg/day
Percent absorbed	2	%	5	%
Absorbed dose	0.0625	mg/day	0.80625	mg/day

INHALATION EXPOSURE DURING SPRAYING

Inhalation exposure	0.01	ml/h
Duration of exposure	6	h
Concentration of a.s. in spray	2.5	mg/ml
Inhalation exposure to a.s.	0.15	mg/day
Percent absorbed	100	%
Absorbed dose	0.15	mg/day

PREDICTED EXPOSURE

Total absorbed dose	1.01875	mg/day
Operator body weight	60	kg
Operator exposure	0.016979167	mg/kg bw/day

Respiration rates

A wide range of values is available. Those used routinely by the CRD are from NAFTA (1998). Long-term inhalation rates (m^3 24 h^{-1}) are as follows.

Males	15.2
Females	11.3
Males and females combined	13.2

Short and intermediate-term inhalation rates (m^3 h^{-1}) for males and females; actual values used are dependent on the specific task, as given below.

Resting rate (lying down)	0.4
Sedentary activity (driving tractor)	0.5
Light activity (mix or load <22 kg)	1.0
Moderate activity (backpack sprayer)	1.6
Heavy activity (not typical for pesticides)	3.2

Inhalation rates for children are taken from the US EPA Exposure Factors Handbook (US EPA, 2002).

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4 Food Standards Agency's Approach to Exposure Modelling

4.1 Introduction

Exposure modelling is critical to the Food Standards Agency's (FSA) work in risk assessment of food chemicals to ensure adequate protection for consumers. There are several aspects to consider when assessing exposure to chemicals from the consumption of food and drink. Most chemicals are natural constituents of food, but some are added intentionally. These include food additives and supplements. The use of food additives is governed by European legislation that applies in all member states, which identifies the additives that are permitted for use, the categories of foods in which they can be used and the maximum amount that can be added.

Food additives are permitted for use only after undergoing safety evaluations by the independent scientific committees that advise the European Commission and the UK government. Even when approved, the use of a permitted additive continues to undergo careful scrutiny. Intake surveys are carried out to ensure that consumers are not exceeding the acceptable daily intake (ADI) levels advised by the committees referred to above.

Some chemicals are present in food as a result of the way the food is produced, but not intentionally added to food as eaten. These include pesticides and veterinary medicine residues. Chemicals can also be present in food through migration from food packaging or kitchenware. There is legislation in place to ensure that the transfer of such chemicals into food does not endanger health or adversely affect the quality of the food.

Maximum limits and action levels have been set by the European Union for some environmental pollutants, process contaminants (including substances formed during cooking) and naturally occurring toxins like mycotoxins and marine biotoxins, but many chemicals in these categories are not regulated.

4.2 Exposure assessment

Exposure assessment takes as a starting point the levels of chemicals measured or calculated in food and combines this information with the amount of that food consumed – see Equation 4.1, or, on a body weight basis, Equation 4.2.

Equation 4.1

$$Dietary\ Exposure = \sum \left(Food\ chemical\ concentration \times Food\ consumption \right)$$

Where: *Food chemical concentration* is the concentration of the contaminant in the food, mg
Food consumption is the amount of that food that is eaten, g

Equation 4.2

$$Dietary\ Exposure = \sum \frac{\left(Food\ chemical\ concentration \times Food\ consumption \right)}{BW}$$

Where: *Food chemical concentration* is the concentration of the contaminant in the food, mg
Food consumption is the amount of that food that is eaten, g
BW is the body weight, kg

The sources of chemical concentration and food consumption data are discussed in Section 4.2.

Figure 4.1 shows the steps in a dietary exposure assessment. If the estimate of exposure is within the limit set by a reference dose such as the acceptable daily intake (ADI), then the exposure assessment does not proceed. (The ADI is an estimate of the amount of a substance in food, expressed on a body weight basis, which can be ingested daily over a lifetime by humans without appreciable health risk.) If necessary, the exposure assessment could be further refined to get a more accurate level of exposure.

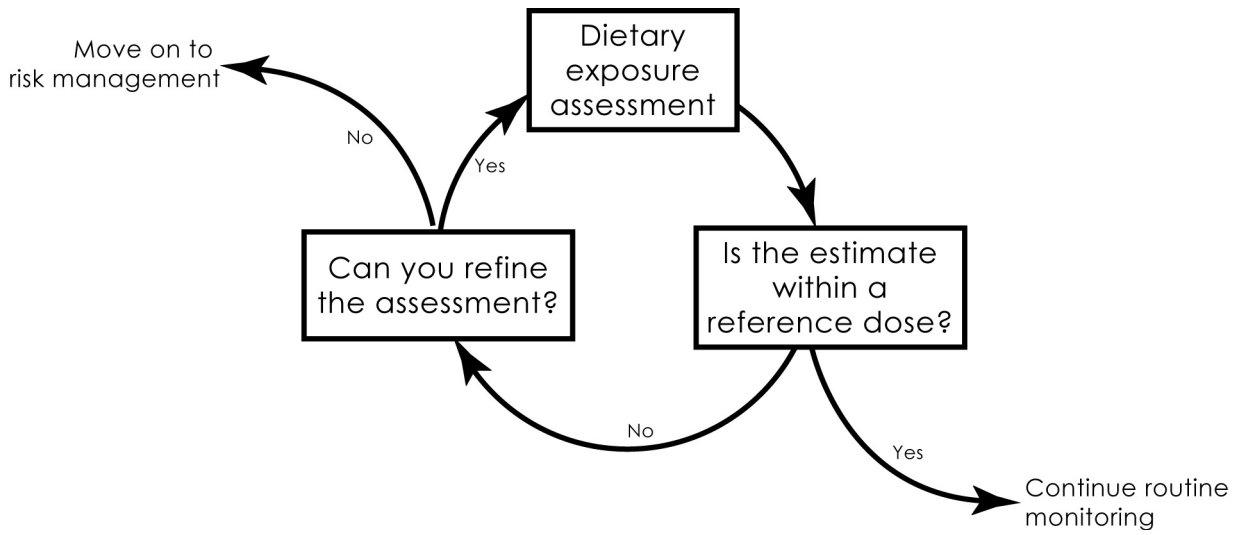
4.3 Data sources

The main source of data used by the FSA for estimating consumption is the National Diet and Nutrition Survey programme (NDNS). The NDNS programme was originally set up as a series of cross-sectional surveys of diet and nutritional status covering the population from age 18 months upwards; data were collected from approximately 2000 individuals in each of four age groups (1.5 to 4.5 years, 4 to 18 years, 19 to 64 years and 65 years and over) between 1992 and 2001(Gregory *et al.*, 1995, 2000; Finch *et al.*, 1998; Henderson *et al.*, 2002). A rolling programme of NDNS has now been set up to collect data on a continuous basis. This new programme will provide more frequent data for tracking trends in food consumption and give more flexibility to respond to changing data needs. One of the major components of the NDNS is a detailed assessment of diet over four or seven days. In previous surveys, participants were asked to weigh and record a description of everything they ate over a four- or seven-day period. However, the rolling programme is not using a weighed record because of concerns about the high burden it places on participants, which can lead to reduced response rates. Following pilot work which tested a 24-hour recall and an unweighed diary method, it has been decided to use a four-day unweighed diary as the dietary assessment method for the NDNS rolling programme.

Other surveys, such as the Food and Nutrition Intakes of British Infants Aged 6–12 Months (Mills & Tyler, 1992), Dietary Survey of Vegetarians (Ministry of Agriculture, Fisheries and Food, 1996) and the Expenditure and Food Survey (EFS; DEFRA, 2008), are also considered for providing supporting information on food consumption. For instance, the EFS is carried out annually and provides data on food purchases at a household level. This has limited value for assessing food safety as the data provided are population averages. However, as it is a continuous survey it is useful for tracking food consumption patterns. A study which tracked the consumption of human milk by 48 infants over an eight-month period can be used to give estimates of the mean consumption of human milk by nursing infants between two and 10 months (Paul *et al.*, 1988).

Data on the concentration of food chemicals and nutrients for use in exposure assessments are obtained from sources such as research projects, surveys and monitoring work. Total diet studies (TDS) provide the FSA with another source of data for exposure assessment. The TDS is a continuous market basket-type survey in which foods representing the average UK diet (based on the EFS) are purchased, prepared and combined into 21 groups of similar foods for analysis. Food samples representative of the UK diet are purchased throughout the year in 24 towns covering the UK. The types and quantities of food required are based on analysis of food consumption recorded in the EFS and from trade statistics. The quantities of food are updated annually to reflect changing eating habits in the UK.

Figure 4.1 Dietary exposure assessment framework



The TDS has been run on a continuous annual basis since the early 1960s and allows the FSA to estimate the population's average exposure to non-nutrients (i.e. contaminants such as heavy metals and dioxins), as well as intakes of some nutrients. The continuous nature of the TDS allows trends over time to be established.

