REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains
Part IV: Supplement Exposure Estimation

June 2010

Important note to the reader

This document has been prepared by a VCI working group as part of the joint Cefic/VCI project to develop tools and guidances for industry – in respect of Chemical Safety Assessments, Chemical Safety Reports and Exposure Scenarios.

It is Part IV of the REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains. It describes the status of development as per Q1 2010. Many activities, both in industry working groups as within ECHA are still ongoing. The guide is therefore not to be regarded as complete, but as a status overview.

The Practical Guide comprises several parts. An overview is given in the preface of Part I.

The structure and the contents of the REACH Practical Guide are described on the following web sites:

VCI: http://www.vci.de/default~cmd~shd~docnr~125022~lastDokNr~102474.htm

All related documents can be downloaded from this site. In addition you find here information on related issues and actual developments.

CEFIC: http://cefic.org/templates/shwPublications.asp?HID=750

REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains

Part IV: Supplement Exposure Estimation

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1   Occupational exposure estimation

1.1   Aim, basic concepts and main determinants of occupational exposure assessment and risk characterisation

This general introduction describes some of the basic ideas behind occupational exposure estimation and risk characterisation (e.g. routes and determinants of exposure), while the more detailed issues (e.g. application and evaluation of commonly used exposure assessment tools) will be dealt with in subsequent sections.

1.1.1   Routes of exposure

Occupational exposure occurs mainly by inhalation and dermal contact (i.e. uptake through the skin). Inhalation exposure may take different forms. For example, solids may become airborne in the form of dust, while a volatile liquid may evaporate and thus generate vapours. The properties of the substance (e.g. dustiness in the case of solids and vapour pressure in the case of liquids) are therefore crucial determinants for the exposure estimation and are generally required by exposure estimation tools (see below).

Although often neglected, dermal exposure may in some cases even be more important than inhalation exposure. In practise, <u>potential dermal exposure</u> (i.e. the amount of substance on the surface of (protective) clothing and the exposed skin surface) and <u>actual dermal exposure</u> (i.e. the amount of substance on the skin available for uptake into the body) are two ways of measuring dermal exposure.

For substances, which predominantly exert local effects such as skin or eye irritation and corrosion and skin sensitisation, it may be difficult to quantify these effects and to derive DNELs for these endpoints. In this case, quantitative dermal exposure estimation may not be meaningful and a qualitative risk characterisation should be carried out to identify suitable risk management measures. For example, protective gloves will certainly be worn when handling a corrosive substance so that exposure will be minimised. A quantitative assessment of the exposure will then not be needed.

In other circumstances dermal contact can be excluded due to the operational conditions of use. If, for example, the operating temperature of an installation would immediately lead to burns upon skin contact, it can reasonably be assumed that no dermal contact to substances processed in this installation may occur.

In contrast to the impact area of consumers, oral exposure (swallowing of the substance) is less relevant at almost all workplaces and is not further discussed below. Although oral exposure may occur, e.g. by mouth contact with contaminated work wear, it is generally controlled by simple good hygiene practices (such as separate eating and drinking facilities, washing facilities etc., e.g. as laid down in the German "Technical Rule for Hazardous

Substances 500: Protective measures: Minimum standards" (TRGS 500)). Such practices are considered to be usually in place on the basis of national occupational safety and health legislation.

The exposure estimation usually results in an <u>external</u> exposure value:

- Inhalation exposure: concentration of the substance in the air (in mg/m^3 or ppm, usually full shift (8 h) averages)

- Dermal exposure: amount of substance on clothing and exposed skin surfaces (i.e. potential dermal exposure; measured actual dermal exposure data may be available in a few cases). The unit of exposure may vary, e.g. $\mu g/cm^2$ x h or mg/d.

It is evident that the result of the exposure estimation will not only depend on the properties of the substance but also on the operational conditions of use and risk management measures (RMM) in place. These issues will be dealt with below in the context of a discussion of the tools for exposure estimation.

1.1.2   Approaches to exposure estimation

Generally, relevant information on the exposure situation and on suitable risk management measures should be available (and should be used for registration purposes) for hazardous substances from assessments of risks made within the framework of the Council Directive 98/24/EC ("Chemicals Agents Directive", CAD). In many cases, measured exposure data (e.g. the concentration of a chemical in the workplace air) may be available. These can be used provided that they adequately represent the exposure scenario (ES) considered and meet some quality criteria (see Chapter 1.2.1).

For substances without an occupational exposure limit, however, workplace measurements are often not available or only exist for a specific application. When workplace measurements are missing, exposure has to be estimated. Tools available for this purpose generally follow a step-wise (tiered) approach. The level of differentiation, and thus the input requirements, increases from lower tier (level 1) to higher tier estimation tools. This step-wise approach ensures that a more detailed, labour-intensive assessment is not carried out for situations, in which negligible exposure is expected.

When estimating exposure, it is important to adequately document all entered values and to provide references for the input data. Some of the tools discussed below allow the generation of reports, which include all input parameters, while other tools only have limited options of documentation and print screens may be the only option available.

Note that some of the tools for exposure estimation, such as the ECETOC TRA model, already include a risk-based approach in that exposure estimates are compared with hazard data.

REACH requires assessing exposure resulting from all conditions of use within an exposure scenario, including risk management measures. The exposure estimation models described

in subsequent sections allow to various degrees to consider the reduction of exposure due to risk management measures. This will be discussed below in the context of each model.