Population dietary exposures are estimated by multiplying the average amount of each food group consumed (based on consumption data from the EFS household survey) by the corresponding elemental concentration in the food group from the TDS, then summing across all food groups. The EFS covers the total number of people in a household, regardless of whether they consumed specific foods or not, and so the EFS consumption data are averaged for the whole population.

In addition to conducting exposure assessments at a population level, the FSA has an interest in assessing exposure at a 'consumer' level. Consumer exposure assessment, in its simplest form, involves combining data on the level of a chemical in a food (measured or predicted) with data on the consumption pattern of the food (usually derived from a dietary survey) in order to estimate the amount of the chemical ingested by an individual over a fixed period of time. The benefits of consumer exposure assessment include the ability to estimate high-level (e.g. 97.5th percentile) consumption, and the facility to remove 'non-consumers' of the food(s) of interest from analyses. Considering consumers only is particularly important for foods that are consumed by a relatively small proportion of the population (e.g. different types of liver), allowing specific 'at risk' population subgroups to be identified for targeted advice.

4.4 Exposure modelling

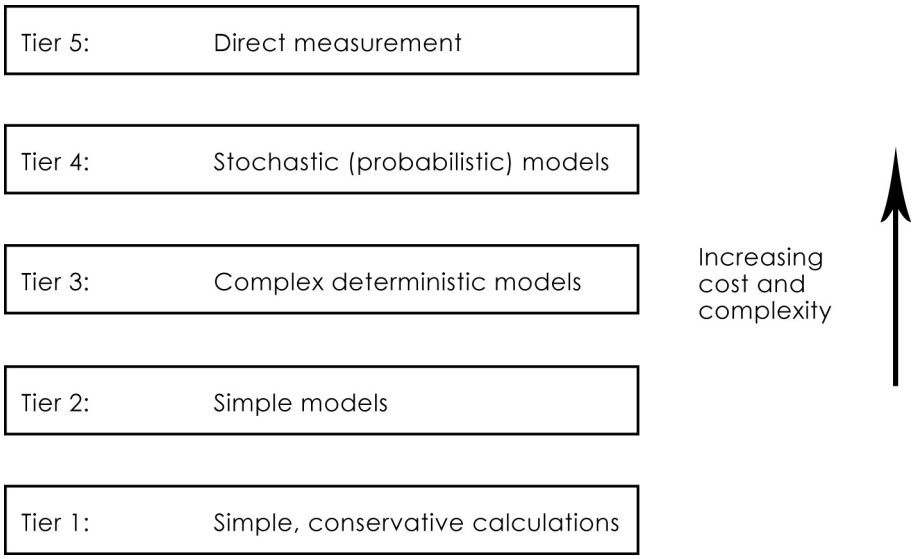
In general, the FSA adopts a hierarchical or tiered approach to selecting the best method to carry out exposure assessment, considering factors such as sources of uncertainty, perceived risk, time, suitability of the method and available resources. The assessment is consistent with the approach adopted by the European Food Safety Authority (EFSA, 2005) and World Health Organization (WHO, 2000). A tiered approach has also been recommended by EFSA for the analysis of uncertainty in exposure assessment (EFSA, 2006).

The hierarchical approach (see Figure 4.2) is a stepwise progression beginning with relatively simple, conservative calculations leading on to more sophisticated computer models which combine distribution data on dietary behaviour with chemical levels to direct measurement of exposure for the target group. Current policy on exposure assessment of chemicals has been to use deterministic and distributional methods. However, the use of more complex methodology such as probabilistic modelling is considered on a case-by-case basis for refining an exposure estimate to a food chemical.

4.4.1 Tier 1

Tier 1 involves basic calculations using conservative worst-case estimates of chemical occurrence and consumption data. These could be based on back calculations (i.e. knowing an ADI and the level of chemical in food, then back calculating how much would have to be eaten to reach the ADI). If the simple estimates are well within safe or agreed limits then the assessment does not proceed further. If the

Figure 4.2 Food Standards Agency tiered approach to exposure assessment



conservative estimate gives any cause for concern it may be necessary to further refine it to give a more realistic picture by taking into account more information. Other methods considered in this tier include using information from measured portion sizes (Ministry of Agriculture, Fisheries and Food, 1993) or manufacturers' feeding instructions (for infant formulae) or recommended dosages (of dietary supplements) to show average exposure, or to assess the number of portions required to achieve a certain level of intake. For foods such as certain types of fish, for which there may be few if any recorded consumers in available surveys, typical portion sizes can be used.

4.4.2 Tier 2

This tier involves using mean or high-level food consumption rates taken from published summary tables of food surveys such as the NDNS. One approach used, which has been found to work reasonably well, is to assume that a high-level consumer might be a high-level consumer of two food categories and would be an average consumer of other foods. This is described in Equation 4.3. It is important to note that the validity of this method is better when using a smaller rather than a larger number of food categories (European Commission, 1998).

4.4.3 Tier 3

The vast majority of FSA exposure assessments utilise Tier 1, 2 or 3 methods. For Tier 3 assessments the FSA uses the Intake program (known as Intake 2). This program makes use of statistical software to predict dietary exposure from individual dietary survey records (such as the NDNS) for different subgroups with single values of a chemical concentration in food. The program uses the 97.5th percentile consumer to represent reasonable high-level consumption. When considering nutrient exposure, a lower-level percentile below 2.5% may be considered.

If an estimate of likely exposure to a chemical in a set of foods is required, Intake 2 can retrieve information on these foods from the relevant survey. Chemical concentrations can be entered into the program for the level of chemical in each group of foods being considered and then Intake 2 will review each participant's dietary record for the foods specified. Where a particular food is eaten, consumption is combined with the relevant chemical concentration for each person in the survey from all the specified foods (provided there are sufficient numbers of recorded consumers of the food(s) in question). If the estimate is for a chemical with a chronic effect, then each person's average daily exposure (ADE) over the length of the survey (four or seven days) is calculated. For a chemical with an acute effect, each person's highest day of exposure to the chemical is selected. If exposure on a body weight basis is required then Intake 2 can calculate that person's exposure using their body weight as recorded in the survey. The full distribution of personal exposure is then plotted, and from this distribution summary statistics (e.g. mean and 97.5th percentile) are extracted. The general statistics used by Intake 2 are provided in the Annex to Section 4.

4.4.4 Tier 4

Tier 4 covers the use of probabilistic modelling. Probabilistic methods represent a higher degree of complexity, allowing consideration of the full range of chemical data and/or other parameters. The models randomly sample the full distribution of chemical levels in individual items of food in addition to the distribution of consumption data provided by the NDNS; the data are combined and presented as a distribution of likely exposures.

Probabilistic modelling offers the possibility of more realistic estimates of exposure and useful refinements in analysis which go beyond routine risk assessment. However, the Agency is currently developing its thinking on determining the most effective use of this methodology.

Probabilistic modelling is particularly suited to assessments of acute exposure since these are well supported by the short-term dietary intake data collected by the FSA (via the NDNS). Assessments of long-term exposure are usually less suited to probabilistic modelling, due to the difficulty in extrapolating from short-term intake data. Spikes of exposure, which may be important to model in relation to acute assessment (e.g. hot spots of pesticide residue in a single apple), tend to average out in long-term assessments.

Where probabilistic modelling has been applied to FSA assessments of longer-term exposure it has

Equation 4.3

$$\textit{Estimated total consumption} = \sum \left(2 \times \textit{highest consumption} + \textit{mean population consumption from the rest of the diet}\right)$$

Where: *Highest consumption* is the amount of food consumed, g
Mean population consumption from rest of the diet is the amount of that food that is consumed, g

usually been in order to model the possible impact of brand loyalty.

The Agency has consulted with other government departments to consider the value of probabilistic modelling for assessing exposure to multiple chemicals from multiple sources. This work is being carried out in the context of addressing the recommendations made by the Committee on Toxicity (COT) Working Group on the Risk Assessment of Mixtures of Pesticides and Similar Substances (COT, 2002).

In addition, the FSA has developed probabilistic models for the terrestrial food chain and is developing similar types of model for the aquatic food chain. This modelling is specifically carried out for radiological assessments and includes calculating the movement of chemicals through the atmospheric, aquatic and terrestrial environments.

4.4.5 Tier 5

This is a direct measure of exposure for a specific critical group, using methods such as biomarkers or duplicate diet studies. A duplicate-diet study of vegetarians has been carried out to determine dietary exposures to inherent natural toxicants, 12 metals and other chemical elements, and nitrate (MAFF, 2000). This information has been used to assess the risks to health of vegetarians by comparison with dietary exposures estimated for the general UK population and with the appropriate maximum recommended exposure levels.

The individuals taking part in the study collected an exact duplicate of everything they ate (except beverages) over a week, and the samples were analysed for 12 metals and other elements. Dietary exposures were calculated from the concentrations of the elements in the duplicate diet samples and from the weights of the samples.

4.5 Case study

Ascorbic acid, also known as vitamin C, is found in a wide variety of fruit and vegetables. Good sources include peppers, broccoli, Brussels sprouts, sweet potatoes, oranges and kiwi fruit. Chronic exposure of adults in the NDNS to ascorbic acid in oranges and orange juice (consumed directly) has been used in this case study. Any food chemical can be treated in a similar fashion. In a risk assessment of ascorbic acid, 'total exposure' would be considered, but there might be some instances in which it is useful to explore contribution from one or two sources, in order to determine contribution to total.

The amount of ascorbic acid in oranges and orange juice is 54 mg 100 g^{-1} and 39 mg 100 g^{-1}, respectively (FSA, 2002).

4.5.1 Tier 1

A simple calculation is used as the start (Equation 4.1). It is assumed that a high-level consumer may drink one average glass of orange juice a day and eat one medium orange a day. An average glass of orange juice weighs 160 g and an average orange with no peel weighs 160 g (Ministry of Agriculture, Fisheries and Food, 1993).

$$\frac{160\text{ g}}{100} \times 39\text{ mg} + \frac{160\text{ g}}{100} \times 54\text{ mg} = 149\text{ mg person}^{-1}\text{ day}^{-1}$$

However, this is a very crude assessment. To refine the assessment, the consumption of oranges and orange juice by the participants in the NDNS survey is considered in the next tier.

4.5.2 Tier 2

Table 4.1 is from the NDNS summary data that show the mean amount of orange and orange juice consumed by all individuals who consumed these foods in the survey. Consumption values at the 97.5th percentile level are also shown in order to represent high-level consumption.

The exposure to ascorbic acid can then be calculated as follows.

Mean exposure to ascorbic acid from oranges = mean consumption of oranges from NDNS survey (g) × ascorbic acid concentration (mg g^{-1})

97.5th percentile exposure to ascorbic acid from oranges = 97.5th percentile consumption from NDNS survey (g) × ascorbic acid concentration (mg g^{-1})

The same calculation is made for exposure from orange juice, and the results for oranges and orange juice combined (Table 4.2).

However, adding the consumption or exposure data together can often lead to an overestimate, because the participants in the survey who consumed a high amount of oranges may not necessarily be extreme consumers of orange juice as well. The Intake 2 program does these calculations more accurately at the next tier.

Table 4.1 Orange and orange juice consumption for adults in the NDNS

	Number of consumers	Mean consumer (g person^{-1} day^{-1})	97.5th percentile consumer (g person^{-1} day^{-1})
Oranges	232	45	171
Orange juice	617	96	310
Combined		141	481

Table 4.2 Exposure to ascorbic acid from oranges and orange juice

Exposure to ascorbic acid	Mean consumer (mg person^{-1} day^{-1})	97.5th percentile consumer (mg person^{-1} day^{-1})
Oranges	24	92
Orange juice	37	121
Combined	61	213

Table 4.3 Exposure to ascorbic acid in oranges and orange juice using Intake 2

Food	Number of consumers	% consumers of total surveyed (1724)	Mean consumer (mg person^{-1} day^{-1})	Median consumer (mg person^{-1} day^{-1})	97.5th percentile consumer (mg person^{-1} day^{-1})
Oranges	232	14	24	16	92
Orange juice	617	36	37	28	121
Oranges and orange juice	750	44	38	28	130

4.5.3 Tier 3

The level of ascorbic acid can be set and exposure can be considered for orange juice separately from oranges, and oranges and orange juice combined together (Table 4.3).

The estimates for oranges and orange juice together are lower than for the combined data from Table 4.2 because the Intake 2 program identifies the participants that consumed both foods in the survey. Using this higher tier shows that tiers 1 and 2 lead to a higher estimate of exposure to ascorbic acid, which would be an overestimate of the intakes for the great majority of consumers.

Similar analysis could be applied to acute exposures to chemicals. This would involve using the Intake 2 program to identify the highest amount of a particular food eaten on one day and multiplying this by a chemical concentration to obtain an exposure value.

Annex: General statistics used by Intake 2

The FSA Intake 2 program is a distributional model for determination of acute or chronic intake of chemicals from food that uses distributional data for one input variable. The system contains raw data about food consumption from the NDNS. If information about the concentration of a chemical in food is available, a concentration value can be assigned to each relevant food description in the database. Acute or chronic chemical intake can be calculated for each participant of the survey based on their personal food consumption records and the concentration data; the intake value can also be expressed according to that person's body weight.

Unless explicitly stated otherwise, the Intake 2 program uses assumptions that are based on the intake of the consumer population, that is, those people in the survey who have eaten the food of interest rather than average consumptions based on the total population of the survey. A number of descriptive statistics are produced, including:

- number of consumers
- mean exposure of consumers and standard deviation
- minimum and maximum exposure

- median exposure
- up to two user-defined percentiles (Percentile1 and Percentile2)
- confidence intervals about the percentiles
- number of people in survey population
- survey population mean
- % consumers.

The following equations (4.4–4.17) are used by Intake 2 to model exposure; they incorporate a weighting factor (*Wi*) to reweight the survey population to better reflect the distribution of the UK population based on age, gender and country. A weighting factor of 1.5, say, means that that person's exposure counts 1.5 times more than a person with weighting factor of 1. The median and percentiles are calculated by ranking the exposures in order, identifying the appropriate rank (based on the sum of the individual weightings), and interpolating between the exposure levels associated with the consumers either side of the rank as detailed in the equations below.

Equation 4.4 Mean of consumers

$$\overline{X}_{Consumers} = \frac{\sum_{i=1}^{N_{consumers}} (W_i X_i)}{\sum_{i=1}^{N_{consumers}} W_i}$$

Where: $X_{consumers}$ is the mean consumer exposure, g person^{-1} day^{-1}
X_i is consumer exposure for each data point, g person^{-1} day^{-1}
W_i is a weighting factor to reflect distribution of the UK population, no units
$N_{consumers}$ is the number of consumers included in the calculation

Equation 4.5 Number of consumers

$$N_{Consumer} = count\left(X_i\right) \text{ for } \left\{i_{Consumer}\right\}$$

Where: $N_{consumer}$ is the number of consumers included in the calculation
X_i is consumer exposure for each data point, g person^{-1} day^{-1}
$i_{Consumer}$ is each individual consumer in the survey, i.e. each data point

Equation 4.6 Standard deviation

$$Sd = \sqrt{\frac{\sum_{i=1}^{N_{consumers}} \left(W_i (X_i - \overline{X}_{consumers})^2\right)}{\left(\sum_{i=1}^{N_{consumers}} W_i\right) - 1}}$$

Where: Sd is the standard deviation of consumer exposure
$X_{consumers}$ is the mean consumer exposure, g person^{-1} day^{-1}
X_i is consumer exposure for each data point, g person^{-1} day^{-1}
W_i is a weighting factor to reflect distribution of the UK population, no units
$N_{consumers}$ is the total number of consumers included in the calculation

Equation 4.7 Standard error

$$STD_{error} = \frac{Sd}{\sqrt{N_{consumers}}}$$

Where: STD_{error} is the standard error of the sample
Sd is the standard deviation of the sample
$N_{consumers}$ is the total number of consumers included in the calculation

Equation 4.8 Minimum

$$Min = minimum\left(X_i\right) \text{ for } \left\{i_{Consumers}\right\}$$

Where: Min is the minimum consumer exposure of all consumers included, g person^{-1} day^{-1}
X_i is consumer exposure for each data point, g person^{-1} day^{-1}
$i_{consumer}$ is each individual consumer in the survey, i.e. each data point

Equation 4.9 Maximum

$$Max = max\left(X_i\right) \text{ for } \left\{i_{Consumers}\right\}$$

Where: Max is the maximum consumer exposure of all consumers included, g person^{-1} day^{-1}
X_i is consumer exposure for each data point, g person^{-1} day^{-1}
$i_{consumer}$ is each individual consumer in the survey, i.e. each data point

The median and up to two user-defined percentiles are calculated by ranking the exposures in order, identifying the appropriate rank (based on the sum of the individual weightings), and interpolating between the exposure levels associated with the consumers either side of the rank, as detailed in the equations below.