1.1.3   Determinants of exposure

Certain core information, the so-called determinants of release and exposure, has already been discussed in relation to ES development (Chapters 6, Part I, and 9.3 of Part II of the practical guide; see also ECHA CSA 2008, Part D, Chapter 2.2). These determinants, such as substance specific properties, conditions of use and risk management measures, are very important in the exposure estimation. For example, the vapour pressure of a liquid substance has a decisive impact on the concentration of that substance in air and thus on inhalation exposure. In relation to conditions of use, a higher process temperature can increase inhalation exposure, which however can be controlled by risk management measures, such as local exhaust ventilation.

Specific information may be available for most of these determinants. However, Tier 1 estimations usually only require very basic information and if a Tier 1 estimate does not identify a risk (i.e. a higher tier estimate is not required), the specific information will not be needed.

The parameters required for Tier 1 and higher tier estimations are listed in Appendix 4.1.3 and 4.1-4. These appendices also give hints on where to get the relevant data from.

1.2   How to assess occupational exposure

In principle, an exposure can be assessed on the basis of measured data or on data generated with one of the tools described below (modelled estimates). ECHA CSA 2008 (Chapter R.14.4.1) proposes the following <u>hierarchy</u>:

1.   Measured data for the actual substance

2.   Measured data for analogous/surrogate substances/activities

3.   Modelled estimates.

While it is clear from this hierarchy that modelled data are only the last option (no completely validated exposure model currently exists), measured data are not preferable *per se* but have to meet certain criteria. For example, measured data for the actual substance should be representative of the ES, robust in terms of the sample size and reliable. Having this in mind, many measured data will not meet one or more of these criteria and analogous/surrogate data may also fail to qualify. If lesser quality measured data are available, these will be used together with results from the application of the tools, i.e. modelled data, being generated in parallel. The plausibility of the values resulting from measurements and model estimates needs to be discussed to arrive at a final estimate.

Besides, several general principles have to be borne in mind:

- The assessment should be transparent and clear.

- The assessment should be of a conservative nature, i.e. be on the safe side, and should be conducted for all activities and routes within the ES presenting the potential for exposure. However, exposure resulting from accidents, deliberate misuse or malfunction should not be covered.[1] Also, extreme estimates resulting from the combination of several maximum assumptions should be avoided.

- Attention should be paid to subsets or subpopulations differing in exposure intensity or vulnerability (such as women of conceptive age and pregnant women).

These and many other general principles, such as the consideration of RMMs, mentioned in ECHA CSA 2008 (Chapter R.14) are not necessarily applicable to all assessments. For example, Tier 1 models are already conservative and no special attention has to be paid to this principle.

1.2.1   Use of measured data

Basically, there are two kinds of measurement data:

- Actual measurement data for the substance;

- Analogous/surrogate measurement data.

These different kinds of data are described in the following matrix. Note that the use of data for similar substances used in similar exposure scenarios involves two extrapolation steps and therefore requires reasonable care. The rationale for using these data must be well explained and documented.

	Actual substance	**Similar substance**
Actual exposure scenario	Actual measurement data	Analogous/surrogate data
Similar exposure scenario	Analogous/surrogate data	Analogous/surrogate data

A similar substance is defined as possessing similar physico-chemical properties relevant for exposure (e.g. vapour pressure, dustiness). To be on the safe side, a more "critical" similar substance has to be used for analogous/surrogate data. As an example, the use of toluene data for a xylene exposure assessment could be appropriate, since toluene is more volatile than xylene and thus results in a conservative exposure estimate.

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[1]   Council Directive 98/24/EC "on the protection of the health and safety of workers from the risks related to chemical agents at work" is (partly) dealing with these situations.

A similar exposure scenario is characterised by activities with similar operational conditions of use and risk management measures, which is likely to give a reliable estimate of the exposure in the scenario under assessment.

Generally, measurement data for the actual substance are preferred. However, high quality analogous/surrogate data are often better than poor quality data for the substance itself.

1.2.2   Sources of measured data

Measurement data may be available from a variety of different sources, such as:

- In-house data
- Databases (as far as publicly available)
- Surveys, e.g. by trade or similar organisations
- Publicly available data (e.g. reviews, literature data)

Appendix 4.1-1 provides examples of publicly available sources for measurement data. Chapter 8.3 (Part I of the practical guide) describes the use of existing data (e.g. the MEGA database) in more detail.

1.2.3   Criteria and selection of appropriate measurement data

Inhalation exposure

As already mentioned above, measurement data must meet some quality criteria in order to be representative, robust and reliable. ECHA CSA 2008 (Chapter R.14.4.5) lists several criteria, of which the most important ones to ensure a sufficient quality of measurement data are:

- Concentration and unit of measured values given
- Large sample size
- Representativeness of the data for the ES under assessment (in particular, operational conditions of use and risk and management measures)
- Personal (breathing zone) sampling is preferred over static sampling.

Measurements obtained using recognised and standardised protocols for sampling and analysis are generally preferred. If the concept of homogenous exposure groups (HEGs) according to European standard EN 689 has been followed in the planning of the workplace measurements this may be especially helpful to understand the representativeness of the data (HEGs are groups of workers who experience similar exposures).

Dermal exposure

In general, there are considerably less data available for dermal exposure than for inhalation exposure. ECHA CSA 2008 (Chapter R.14.4.5) therefore tends to use dermal data without

applying the same strict quality criteria used for inhalation data. Again, the following list gives some criteria necessary to ensure sufficient quality.