Equation 4.10 Median

$$X_{median} = \frac{\left(Rank_{median} - \sum W_{Low}\right) X_{High} + \left(\sum W_{High} - Rank_{median}\right) X_{Low}}{\left(\sum W_{High} - \sum W_{Low}\right)}$$

Where: X_{median} is median consumer exposure, g person^{-1} day^{-1}
$Rank_{median}$ is median rank based on the sum of consumer weightings as defined in the equation below
W_{Low} is weighting factors of consumers below the $Rank_{median}$th consumer
W_{High} is weighting factors of consumers above the $Rank_{median}$th consumer
X_{High} is consumer exposure above $Rank_{median}$th exposure, g person^{-1} day^{-1}
X_{Low} is consumer exposure below $Rank_{median}$th exposure, g person^{-1} day^{-1}

$$Rank_{median} = \left(\left(\sum_{i=1}^{N_{consumers}} W_i\right) \times 0.5\right) + 0.5$$

Where: $Rank_{median}$ is the median ranking of consumers based on their individual weightings
W_i is a weighting factor to reflect distribution of the UK population, no units
$N_{consumers}$ is the total number of consumers included in the sample

Equation 4.11 Percentile 1

$$Rank_{P_1} = \left(\left(\sum_{i=1}^{N_{consumers}} W_i\right) \times p_1\right) + 0.5$$

$$X_{P_1} = \frac{\left(Rank_{P_1} - \sum W_{Low}\right) X_{High} + \left(\sum W_{High} - Rank_{P_1}\right) X_{Low}}{\left(\sum W_{High} - \sum W_{Low}\right)}$$

Where: X_{P_1} is nth percentile consumer exposure, g person^{-1} day^{-1}
p_1 is the nth percentile to be calculated [user defined, typically 97.5%]
$Rank_{p_1}$ is nth percentile rank based on the sum of consumer weightings
$N_{consumers}$ is the total number of consumers included in the sample
W_i is a weighting factor to reflect distribution of the UK population, no units
W_{Low} is weighting factors of consumers below the $Rank_{p_1}$th consumer
W_{High} is weighting factors of consumers above the $Rank_{p_1}$th consumer
X_{High} is consumer exposure above $Rank_{p_1}$th exposure, g person^{-1} day^{-1}
X_{Low} is consumer exposure below $Rank_{p_1}$th exposure, g person^{-1} day^{-1}

Equation 4.12 Percentile 1: Lower 95% confidence interval

$$Rank_{p_1LCI} = \left(\left(\sum_{i=1}^{N_{consumers}} W_i\right) \times p_1\right) + 0.5 - 1.96\sqrt{\left(p_1\right)\left(1 - p_1\right)\left(\sum_{i=1}^{N_{consumers}} W_i\right)}$$

$$X_{p_1LCI} = \frac{\left(Rank_{p_1LCI} - \sum W_{Low}\right) X_{High} + \left(\sum W_{High} - Rank_{p_1LCI}\right) X_{Low}}{\left(\sum W_{High} - \sum W_{Low}\right)}$$

Where: X_{p_1LCI} is lower 95% confidence interval for the nth percentile consumer exposure, g person^{-1} day^{-1}
p_1 is the nth percentile to be calculated [user defined, typically 97.5%]
$Rank_{p_1LCI}$ is the lower 95% confidence interval rank for the nth percentile rank
$N_{consumers}$ is the total number of consumers included in the sample
W_i is a weighting factor to reflect distribution of the UK population, no units
W_{Low} is weighting factors of consumers below the $Rank_{p_1LCI}$th consumer
W_{High} is weighting factors of consumers above the $Rank_{p_1LCI}$th consumer
X_{High} is consumer exposure above $Rank_{p_1LCI}$th exposure, g person^{-1} day^{-1}
X_{Low} is consumer exposure below $Rank_{p_1LCI}$th exposure, g person^{-1} day^{-1}

Equation 4.13 Percentile 1: Upper 95% confidence interval

$$Rank_{p_1UCI} = \left(\left(\sum_{i=1}^{N_{consumers}} W_i \right) \times p_1 \right) + 0.5 + 1.96 \sqrt{(p_1)(1-p_1)\left(\sum_{i=1}^{N_{consumers}} W_i \right)}$$

$$X_{p_1UCI} = \frac{\left(Rank_{p_1UCI} - \sum W_{Low}\right) X_{High} + \left(\sum W_{High} - Rank_{p_1UCI}\right) X_{Low}}{\left(\sum W_{High} - \sum W_{Low}\right)}$$

Where: X_{p_1UCI} is upper 95% confidence interval for the *n*th percentile consumer exposure, g person^{-1} day^{-1}
p_1 is the *n*th percentile to be calculated [user defined, typically 97.5%]
$Rank_{p_1UCI}$ is the upper 95% confidence interval rank for the *n*th percentile rank
$N_{consumers}$ is the total number of consumers included in the sample
W_i is a weighting factor to reflect distribution of the UK population, no units
W_{Low} is weighting factors of consumers below the $Rank_{p_1UCI}$ th consumer
W_{High} is weighting factors of consumers above the $Rank_{p_1UCI}$ th consumer
X_{High} is consumer exposure above $Rank_{p_1UCI}$ th exposure, g person^{-1} day^{-1}
X_{Low} is consumer exposure below $Rank_{p_1UCI}$ th exposure, g person^{-1} day^{-1}

Equation 4.14 Percentile 2

A second user-defined percentile of exposure can be calculated in a similar manner to Percentile 1, as detailed above.

Equation 4.15 Number in population

$$N_{population} = count\left(X_i\right) \text{ for } \left\{ i_{population} \right\}$$

Equation 4.16 Percentage of consumers

$$p_{consumers} = \frac{\sum_{i=1}^{N_{consumers}} W_i}{\sum_{i=1}^{N_{population}} W_i}$$

Equation 4.17 Mean of population

$$\overline{X}_{population} = \frac{\sum_{i=1}^{N_{population}} (W_i X_i)}{\sum_{i=1}^{N_{population}} W_i}$$

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5 Summary

5.1 Introduction

Exposure assessment is, alongside hazard characterisation, a key step in the risk assessment process. Risk assessment is frequently a requirement of regulations and legislation, and exists to protect the populace from environmental and occupational risks. A number of UK government departments and agencies have responsibility for assessing risk to human health from chemicals in the air, soil, drinking water, food, occupational environment, consumer products, animal feed and human and veterinary medicines. There are therefore many different chemicals for which human exposure is likely to occur via a range of potential pathways. As data regarding exposures are commonly absent and, if available, limited to specific scenarios and circumstances, assessments of exposure contain inherent uncertainties and may result in risk assessments that do not necessarily reflect the risk of a particular situation. Exposure modelling enables assessments to take place in the absence of situation-specific data using clearly defined assumptions; where data are uncertain deterministic and probabilistic assessments can be conducted. By clearly defining the assumptions used in exposure models, including the use of default values on occasions where no data exist, the exposure assessment and resulting risk assessment can be evaluated for validity.

The purpose of this document has been to evaluate some of the main exposure models used by UK government regulators, risk assessors and policy makers, and explain the underlying processes of the modelling approaches utilised. By increasing transparency of the models, it is possible to determine how the outcomes are derived for specific scenarios and hence inform decisions regarding risk to human health from exposure to chemicals in the environment and at work.

5.2 Exposure models

Many UK government departments and agencies use chemical exposure assessments for which certain exposure modelling approaches are used or have been developed. This document describes the models used by three government agencies (Table 5.1) and the integration of the specific models into the exposure assessment framework.

The Environment Agency's Contaminated Land Exposure Assessment (CLEA) model was first developed to derive soil guideline values (SGV) for contaminated land in the UK, and hence may be considered a generic exposure assessment tool. CLEA is used to evaluate ingestion, inhalation and dermal exposures for adults and children in contact with contaminated soils through living, working and playing on contaminated sites over long periods of time; as such, it may also be considered applicable to site-specific exposure assessments. Using deterministic assessments, the CLEA model benefits from an ability to perform aggregate exposure assessments for up to ten exposure pathways (involving soils, vegetable consumption, indoor and outdoor vapours, and indoor and outdoor dust), providing separate age and gender categories, as well as the ability to integrate background factors (other sources of exposure to contaminants of concern). Designed to be specifically applicable to the UK situation, CLEA does also possess a number of potential limitations. These include the use of conservative default values and exposure scenario assumptions, the absence of acute exposure assessment (for periods of less than one year), and the exclusion of exposure pathways involving groundwater, surface water and food substances other than fruit and vegetables. The outcome of the model is the average daily exposure (ADE) from all or individual exposure routes applicable to the conceptual model developed for a particular scenario. The ADE is used to calculate SGV by comparing to

Table 5.1 Comparison of exposure models used by UK government department and agencies (in the absence of measured data)

Dept, Agency	Model	Use	Solution	Input	Pathway	Duration	Receptor	Aggregate exposure[1]	Cumulative assessment[2]	Variability and uncertainty
Environment Agency	CLEA	Adult/child exposure to contaminated land	Deterministic	Measured, estimated and/or default data	Ingestion, inhalation, dermal – dust, vapours soil, vegetables	One childhood year to lifetime	Children (16 age groups), working adults, retired – all local population	Yes	No	Distribution data and Monte Carlo simulation
Health and Safety Executive	EASE	Workplace exposures to hazardous chemicals	Deterministic	Measured, estimated and/or default data	Inhalation, dermal – dust vapours/gas solid, liquid	Daily exposures	Workforce	No	No	Exposure ranges rather than single values
Health and Safety Executive	ConsExpo	Exposure to and and uptake of chemicals in consumer products e.g.biocides	Probabilistic/ deterministic	Measured, estimated and/ or default data	Ingestion, inhalation, dermal – air, food, surfaces	Single events to yearly exposures	Users/consumers; non-users exposed at time of application	Yes	No	Distribution data and methodology for sensitive analysis
Health and Safety Executive	BEAT	Workplace exposures, e.g. biocides	Probabilistic/ distributional	Estimated and/ default data	Dermal	Task-based	Workforce	Yes	No	Distribution data
Health and Safety Executive	POEM	Workers exposed to agricultural pesticides	Deterministic	Default values	Inhalation, dermal – solid/ liquid conc., spray	Daily exposures pesticides	Operators applying/ preparing agricultural	Yes	No	Conservative model
Health and Safety Executive	Consumer Exposure model	Consumer dietary exposures to pesticides	Deterministic	Estimated and/or default values	Ingestion – agricultural commodities	Daily to lifetime	Children (three age groups), working adults	No	No	Consumption data – some variation considered
Food Standards Agency	Intake 2 program	UK population exposure to dietary contaminants	Distributional/ deterministic	Estimated and/ or default data	Ingestion – food/water	Daily to one week (chronic)	Children (three age groups), working adults, retired adults, vegetarians	No	No	Distribution data

Adapted from Fryer *et al.* (2004)

[1] Combined exposures from all sources (multiple pathways, single agent)

[2] Combined exposures to different chemicals (numerous agents)

health criteria values (HCV), which are contaminant-specific toxicological benchmark values that also provide a measure of risk associated with exposure.