- Concentration and unit of measured values (e.g. mass per unit area, including conditions of the measurement such as data on surface size sampled, mass of contaminant and duration of sampling)
- Large sample size
- Representativeness of the data for the ES under assessment (in particular, operational conditions of use and risk and management measures)
- It has to be clearly indicated whether data stand for exposure to a substance or exposure to the mixture used

There are many different units of expressing dermal exposure (e.g. in mg/person, mg/cm^2 of skin or mg/cm^2 x h). If the DNEL has a different unit than the exposure value, the latter may have to be converted to the unit of the DNEL.

In addition to ECHA CSA 2008, several other documents, such as the German TRGS 401 (skin contact) and 402 (inhalation),[2] provide important information to ensure a good quality of measurement data.

Discussion of adequacy/applicability

In order to differentiate between differences in quality of measurement data, the following three levels are introduced:

- High quality,
- Intermediate quality and
- Lower quality.

The types of data representing the three different levels are illustrated in the following examples:

- A measurement value (e.g. expressed as a median or 90th percentile) obtained from 26 personal sampling measurements under conditions representative of the ES under assessment, will most probably enter the exposure estimation as a value of high quality. Such a value might be given in branch-specific measurement reports or in an EU Risk Assessment Report.
- A mean from 3 measurements with personal sampling for the ES under assessment (e.g. from an original literature study) is likely to be an intermediate quality value for the exposure assessment.

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[2] Bundesanstalt für Arbeitsschutz und Arbeitsmedizin: Technical Rules for Hazardous Substances (TRGS): Risks resulting from skin contact – determination, evaluation, measures (TRGS 401) Ermitteln und Beurteilen der Gefährdungen bei Tätigkeiten mit Gefahrstoffen: Inhalative Exposition (TRGS 402) (available only in German). http://www.baua.de

- A value given only as a mean without the number of measurements and details on sampling is most probably a lower quality value, especially if it is not fully representative of the activity described in the ES in question. This type of data presentation is common in reviews (e.g. the Environmental Health Criteria series published by the World Health Organization).

These criteria can be applied both to measurement data for the actual substance in the ES under assessment and for analogous/surrogate data. In principle, a high quality value for the actual substance in the ES under assessment may be used alone. An intermediate quality value will most likely require additional analogous/surrogate measurement data or modelling (i.e. application of estimation tools). As a general rule, it can be suggested that the lower the quality gets, the more approaches should be taken in parallel. It may well be the case that three approaches (e.g. lower quality measurement data for the actual substance in the ES, intermediate quality analogous/surrogate measurement data and modelled estimates) have to be followed and the various estimates integrated.

1.2.4   Use of exposure estimation tools – Tier 1

In the following sections, Tier 1 tools as proposed in ECHA CSA 2008 (Chapter R.14.4.6-R.14.4.8) are explained. A brief overview and sources of Tier 1 tools are given in Appendix 4.1-2.

Users of exposure estimation tools should keep in mind that most tools are of a very conservative nature (i.e. in most cases they tend to the cautious, higher side of exposure estimates) and that they are only validated to a limited extend and/or for some uses. Application of higher tier models in particular will in many situations require in depth understanding of exposure estimation and expertise in handling the tools to avoid highly inaccurate estimates.

ECETOC Targeted Risk Assessment (TRA)

The completely revised version of ECETOC TRA (see Appendix 4.1-2 for access and documentation) allows the estimation of both inhalation and dermal exposure of workers. Compared to the previous web-based version, ECETOC TRA is now implemented as a Microsoft Excel® tool and includes many changes, which are described in more detail in the accompanying Technical Report (see Appendix 4.1-2).

Many of the revisions implemented in the new version are aimed towards better integration into the exposure assessment process under REACH (e.g. adoption of the PROCs). Consequently, ECETOC TRA is now more an exposure assessment tool than a targeted risk assessment tool (as was the previous version). However, it is still possible to calculate risk values after entering DNELs or analogous values. Again, more details on the background of the changes and the scope of the new version can be found in the Technical Report.

The tool is considered to be the preferred Tier 1 model for occupational exposure estimation (ECHA CSA 2008, Part D, Chapter 5.3).

ECETOC TRA consists of individual MS Excel® spreadsheets for the impact areas workers and consumers. In addition, an integrated tool has been developed which covers also environmental assessments (beside assessments of workers and consumers) (Info-Box 1)

User guides are available for all these components. The following description is based on the stand-alone ECE-TOC TRA Worker tool.

The stand-alone ECE-TOC TRA Worker tool consists of a single MS Excel® file and an accompanying user guide. Before starting the tool, it is wise to keep a copy of the original MS Excel® file. Depending on the security settings in MS Excel®, the user may have to enable macros upon opening the tool.

Info-Box 1

The integrated tool is much more complex than the individual tools (using 9 different files) and follows the principles of the previous version by:

- providing a common user interface for data input and output for all three impact areas

- building on a database to store data for numerous substances with multiple use scenarios

- the possibility to alter entry data stored in the database

In addition, the integrated tool of the new ECETOC TRA version now incorporates the possibility to run a batch mode for multiple substances / scenarios. This may especially be helpful as a first screening step to gain a complete overview.

For more information on the integrated tool, users may consult the Technical Report and the respective user guide.

The tool starts with an example (substance "demosub1" with artificial CAS number 01-02-03) already filled in. This may be helpful in gaining a first overview of the tool. However, before using the tool for exposure estimation, it is useful to first select the "Clear all" button at the end of the "InputModule" (rather than trying to overwrite the example).

There are nine tabs visible in the bottom tab bar, representing the following worksheets:

- "InputModule": this is the central data entry screen

- "Fugacity", "Value look up", "PROC", "Duration of Activity", "RPE", "Mixtures" and "Dermal": these worksheets contain all the values used in the calculation, e.g. exposure reduction factors for respiratory protection, and provides a rationale for their selection (e.g. when the new TRA exposure predictions deviate from the underlying EASE model or from the previous TRA version); they are helpful to better understand the calculation and also to get an idea of the influence of individual exposure determinants.

- Demosub1 (01-02-03): contains the results of the exposure estimation (called "linear report" in the tool) for the example.

The tool provides notes on use in the "InputModule", which basically describe the step-by-step approach (comments on each parameter are available in the fields with question marks):

▪ START: First enter the substance-specific data (name, CAS number, molecular weight and data on the likelihood to become airborne). Indicative reference values (e.g. a DNEL or some other value such as an OEL) can be entered and the tool then calculates whether predicted exposures are higher than the reference value. However, the user may leave these fields empty and estimate exposure only (but see limitations below).

The "likelihood to become airborne" (fugacity) section represents a combination of determinants, which are summarised in the following figure.
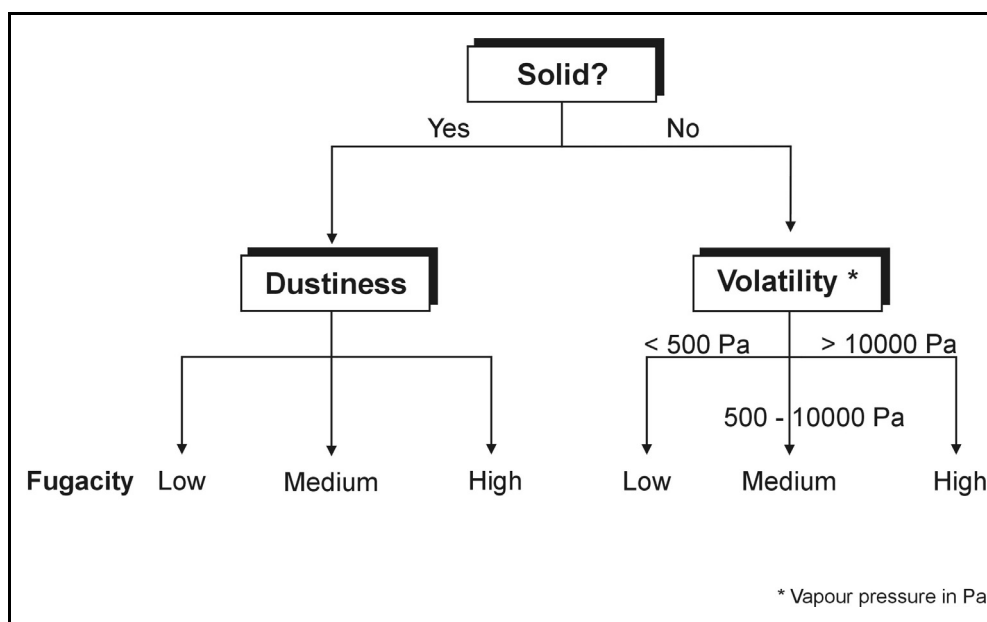
Figure 1-1:   Schematic representation of the fugacity decision tree

The decision on the dustiness of the substance involves a subjective element (see also discussion of the EMKG-EXPO-TOOL below). The ECETOC TRA Worker tool provides some guidance on the dustiness in the "Fugacity" worksheet (for more detailed information, see the Technical Report (ECETOC 2004, section 2.1.1 and Appendix C as well as the addendum to it (ECETOC 2009)) as well as Chapter R.14 of ECHA CSA (2008, draft version 2010). It must also be stressed that for volatiles, the vapour pressure at the process temperature has to be chosen as the basis. Therefore, ECETOC TRA may have to be run several times, if a substance is handled under similar conditions but at different temperatures.

After completion of the "input parameters" mentioned above (substance-specific data and likelihood to become airborne) users are required to specify the conditions of use in the

"exposure scenario builder" section of the "InputModule". The difference between the two sections "input parameters" and "exposure scenario builder" is important since it is possible to retain the "input parameters" and run exposure estimations for different scenarios (see below).

In the "exposure scenario builder", a name should be given for the scenario, followed by selection of the appropriate PROC and choosing either "industrial activity" or "public domain (professional) activity" (STEP 1 in the tool). Selection of the correct PROC is not dealt with here in detail, because this is already described in the context of ES development (Part II of the practical guide, chapter 9.3.1). The tool automatically assigns industrial or professional activity to some of the PROCs by disabling the alternative choice. For example, if industrial spraying (PROC 7) is chosen, the option "public domain (professional) activity" is automatically disabled.

STEP 2 in the "exposure scenario builder" involves application of "exposure modifiers" (operational conditions). It is at this stage that ECETOC TRA allows user to "play around" with the parameters and to examine the impact of these parameters on the exposure estimation ("iteration"). For example, a liquid substance with a vapour pressure of 1000 Pa (medium fugacity) may give the following estimates for PROC 7 (industrial spaying) at extreme ends.