Exposure modelling by the Health and Safety Executive (HSE) differs from that of the Environment Agency (EA) due to a focus on exposure to particular chemicals and groups of chemicals in the workplace, specifically occupational exposure to industrial chemicals, biocides and pesticides, rather than environmental pathways (e.g. contaminated land). With regard to industrial chemicals in the context of REACH, the ECETOC targeted risk assessment (TRA) tool is the primary model used. The ECETOC TRA tool is based on the EASE (estimation and assessment of substance exposure) model, which assesses the exposure of workers to substances hazardous to human health in the workplace. It is a deterministic, empirical knowledge-based model that adopts a decision-tree approach to the assessment of inhalation (dust or gas/vapour/aerosol) and dermal (gas, liquid or solid substance) exposures based on the physical properties of the substance, patterns of use, the processes being undertaken, and any control measures in place. Ingestion is not usually considered an occupational exposure pathway for industrial chemicals. EASE can be applied to a variety of occupational situations, has application to a wide range of chemical substances and has been extensively validated (including adoption as part of the European Union System for the Evaluation of New Substances, EUSES). However, it is unable to consider acute worker exposures, only includes normal (i.e. not accidental) exposure scenarios and cannot aggregate exposure pathways (i.e. exposure via inhalation and dermal exposures) or provide a cumulative assessment for groups of chemicals. EASE evaluates exposure based on chemicals present in the workplace environment and does not model intake of the chemical, and hence does not include parameters concerning, for example, body weight. The decision-tree approach provides for ease of use, but the categorical and numerical features lead to a semi-quantitative model that only predicts exposure ranges rather than providing distinct values; this makes EASE more suitable for use at lower tiers of the risk assessment hierarchy (simple to deterministic models). However, EASE does give preference to the use of measured exposure data, particularly for inhalation, from representative UK workplace environments; default assumptions are only used if analogous or surrogate data cannot be used in the absence of measured values, and are more applicable to dermal models. EASE outputs can be used to derive inhalation time-weighted averages (TWA), although caution is urged on their use due to the semi-quantitative nature of the model. More recently, it has been proposed that EASE be redeveloped to include a probabilistic model and exposure database to help predict exposure variability and uncertainty.

For biocides, HSE uses a similar approach to the EASE model through the determination of patterns of use, population at risk (primary or occupational exposure and secondary or bystander/consumer exposure), routes of exposure and exposure scenario, and uses measured data rather than generic (analogous or surrogate) or modelled data. When measured exposure data are not available and the application of generic data is necessary, two exposure models can be applied to the assessment of biocides – Bayesian Exposure Assessment Toolkit (BEAT) and Consumer Exposure (ConsExpo). Unlike EASE, BEAT provides a probabilistic tool and an integrated exposure database able to generate estimates of dermal exposure based on specified scenarios, including indications of variability and uncertainty. ConsExpo, also adopted as part of EUSES, is a deterministic and probabilistic model that assists in the estimation of dermal, inhalation and oral exposures of consumers to products containing chemical compounds (paint, cosmetics, children's toys, disinfectants, cleaning and pest-control products). ConsExpo can consider complex scenarios, evaluating multiple routes and pathways of exposure for a wide range of substances and including acute and chronic exposures; however, the model is complex, relates to consumer products only, and does not consider susceptible populations or provide cumulative assessments for multiple chemicals. Some of the ConsExpo models have been validated against measured data sets.

For pesticide, HSE uses the Predictive Operator Exposure Model (POEM) to predict the level of exposure likely to be experienced by operators preparing and applying agricultural pesticides in the UK. Based on an Excel spreadsheet, POEM divides operator exposures into two distinct parts: preparation of the pesticide from the solid or liquid concentrated formulation (dermal exposure to hands only) and application of the diluted formulation as a spray (dermal and inhalation exposures). Ingestion is not considered in occupational exposure assessments. Exposure levels, including absorption factors, are predicted from a series of conservative assumptions and default values derived from generic monitoring studies and application for single-day exposure, with the output of the model compared to a relevant reference dose, most commonly the no observed adverse effect level (NOAEL) or acceptable operator exposure level (AOEL). Default values can be changed if product-specific information is available, with the model using the 75th percentile of measured values. While designed for UK situations, the semi-quantitative/deterministic model is only applicable to occupational pesticide exposure scenarios and cannot be used to assess cumulative exposure to pesticides.

POEM does not consider work re-entry or bystander exposures, but is being expanded upon in Europe for a greater range of exposures to plant protection products (EUROPOEM). Workers (non-operators), bystanders and residents are considered separately to operators (pesticide applicators). Modelling of dermal, inhalation and ingestion (for children living close to application sites) exposures for non-operator susceptible groups involves consideration of a number of parameters including application-specific variables and variables affecting the receptor (namely, work rate, clothing penetration, inhalation rates, etc.), many of which are provided with default values. The EUROPOEM model provides an option to consider a re-entry group and includes various default values (for transfer coefficients, task-specific factors, etc.) to assist in calculations. Generally, however, exposure estimates for workers, bystanders and residents are calculated manually rather than by a specific or even a generic model program.

HSE also assesses consumer exposure to pesticide residues using the Consumer Exposure Model (ConsExpo), linked to the FSA's Intake program. The ConsExpo Model only considers exposures to pesticides via the ingestion of residues in agricultural commodities by the UK population. The deterministic model uses data on the consumption of agricultural commodities, pesticide residue levels, factors affecting pesticide concentration, acceptable daily intake (ADI) levels and population body weights to calculate conservative pesticide intake values. For single-day exposures, the model calculates a national estimate of short-term intake (NESTI) by multiplying consumption by the highest residue (HR) level in a commodity. For lifetime exposures, a national estimate of dietary intake (NEDI) is determined from consumption and pesticide residue levels (provided as supervised trial median residue, STMR). Total NEDI can be obtained for each subpopulation and food type considered. More conservative exposure values can be obtained from the model, which calculates theoretical maximum daily intake (TMDI) using maximum residue levels and so provides a 'worst-case scenario' of exposure. If expanding to total dietary intake, the Rees–Day model can be used.