Table 1-1   Extreme estimates for a substance with medium fugacity in PROC 7

Parameter	Exposure estimate	
	Lowest	**Highest**
Does this activity take place <u>indoors</u> or <u>outdoors</u>?	Outdoors	Indoors
Is <u>Local Exhaust Ventilation</u> present?	N/A	No
What is the <u>Duration</u> of the Activity?	15 minutes	>4 hours
What type of <u>respiratory protection</u> is used?	95% reduction*	No protection
Is the substance used in a <u>Mixture</u>?	Yes	No
Select the <u>concentration range</u> (w/w)	<1%	N/A
Result	0.0875 ppm	250 ppm

Respiratory protection capable offering a 95% reduction in inhaled concentrations of the substance

This example shows that exposure estimates can vary over a wide range depending on the parameters selected. ECETOC TRA only states a default for the duration (>4 hours). For Tier 1 screening purposes, it might be a good idea to start with the most conservative parameters (see last column in the table above). If safe use can be shown with this screening procedure,

no further refinement is necessary. If safe use can not be demonstrated with the most conservative parameters, users can subsequently choose less conservative parameters in a step-by-step approach. The effect of selecting different values is detailed in the tabs for the individual parameters. For example, changing the duration of the activity from >4 hours to 1-4 hours will reduce the estimated exposure by 40%.

When all parameters have been selected, there are two ways of presenting results:

▪ "Generate report" will display a report on the exposure estimation in the same work-sheet ("InputModule", green box to the right of the input section). This is somewhat confusing since this is actually the result and not an input. This report will be displayed no matter if indicative reference values were entered or not. The result can be used in the risk characterisation performed in a different IT environment. The "generate report" option is particularly helpful for the iteration described above since the report is automatically updated once parameters are altered and the button is clicked again. Note that this report is overwritten every time the user clicks the "Generate report" button.

▪ "Copy scenario results to the linear report" will create a new tab (substance name and CAS number constitute the name of this new tab), which includes the results including a basic risk characterisation when all reference values have been entered in the "InputModule" (but see Info-Box 2 for limitations). This functionality is especially helpful for running different scenarios for the same substance. Each scenario is stored in the worksheet for the substance in a new row. Use the "clear scenario" button to run an assessment of a different scenario for the same substance. Note that this is the report actually stored for future reference (but see discussion below).

Info-Box 2

Note that a linear report will only be properly created when reference values for both inhalation and dermal exposure have been entered. If not, an error message will appear but the user can nonetheless move to the linear report. This is somewhat disturbing and the user may be uncertain whether calculations have been carried out correctly. According to the User Guide, this issue will be solved in the next revision of the tool.

Also, remember that the automatically generated tab name for the result worksheet is limited to 31 characters (28 characters for name and CAS number + 3 for a blank and two brackets). Therefore, use short abbreviations or acronyms for the substance name when starting the estimation.

In summary, the most helpful approach seems to be the iteration mentioned above, followed by copying the results of the final iteration to the linear report and repeating the procedure for all scenarios to be evaluated.

As an example, exposure was estimated for a liquid with a vapour pressure of 30.000 Pa (high fugacity). All other input parameters are included in the report produced with the "generate report" function (Figure 1-2).

Worker Exposure report for Substance test 3 (CAS NO. 456-78-9)	
High fugacity	**Exposure Estimate (Units ppm)**
Exposure scenario (Test scenario 3)	
Process Category 7 -Industrial spraying.	
Industrial activity	
Initial Exposure Estimate	500
Exposure modifiers	
The activity takes place **Indoors**	
Ventilation is present with an assumed **efficiency of 95%**	25
The maximum duration of the activity is **>4 hours (default)**	25
Respiratory protection is not used	25
Is this substance part of a preparation? No	
Assessment factor applied is 1	25
The Inhalative Exposure Estimate for this Exposure Scenario is	**25 ppm**
Dermal exposures may arise from this Exposure Scenario and assuming a maximal exposed skin area	1500 (sq cm)
are estimated at	**2.1429 mg/kg/day**

Figure 1-2   Printscreen of the result report for a liquid used in industrial spraying

This example (highly volatile liquid) has also been assessed using the EMKG-EXPO-TOOL (chapter 1.2.4.2).

Discussion of adequacy/applicability

It is not always clear in the tool if a field has been disabled. For example, for a solid, the field volatility (vapour pressure) is disabled. However, it is still possible to enter a value in the larger cell (of which the field volatility forms part; see Figure 1-3). This does not appear to result in erroneous calculations but may in cases be misleading for the user.

Figure 1-3   Printscreen of fields in worksheet "InputModule"

Also, once a report has been generated, the input parameters (substance-specific) cannot be altered. The "clear all" button" has to be clicked in order to enter data for a new substance. This is somewhat unusual but users will get used to it after a couple of data entries.

More problematic in terms of content is the question of solids being used in liquid mixtures. For example, if a solid substance is evaluated and PROC 7 ("Industrial spraying") or PROC 10 ("Roller application or brushing") is chosen, it is impossible to select "Yes" for the question "Is the substance used in a Mixture?" This is not immediately plausible since some solids will be used in liquid mixtures in these processes. In addition, ECETOC (2009) defines PROC 7 as "Spraying of the substance or <u>mixtures containing the substance</u> in industrial applications e.g. coatings" (our emphasis). Users are left alone and this issue is not dealt with in the Technical Report or the brief User Guide.

Another issue is related to local effects (e.g. skin irritation and sensitisation) following dermal exposure. The tool has a focus on calculating a body dose (in mg/kg x d) for dermal exposure. Within the approach of the tool this makes sense, since for the calculation of total exposure both inhalation and dermal exposure have to be given in an identical unit. However, a dose given in $\mu g/cm^2$ skin may be more relevant for dermal risk characterisation in some cases. A dose related to skin area is not automatically calculated in the tool, but may be looked up in the "Dermal" worksheet. In addition, the tool does not offer the possibility to enter a reference value in $\mu g/cm^2$. Therefore, a risk characterisation on the basis of skin area (e.g. for skin sensitisation) has to be conducted manually. The same problem does not exist for inhalation, since concentrations are calculated in the report generated in the "InputModule" worksheet and in the linear report.

It has to be noted that, according to ECHA CSA (2008, Chapter R.14), ECETOC TRA in some cases substantially underestimates dermal exposure in the presence of LEV (local exhaust ventilation) by assigning a very high efficiency to LEV for dermal exposure. ECHA CSA (2008, Chapter R.14, draft version 2010) therefore recommends to reduce LEV efficiency outside the tool to zero or at least a factor clearly below 90% in order to obtain a conservative estimate.

More generally, the ECETOC TRA Worker tool is based on the EASE model and thus the limitations of the latter apply. Basically, exposure to mists and process fumes cannot adequately be estimated.

It is one of the very helpful features that the ECETOC TRA Worker tool allows to run several scenarios for the same substance. These are stored as separate rows in the same worksheet. The respective tabs are named according to substance name and CAS number (Info-Box 2). This is very useful, if several substances are assessed within a single file, since the resulting tabs (one for each substance) allow easy navigation between the results of the different substances. Running more and more substances/scenarios within a single MS Excel® file may, at a certain point, become confusing. It may thus be helpful to get an idea about the number of substances and scenarios that require exposure estimation before starting to work with the tool. Depending on number/scale of estimations, the user may then decide, for example:

- to work with one file only (few substances with few scenarios),

- to work with three files (three groups of substances with few scenarios each),

- to have a separate file for each substance because many scenarios have to be evaluated per substance or

- to use the integrated version (Info-Box 1) since many substances and scenarios have to be evaluated and the batch mode is considered helpful.

Note that the linear report (i.e. the result section actually stored and accessible after a series of evaluations) does not contain the vapour pressure actually entered but only the fugacity assigned to this vapour pressure. It may be helpful to manually enter the vapour pressure in the linear report for future reference and documentation purposes.

The limitations mentioned notwithstanding, the ECETOC TRA Worker tool is very transparent in its assumptions. It is also user-friendly due to its implementation in MS Excel®, the possibilities of calculating different scenarios in a single file and the brief User Guide detailing the key features.

The following example shows how ECETOC TRA may be used in the "Iterative 3-step approach for exposure assessment" (Part II of the Practical Guide, chapter 9.8). This approach is part of CEFICs "Guidance on Use and ES development and Supply Chain Communication", which is discussed in more detail in Part II of the Practical Guide, chapter 10.3).

Example:

"*Iterative 3-Step approach to exposure assessment*"

For substances with many uses and complicated supply chains it is laborious and sometimes impossible for the substance manufacturer to get to know all uses. The following iterative 3-step approach to exposure assessment was developed especially for companies dealing with a large amount of substances. It offers a way to use the wide range of existing activities in the development and shaping of exposure scenarios, integrating them in a clear-cut overall structure and intends to make downstream communication more efficient.

Step 1: Basic exposure assessment using ECETOC TRA

In the first step, ECETOC TRA, which is considered as a conservative IT tool, is used to make a Tier 1 exposure assessment using **all** process categories (PROCs) as listed in the Guidance (ECHA CSA 2008, R.12). It is assumed that the complete list of PROCs comprises all possible uses of the substance in question. This can be done with a minimum of substance- and use-specific information. The following table shows the output of ECETOC TRA for a test substance. It indicates for which of the PROCs a further assessment is warranted to assure safe use (answer "Yes" in right column). PROCs for which this Tier 1 assessment already signals safe use receive the answer "No".

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process cate-gories [PROC]	Use Scenarios	Duration of activity [hours]	LEV (Y/N)	Estimated Exposition [ppm]	MoE [DNEL/ est expo]	Further assessment required
PROC 1	Use in a closed process with no likelihood of exposure	> 4 hours	Yes	0,01	31,8	No
PROC 2	Use in closed process with occasional controlled exposures e.g. during sampling	> 4 hours	Yes	0,5	0,636	Yes **no refinement done – if needed, please contact manufacturer**
PROC 3	Use in a closed batch process i.e. where only limited opportunity for breaching arises e.g. sampling	> 4 hours	Yes	0,1	3,18	No
PROC 4	Use in a batch or other process (including related process stages e.g. filtration, drying) where opportunities for exposure arise e.g. sampling, dis-/charging of materials	> 4 hours	Yes	1	0,318	Yes **no refinement done – if needed, please contact manufacturer**
PROC 5	Use in a batch process including chemical reactions and/or the formulation by mixing, blending or calen-daring of liquid and solid-based products	> 4 hours	Yes	1	0,318	Yes **for refinement see Chapter 9.2**
PROC 6	Spraying of the substance or mixtures containing the substance in industrial applications e.g. coatings	1–4 hours	Yes	12	0,026	Yes **for refinement see Chapter 9.2**
PROC 7	Dis-/charging the substance (or mixtures containing the substance) to/from vessels	1–4 hours	No	6	0,053	Yes **for refinement see Chapter 9.2**
PROC 8	Filling containers with the substance or its mixtures (including weighing)	1–4 hours	No	6	0,053	Yes **for refinement see Chapter 9.2**
PROC 9	Roller application or brushing of adhesives and other surface coatings	1–4 hours	No	300	0,001	Yes **for refinement see Chapter 9.2**
PROC 10	Use as a blowing agent in the manufacture of foams, etc.	> 4 hours	Yes	0,5	0,636	Yes **no relevant PROC**
PROC 11	Use for coating/treatment of articles, etc. (including	> 4 hours	Yes	3	0,106	Yes **for refinement**