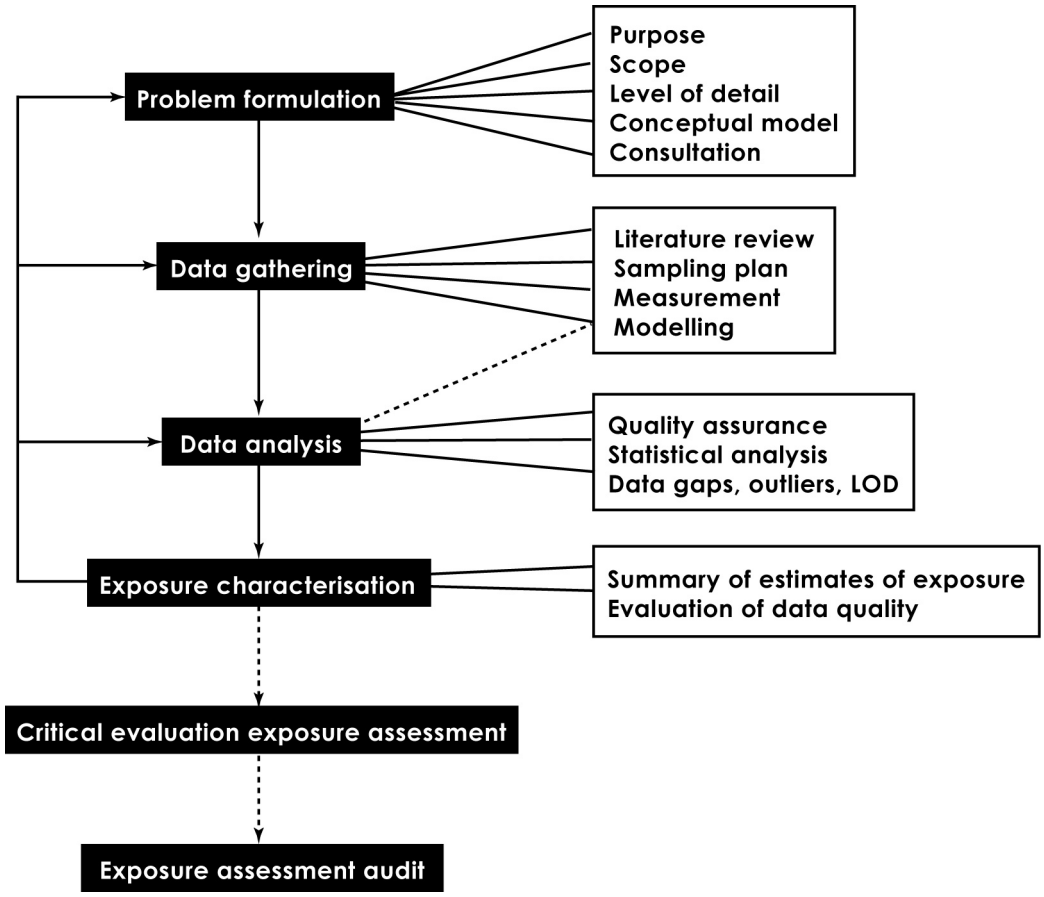
The Food Standards Agency (FSA) uses the Intake program (Intake 2) to assess acute and chronic dietary chemical exposures for the UK population, based upon consumption data from UK dietary surveys. It is a deterministic model which assigns a unique numerical code to every food item; this code is linked to the Risk Recipe database, which defines the chemical content of each ingredient, specifically food additives, pesticides and veterinary medicine residues. Maximum limits and action levels have been set by the European Union for some environmental pollutants, process contaminants and naturally occurring toxins such as mycotoxins, but many chemicals are not regulated. Using a sample of the UK population, the outcomes of the model can be compared to these limits as well as to reference doses such as the ADI, which is an estimate of the amount of a substance that can be ingested on a daily basis over a lifetime on a body weight basis without an appreciable health risk. Relatively few input parameters are required, it is UK-specific, and considers a range of age groups, diets (e.g. vegetarian) and chemicals as well as interindividual variability in consumption patterns. Weighting factors can be used to reweight the sample population to better reflect the distribution of the UK population. However, the Intake program does not consider multiple substances concurrently or incorporate variability and uncertainty into concentration levels, nor does it assess exposures for time periods in excess of one week (chronic exposure). Intake 2 does consider multiple food sources for one substance and hence prevents 'double accounting' of intakes from different food types. It is a proprietary FSA tool and so is not widely used beyond the FSA. Probabilistic models have been developed by the FSA for higher-tier exposure assessments, but such models are not frequently used and it is common for most exposure assessments to stop at the Intake 2 modelling step.

5.3 Similarities of approach

The exposure models summarised in Section 5.2 and Table 5.1 reflect the very different focus of the three government departments and agencies, involving different types of chemicals, routes of exposure and receptor categories. However, there are a number of similarities of approach adopted by each of the exposure models, including the stage at which the exposure model is used, the tiered approach to modelling, the recognition of the source–pathway–receptor methodology, and similar pathways and parameters.

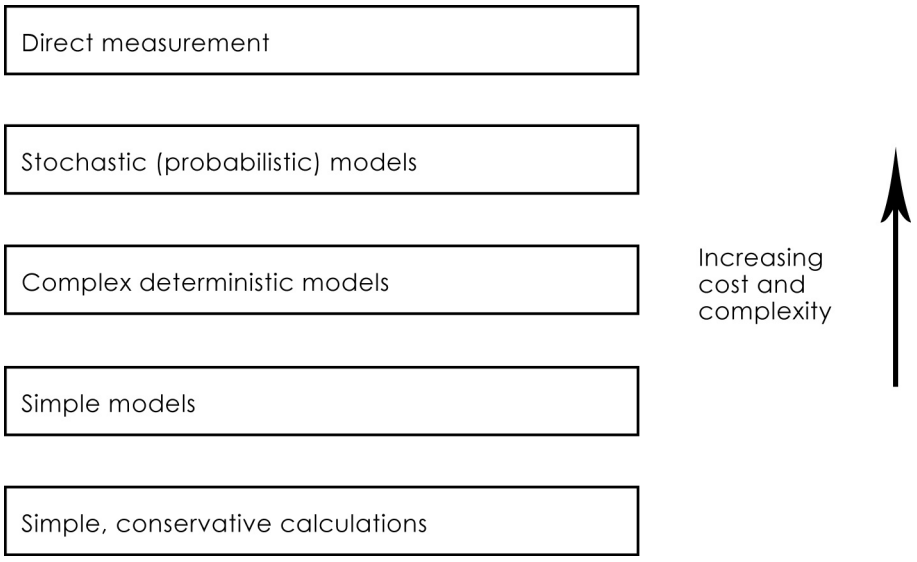
Modelling is one element of the exposure assessment approach, which includes a number of steps and subdivisions as shown in Figure 5.1. Modelling can be used at the data-gathering stage, if measured data are unavailable or limited, or during data analysis to obtain statistical descriptions of the exposure scenario and the consequences that occur as a result. Simple models are widely used to generate data in the absence of measured values whilst more complex models are able to generate estimates, combine the estimates with measured or default data, if available, and interpret the result. As such, exposure modelling adopts a tiered approach, using simple calculations to obtain data for single pathway and receptor scenarios (Tier 1) and

Figure 5.1 Stepwise approach to exposure assessment



LOD, Limit of detection

Figure 5.2 Tiered approach to exposure modelling, based on Figure 4.2



progressing through to stochastic or probabilistic models for more complicated scenarios involving a number of different pathways and receptors (Figure 5.2). Direct measurement of exposure is the ultimate approach to data gathering, although this need not exclude modelling for analytical purposes.

The dotted line between modelling and data analysis in Figure 5.1 indicates that modelling can be used for both data gathering and data analysis. After exposure characterisation, the exposure assessment is complete and subsequent steps (as shown connected by dotted arrows) exist to ensure consistency and validity [after IGHRC, 2004].

The source–pathway–receptor approach applies to exposure assessment, hazard assessment and risk assessment. All models used by UK government departments and agencies apply the general risk linkages of source, pathway and receptor (Table 5.1). While all the sources involve exposure to a chemical, albeit a specific pesticide, a soil contaminant or a chemical within a consumer product or food, the specifics of the exposure vary according to the role of the department or agency. One or more pathways from inhalation, ingestion and/or dermal exposure are considered, whilst the receptors include any combination from children (of varying age-group categories) to working adults (16–64 years), retired adults (65+ years) and occupationally exposed individuals (a specific proportion of the 16–64-year working adult group). Bystanders, defined as individuals not applying or using the product but exposed through proximity to application or usage site, are also frequently considered.

Many exposure assessment models utilise default values based on generic situations and derived from measured exposure values; the default values may be used instead of or alongside measured variables. The parameters used by each of the exposure models described in this document (see Table 5.1) vary according to the specific source, pathway or receptor. Nevertheless, there are a number of parameters that are required for all the models, examples of which are provided in Table 5.2. Body weight, as appropriate for the specific receptor category (namely adult or child), is considered by almost all the models; the most common default value being 60/70 kg for an average adult. Consumption, use and application rate are also required by the models to determine likely exposure, as are intake, or even uptake, levels which are frequently a default proportion of the exposure level. Duration of exposure varies from acute to chronic, with time scales tied to the type of exposure (hazardous chemical in the workplace compared to food contaminant); a daily exposure is the most common period of exposure duration modelled. Intake rates for inhalation are provided for some models, as are dermal absorption rates. However, there are a number of parameters that are specific to the scenario being modelled, such as the dislodgeable foliar residue (DFR) used in bystander and occupational exposure models to predict exposure to pesticide residues after application of the product to a crop. This example provides one difference between the models described herein, a factor that is expanded upon in Section 5.4.

5.4 Critical differences in approach

The models used by UK government departments and agencies have all been developed for different purposes, whether to assess exposure of workers to industrial chemicals or pesticides, or consumer exposure to contaminated land, food or pesticides (Table 5.1). While they all share the same tiered source–pathway–receptor approach, the models frequently include different parameters, including the types of exposure pathway considered, the environmental media these pathways operate through and the types of receptor considered. It is the

Table 5.2 Examples of the common exposure parameters considered by the models

Parameter	CLEA	EASE	ConsExpo	BEAT	Intake 2	POEM	Consumer Exposure Model
Body weight	✓	–	✓	✓	✓	✓	✓
Consumption, use rates e.g. vegetables eaten	✓	–	–	–	✓	–	✓
Inhalation rate	✓	–	✓	–	–	✓	–
Rate of dermal absorption	✓	–	✓	–	–	✓	–
Ingestion rate	✓	–	–	–	✓	–	✓
Environmentally available levels	✓	✓	✓	✓	✓	✓	✓
Exposure duration (Long-term: >1 year)	✓	–	✓	✓	–	–	✓
Exposure duration (Short-term: day to year)	–	✓	✓	✓	✓	✓	✓

✓parameter included, – parameter not included

individual roles of the departments and agencies that dictate the parameters included in the model. One important example of this is the absence of ingestion as an exposure pathway for occupational exposures to chemicals, ingestion not being perceived as a relevant exposure route in the workplace.