	cleaning) by dipping or pouring					**see Chapter 9.2**
PROC 12	Production of products or articles from substance by compression, tabletting, extrusion or pelletisation	> 4 hours	Yes	3	0,106	Yes **no refinement done – if needed, please contact manufacturer**
PROC 13	Use as a laboratory reagent	1–4 hours	Yes	0,06	5,3	No
PROC 14	Use as a fuel	< 15 min	No	0,1	3,18	No
PROC 15	Use as a lubricant (including metal working fluids)	> 4 hours	Yes	50	0,006	Yes **no refinement done – if needed, please contact manufacturer**

LEV: local exhaust ventilation; MoE: margin of exposure; DNEL: derived no effect level

Only those uses with answers "Yes" are further considered in step 2.

Step 2: Generic exposure assessment

Refinement of exposure assessment for selected uses is carried out by use of generic exposure scenarios (GES). GES are under development in various industry sectors and branches and it is expected that a broad range of GES will be publicly available in the future. Only at this stage more detailed RMMs are introduced into the exposure assessment and will lead to assurance of safe use conditions. In Step 2, various exposure estimation tools may be used, depending on the scenario and substance properties. If available, higher tier models can be used for consideration of exposure reduction by RMMs.

Step 3: Specific exposure assessment

If step 2 does not lead to a description of conditions and RMMs for safe use, a specific assessment, including information from individual downstream users and refinement of RMMs, is carried out. The exposure scenario is further developed and RMMs are proposed for implementation, which ensure safe use of the substance for this specific use.

EMKG Exposure assessment tool

The EMKG exposure assessment tool (EMKG-EXPO-TOOL, MS Excel®) is part of the "Easy-to-use workplace control scheme for hazardous substances" (EMKG: "Einfaches Maß-nahmenkonzept für Gefahrstoffe") of the German Federal Institute for Occupational Safety and Health (BAuA). The tool uses a "banding approach" for the exposure assessment, which is largely based on COSHH Essentials (Control of Substances Hazardous to Health

Regulations), developed by the UK Health and Safety Executive (HSE). The concept of banding means here that both input data and the result are expressed in categories (bands), which often differ by at least one order of magnitude (see different bands in Figure 1-).

Important issues in relation to the EMKG-EXPO-TOOL are:

- Requires MS Excel® 97 or later (MS Excel® 2002 not yet tested)

- Estimates inhalation exposure only

- Some applications and substances should not be assessed with the tool (e.g. open spray applications, CMR substances; see worksheet "Limitations" in the tool)

The tool consists of three different worksheets, one detailing the limitations and one each for solids and liquids. The input data required by the tool are rather basic and are listed in. Appendix 4.1-3.

(For the occupational exposure assessment of metals and inorganic substances the MEASE tool was developed (online available at: http://www.ebrc.de/ebrc/ebrc-mease.php), based on the exposure estimation model EASE (see http://www.hse.gov.uk/research/rrhtm/rr136.htm) and some measured data (see also chapter 1.2.5).).

Background information on the input parameters for the EMKG_EXPO-TOOL can be found in ECHA CSA 2008 (Chapter R.14.4.8.1). In addition, some basic help and advice for tool application (e.g. data entry for mixtures) is provided in fields with a question mark.

Fig. 1-4 illustrates the worksheet for liquids.

EMKG - Exposure assessment part for liquids

baua:
Bundesanstalt für Arbeitsschutz und Arbeitsmedizin

Definition of volatility bands ?

Band	At normal temperature (~20°C)	Operating temp. (o.t.)	Vapour pressure (kPa at o.t.)
Low	boiling point above 150°C	b.p. ≥ 5 x o.t. + 50	< 0.5
Medium	boiling point between 50 and 150°C	other cases	0.5 - 25
High	boiling point below 50°C	b.p. ≤ 2 x o.t. + 10	> 25

Alternative input of ?
boiling point [°C] **and** operating temperature [°C]

input b.p.	input o.t.

Scale of use bands ?

Band	Description
Small	millilitres up to 1 litre for liquids
Medium	litres (batch sizes between 1 and 1000 litres for liquids)
Large	cubic metres (batch sizes of greater than 1 m³ for liquids)

Short term exposure ?
Activity < 15 min. during a full 8 h shift?

Yes	No

Applications on surfaces > 1m² ?
e.g. painting, applying adhesives etc. and more than 1 litre product used per shift!

Yes	No

Control strategies ?

Control Approac	Type	Description
1	General ventilation	Good general ventilation and good work practice
2	Engineering control	Local exhaust ventilation (e.g. single point extract, partial enclosure, not complete containment) and good work practice
3	Containment	Enclosed, but small breaches may be acceptable. Good work practice.