The critical receptor varies as an end point for many of the exposure models. Occupational exposure models focus on the working population, age group 16–65 years, as the receptor, and yet a consumer model must include provision for other age group (<16 years and 65+ years). Nevertheless, the different receptors are all valid within the context of the models used.

Measured exposures are not always available for a complete exposure scenario, but there may be measured values for some aspects of the scenario. Where there is an absence of information, it may be possible to estimate exposure values, or an exposure range, based upon other scenarios, provided that any assumptions are made clear. Some models contain such estimates as default values within the model, with clearly defined assumptions, and frequently have the option to replace the default values with alternative estimates or measured data should the latter be available and defaults invalid for the scenario. One model's default values may differ from the values used in another model as a result of the different pathways, receptors or scenarios considered. Thus, a default body weight of 60 kg or 70 kg may be applicable to occupational exposure assessments, but should the receptor be children, the resulting model would considerably underestimate the level of exposure and hence the risk. The models used by UK government departments and agencies integrate such considerations into the appropriate default parameters.

The use of single value and data ranges varies between models; in some cases, this variation in usage also applies within models. Thus, some models only use single value estimates for a particular parameter while another will provide a range of values (e.g. minimum, maximum and mean) for which Monte Carlo simulation will sample for a probabilistic output. The use of probabilistic modelling provides for a higher-tier exposure assessment. Within models, some parameters may only require a single value (e.g. body weight) whilst others may use data ranges (e.g. contaminant concentration).

There are differences in the transparency of the modelling approach adopted, with some models operating a 'black box' methodology. Part of the difference in transparency is a consequence of the language and use of acronyms that are variously adopted for the models and there is a need for a more consistent approach to be developed for use across all the models; for instance, the term 'conceptual model' has been defined as the exposure scenario in some models, but in others it is the graphical representation of the relationship between source, pathway and receptor.

Differences in approach can therefore be seen to reflect the different goals of the departments and agencies. Thus the main role of the HSE is to ensure health and safety in the workplace, hence the focus on occupational exposures, although secondary exposures to children and bystanders may sometimes also be considered. The FSA focus is on dietary matters and hence the ingestion of food and water is the main pathway of concern. The EA considers more diffuse environmental sources of exposure to chemicals – whether contaminated land or other sources (landfills, incinerators, sewage works, etc.) While parameters, pathways and receptors may differ between models, and the language and acronyms used may act as a diversion, the tiered and hierarchical approach is a consistent feature of the models evaluated in this document.

5.5 Concluding remarks

The UK government has a cross-departmental, coordinated approach to assessing risks, with exposure assessment being part of that process. Exposure assessment adopts a stepwise approach which includes provision for exposure modelling at the data gathering and analysis stages. The models developed by government departments and agencies seek to generate data for generally different scenarios, from exposure to contaminated land, to pesticide spray drift or food contaminant intake. Despite the inclusion of different parameters in models that evaluate different sources, pathways and receptors across the source–pathway–receptor framework, all follow a tiered approach to exposure assessment that uses simple or complex models determined by the particular scenario and the reliability or availability of measured data or applicability of default values. This report provides examples of the exposure models used by three government departments and agencies that demonstrate the degree of similarity and difference, predominantly in the language, terminology and acronyms used in the different models, that exist between the models, with the central aim of increasing transparency of the approaches to exposure modelling adopted by the UK government.

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Glossary

A number of the chapters within this document provide definitions for the terms used. However, different models use different terms for what is frequently the same meaning. This glossary provides definitions for all relevant exposure modelling terminology used in the document and highlights areas of congruence and overlap.

Acceptable daily intake (ADI): Estimate of the amount of a substance in food or drinking water, expressed on a body mass basis (usually mg/kg body weight), which can be ingested daily over a lifetime by humans without appreciable health risk. For calculation of the daily intake per person, a standard body mass of 60 kg is used. ADI is normally used for food additives (tolerable daily intake is used for contaminants).

Acceptable margin of exposure: Margin of exposure (MOE) is a ratio defined by the US EPA as a dose derived from a tumour bioassay, epidemiologic study or biologic marker study, such as the dose associated with a 10% response rate, divided by an actual or projected human exposure. MOE is often used to determine acute risks for single chemicals and a MOE of >100 or >10 is usually considered acceptable when derived from toxicological data from animal and human studies, respectively.

Acceptable operator exposure level (AOEL): The maximum amount of active substance to which the operator, worker or bystander may be exposed without any adverse health effects. The AOEL is expressed as mg of the chemical per kg body weight of the operator.

Acute reference dose (ArfD): An estimate of the amount of a substance in food and/or drinking water, normally expressed on a body weight basis, that can be ingested in a period of 24 hours or less without appreciable health risk to the consumer on the basis of all known facts at the time of the evaluation.

Advance REACH Tool (ART): Higher-tier assessment tool for assessment of occupational exposure.

Age class system: Used by the CLEA model to divide human exposure into discrete time periods, where exposure characteristics change over a human lifetime. There are 18 age classes, 16 covering childhood from birth to 16 years old, and two covering the working and retirement periods of adult life.

Average daily exposure (ADE): The average daily amount of a chemical to which a critical human receptor is exposed over the duration of exposure.

Bayesian Exposure Assessment Toolkit (BEAT):
A Bayesian task-based exposure model for computing dermal exposure in a wide variety of circumstances. The model is mainly aimed at assessing primary exposure of those applying the biocide product, but is also widely applicable to assessment of formulations of chemical substances.

Biocide: Biocidal products are used in a variety of industries to control unwanted organisms, such as animals, insects, bacteria, viruses and fungi. They are intended to kill or otherwise exert a controlling effect by chemical or biological means.

Breathing zone: The area around the nose and mouth from which air is inhaled.

Bystander: Person located within or directly adjacent to the area where pesticide application or treatment is in process, whose presence is quite incidental and unrelated to work involving pesticides but whose position may put them at risk of potential exposure, who takes no action to avoid or control exposure and who, it is assumed, wears no protective clothing and perhaps little ordinary clothing.

Chemicals Regulation Directorate (CRD): A directorate of the Health and Safety Executive (HSE) whose primary aim is to ensure the safe use of biocides, industrial chemicals, pesticides and detergents to protect the health of people and the environment.

Commercial/industrial Conceptual Exposure Model: See 'Conceptual Exposure Model', with application to commercial and/or industrial situations only.

Committee on Toxicity of Chemicals in Food, Consumer Products and the Environment (COT): An independent scientific committee that provides advice to the Food Standards Agency, the Department of Health and other government departments and agencies on matters concerning the toxicity of chemicals.

Commodity: The edible part of a plant after harvest, that may or may not need further processing before consumption.

Conceptual Model: See 'Conceptual Exposure Model' or, for other models, 'Exposure scenario'.

Conceptual Exposure Model: A textual or graphical representation of the relationship(s) between source(s), pathway(s) and receptor(s) for an exposure situation.

Consumer Exposure Model (ConsExpo): A mathematically based computer model for estimating consumer exposure and uptake to chemical compounds used in consumer products.

Contaminated Land Exposure Assessment (CLEA): Deterministic exposure model used to derive soil guideline values (SGV).

Crop: A plant that is being cultivated

Derived minimal-effect level (DMEL): Represents a level of exposure at which there is anticipated to be a minimal residual risk of adverse effects to human health, which is regarded to be of low concern from a risk management point of view. DMEL, when available, are used in REACH as benchmarks against which to assess the acceptability of exposure to substances where the critical effect is considered to arise through a mode of action for which it is not possible to identify with confidence whether or not a threshold dose exists.

Derived no-effect level (DNEL): Represents a level of exposure above which humans should not be exposed. DNEL are used in REACH as benchmarks against which to assess the acceptability of exposure to substances where the critical effect arises through a mode of action for which a threshold can be anticipated.

EASE: Estimation and Assessment of Substance Exposure model. A deterministic exposure estimation tool to assess workplace exposure by the inhalation and dermal routes.

E-Fast: Exposure and Fate Assessment Screening Tool. A tool to assess exposure to chemicals resulting from release to air, land or water.

EMKG-Expo: A Tier 1 screening tool to estimate workplace inhalation exposure. EMKG stands for Einfaches Maßnahmenkonzept Gefahrstoffe.

Environment Agency (EA): A UK government agency.

Environmental assessment level (EAL): EA-derived provisional benchmarks for substances released to each environmental medium, taken from a variety of published UK and international sources.

European Food Safety Authority (EFSA): EU risk assessment body for food and feed safety.

EUROPOEM: Expansion of POEM by European group to provide a greater range of exposures to plant protection products.

EUSES: European Union System for the Evaluation of New Substances.

Expenditure Food Survey (EFS): A continuous survey of household expenditure, food consumption and income commissioned by the Social Survey Division (SSD) of the Office for National Statistics (ONS) and by the Department for Environment, Food and Rural Affairs (DEFRA).

Exposure scenario: A representation of an activity constructed from pattern of use information, together with assumptions and inferences about how exposure takes place for the defined population. The exposure scenario is used by the exposure assessor to evaluate, estimate or quantify exposures for the defined population. In the context of REACH, exposure scenario is defined as the set of conditions, including operational conditions and risk management measures, that describes how the substance is manufactured or used during its life cycle and how the manufacturer or importer controls, or recommends downstream users to control exposures of humans and the environment.

Food Standards Agency (FSA): A UK government agency.

Foodstuff: Containing one or more commodities in a form ready for consumption.

Geometric standard deviation (GSD): A statistical tool expressing the variability in a set of data.

GExFrame: GlobalExpoFrame, a web-based software system hosted by the European Joint Research Centre to estimate exposure to chemical substances in consumer products.

Good agricultural practice (GAP): A practice that minimises the risk of causing pollution while protecting natural resources and allowing economic agriculture to continue.

Health and Safety Executive (HSE): A UK government agency.

Health criteria value (HCV): Benchmark criteria that represent an assessment of levels of exposure that pose a risk to human health, for example, tolerable daily intake (TDI) and index dose.

Highest residue (HR): The highest residue (in mg of pesticide/kg food) in trials performed according to good agricultural practice.

Index dose: An estimate of the amount of a soil contaminant (expressed as a daily intake) that can be experienced over a lifetime with minimal cancer risk.

Intake 2: Proprietary FSA Tier 3 assessment tool.

Interdepartmental Group on Health Risks from Chemicals (IGHRC): Comprises representatives of UK government departments, research councils and agencies, and aims to stimulate the development of new, improved approaches to the assessment of risks to human health from chemicals.

Ministry of Agriculture Fisheries and Food (MAFF): UK government department responsible for agriculture, fisheries and food; dissolved in 2002.

Maximum residue level (MRL): Derived statistically from the residue trials performed to support authorisation. The MRL is greater than the HR. An MRL is a statutory limit, the maximum concentration of pesticide residue (expressed as milligrams of residue per kilogram of food) likely to occur in or on the food after the use of pesticides according to good agricultural practice (GAP).

Monte Carlo simulation: A problem solving technique used to approximate the probability of certain outcomes by running multiple trial runs, called simulations, using random variables.

National Diet and Nutrition Survey (NDNS): A series of cross-sectional surveys of diet and nutritional status covering the population from age 18 months upwards; data from approximately 2000 individuals in four age groups have been collected.

National estimates of dietary intakes (NEDI): An estimate of intake of pesticide in the diet over the long term to compare to the ADI. The NEDI is based on median or mean residue levels and a high-level consumption (97.5th percentile value) for the daily amounts of the food item consumed over the long term. These are a first estimate of 'long-term' or chronic pesticide intake or as a primary screen of total dietary intake for pesticides.

National estimate of short-term intake (NESTI): An estimate of peak intake of pesticide in the diet to compare to the ARfD. The NESTI is based on the highest residue found multiplied by a variability factor and a high-level consumption (97.5th percentile value) for the amount of the food item consumed over a single day.

No observed adverse effect level (NOAEL): The level of exposure of an organism, found by experiment or observation, at which there is no biologically or statistically significant increase in the frequency or severity of any adverse effects in the exposed population when compared to its appropriate control.

Operator: Person involved in activities relating to the application of a pesticide product; such activities include mixing or loading the product into the application machinery, operation of the application machinery, repair of the application machinery while it contains the pesticide product, and emptying and cleaning of the machinery or containers after use.

Pattern of use: Information on where, when (duration and frequency) and how the product is applied, and on how the defined population could be exposed during and post application.

Personal protective equipment (PPE): Equipment (including clothing affording protection against the weather) which is intended to be worn or held by a person at work and which protects against one or more risks to a person's health or safety, for example, safety helmets, gloves, eye protection, high visibility clothing, safety footwear and safety harnesses.

Predictive Operator Exposure Model (POEM): POEM is based on a Microsoft Excel spreadsheet and contains information on nine types of application technique for pesticides. Default values for work rate and duration of spraying are triggered by particular application techniques (e.g. spraying with a knapsack), but can be altered if appropriate product-specific data are available.

REACH: European regulatory framework for the registration, evaluation, authorisation and restriction of chemicals.

Reasonable worst case (RWC): An exposure scenario covering normal (but not unrealistic) use patterns whereby a defined population could be exposed to the higher end of the potential exposure, dose or risk arising.

Reverse reference scenario: This scenario can be used to determine an estimate of the maximum amount of exposure that might be acceptable and its likelihood of occurrence as a reasonable worst case. Using a relevant no-effect level, it is possible to compute the amount of a product that would lead to that dose by a specific route. The amount of product can then be related to the likelihood of this exposure occurring.

Risk management measure (RMM): A measure that controls the emission of a substance and/or exposure to it, thereby controlling the risks to human health or the environment. Risk management measures include, for example, containment of process, local exhaust ventilation, gloves, waste water treatment, exhaust air filters. More generally, risk management measures include any action, use of tool, change of parameter state that is introduced during manufacture or use of a substance (either in a pure state or in a preparation) in order to prevent, control, or reduce exposure of humans and/or the environment.

RISKOFDERM: A higher-tier modelling tool for estimating potential dermal exposure to chemicals.

Soil guideline value (SGV): Generic assessment criteria to evaluate long-term risks to human health from chemical contamination in soil; intervention values which, if exceeded, may be a cause for concern to human health.

Stoffenmanager Tool: A higher-tier modelling tool for estimating potential worker inhalation exposure to chemicals.

Supervised trial median residue (STMR): The median residue (in mg of pesticide/kg food) in trials performed according to good agricultural practice.

Targeted Risk Assessment (TRA): A Tier 1 screening tool to estimate exposure to chemicals.

Theoretical maximum daily intake (TMDI): Similar to a NEDI, but is a conservative assessment for chronic exposure to pesticides where data may be scarce, which uses a maximum residue level instead of a STMR

Tolerable daily intake (TDI): Regulatory value equivalent to the acceptable daily intake established by the European Commission Scientific Committee on Food. Unlike the ADI, the TDI is expressed in mg/person, assuming a body weight of 60 kg. TDI is normally used for food contaminants.

Total diet study (TDS): The TDS is a continuous market basket-type survey in which foods representing the average UK diet are purchased, prepared and combined into 21 groups of similar foods for analysis.

Time-weighted average (TWA): Term used in the specification of occupational exposure limits to define the average concentration of a chemical to which it is permissible to expose a worker over a period of time, typically eight hours.

World Health Organization (WHO): The directing and coordinating authority for health within the United Nations system.

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The MHRA, NERC and VMD do not have representatives on the Executive Committee.

Publications

Risk Assessment and Toxicology Steering Committee

cr1 Developing New Approaches to Assessing Risk to Human Health from Chemicals

cr2 Risk Assessment Approaches used by UK Government for Evaluating Human Health Effects of Chemicals

cr3 Risk Assessment Strategies in Relation to Population Subgroups

cr4 Physiologically-Based Pharmacokinetic Modelling: A Potential Tool for Use in Risk Assessment

cr5 Exposure Assessment in the Evaluation of Risk to Human Health

cr6 From Risk Assessment to Risk Management: Dealing with Uncertainty

The Interdepartmental Group on Health Risks from Chemicals (IGHRC)

cr7 The Interdepartmental Group on Health Risks from Chemicals: First Report and Forward Plan to 2002

cr7A The Interdepartmental Group on Health Risks from Chemicals: Annexes to First Report and Forward Plan to 2002

cr8 Assessment of Chemical Carcinogens: Background to General Principles of a Weight of Evidence Approach

cr9 Uncertainty Factors: Their use in Human Health Risk Assessment by UK Government

cr10 Guidelines for Good Exposure Assessment Practice for Human Health Effects of Chemicals

cr11 The Interdepartmental Group on Health Risks from Chemicals: Final Report for Phase 1, 1999–2003 and Forward Plan to 2006

cr12 Guidelines on Route-to-Route Extrapolation of Toxicity Data when Assessing Health Risks of Chemicals

cr13 The Interdepartmental Group on Health Risks from Chemicals: Final Report for Phase 2 (2003–2007) and Forward Plan for Phase 3 (2007–2010)

cr14 Chemical Mixtures: A Framework for Assessing Risks to Human Health

cr15 Current Approaches to Exposure Modelling in UK Government Departments and Agencies

All reports are available for download from the IGHRC website, http://ieh.cranfield.ac.uk/ighrc/ighrc.html, or by post from the IGHRC Secretariat, Institute of Environment and Health, Vincent Building, Cranfield University, Cranfield, Bedfordshire MK43 0AL, Tel: +44 (0)1234 758281, Email: e.jones@cranfield.ac.uk