Exposure potential bands (EP)

Solids – EP band	Use band	Volatility band	Description
1	Small	Low	Millilitres of low volatility liquid
2	Small	Medium or High	Millilitres of medium / high volatility liquid, litres / cubic metres of low volatility liquid
2	Medium or Large	Low	
3	Large	Medium	Cubic metres of medium volatility liquid, litres of medium / high volatility liquid
3	Medium	Medium or High	
4	Large	High	Cubic metres of high volatility liquid

Predicted exposure ranges: Liquids

Control Approach	Predicted exposure level for vapour, ppm			
	Solids EP Band 1 (mL of low VP liquid)	**Solids EP Band 2** (mL of med. / high VP liquid or L / m³ of low VP liquid)	**Solids EP Band 3** (m³ of med. VP liquid or L of med. / high VP liquid)	**Solids EP Band 4** (m³ of high VP liquid)
1	< 5	5 - 50	50 - 500	> 500
2	< 0.5	0.5 - 5	5 - 50	5 - 500
3	< 0.05	0.05 - 0.5	0.5 - 5	0.5 - 5

Limitations / Solids \ Liquids /

Figure 1-4   Print screen of the worksheet for liquids in the EMKG-EXPO-TOOL

Application of the tool is straightforward and (with the exception of alternative input for boiling point and operating temperature) only requires the user to click the fields highlighted in italics and red (e.g. "Medium" in the volatility band). Tool application includes the following steps:

- Define dustiness (solids) or volatility (liquids), i.e. tendency to become airborne
- Indicate the scale of use band (amount of substance)

These two steps alone define the exposure potential (EP) band, which is then converted into predicted exposure ranges in the lower right table of the worksheet (this table can be considered the result table).

- Select control strategy

This last step modifies the predicted exposure range in the respective EP column.

The output generated by the tool is in the form of ranges for the concentration of the substance in air, given in mg/m³ for solids and in ppm (parts per million, mL/m³) for liquids. For example, the concentration resulting for a liquid in EP 3 with LEV is 5-50 ppm (Figure 1-4). The upper value of the range given, i.e. 50 ppm in this example, will be used for the comparison with the DNEL (ECHA CSA 2008, Chapter R.14.4.8.5).

Discussion of adequacy/applicability

As already mentioned above, the EMKG-EXPO-TOOL cannot be used for some applications/substances and the user should always consult the description provided in the tool.

In addition, the estimates are generic and therefore comprise uncertainty. However, the tool makes several conservative assumptions, such as:

- The concentration of a substance (in a mixture) is assumed to be 100%.
- The exposure duration is assumed to be full shift length (with the only exception of exposures below 15 minutes).

Together with the use of the upper value of the predicted exposure range for comparison with the DNEL, it is therefore assumed that the tool can predict safe use despite its uncertainties.

In addition, the user should select more conservative parameters whenever uncertain about a particular input. This is especially the case for the rating of dustiness, which contains an element of subjectivity.

Both for solids and liquids, the exposure range predicted can become very high and will be given as > 10 mg/m^3 (solids) and > 500 ppm (liquids), respectively (EP 4 in combination with general ventilation only). These values are close to the German OEL for total dust of 10 mg/m^3 and close to the highest German OEL for vapours of 1000 ppm (both according to TRGS 900). According to ECHA CSA 2008 (Chapter R.14.4.8.3), use of these values is not recommended.

In general,

- a higher tier assessment is required if the DNEL is below the upper exposure predicted (e.g. DNEL = 20 ppm versus exposure predicted = 50 ppm in the example above).
- safe use is shown if the DNEL is above the upper exposure predicted (e.g. DNEL = 150 ppm versus exposure predicted = 50 ppm in the example above).

ECHA CSA 2008 (Chapter R.14.4.8.5) states that safe use in the latter case is only evident in combination with the appropriate control guidance sheet (CGS) issued by HSE (http://www.coshh-essentials.org.uk/assets/live/g###.pdf, with ### to be replaced by the appropriate CGS number, which in turn can be found in Appendix R.14-2 of ECHA CSA 2008; German versions with the same numbering system are available from BAuA at http://www.baua.de/de/Themen-von-A-Z/Gefahrstoffe/EMKG/Schutzleitfaeden.html?__ nnn=true&__nnn=true).[3]

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[3]   COSHH Essentials, which is very similar to the EMKG-EXPO-TOOL is available as a web-based application (http://www.coshh-essentials.org.uk/). The output of this tool is not as straightforward in terms of an exposure estimate as the EMKG-EXPO-TOOL and is therefore not considered here further.
Note that there is also an "S" series of the CGS, e.g. S101 for the selection of personal protective equipment (http://www.coshh-essentials.org.uk/assets/live/S101.pdf).

These CGSs contain good practice advice on the use of the respective control measures (e.g. on design and equipment, maintenance and personal protective equipment, if applicable).

1.2.5   Use of exposure estimation tools – higher tier

Several higher tier tools are available that can be used for exposure assessment. One of the main problems is that they are partly still under development and any description may soon be outdated by a new version. A brief overview and sources of higher tier tools are given in Appendix 4.1-2.

In order to account for the specifics of metals and inorganic substances in the occupational exposure assessment, the MEASE tool was developed (online available at:

http://www.ebrc.de/ebrc/ebrc-mease.php). It is based on the exposure estimation model EASE (see http://www.hse.gov.uk/research/rrhtm/rr136.htm) and some measured data. It offers a higher level of differentiation than ECETOC TRA for some parameters. For example, the fugacity of a solid substance may not only be described in terms of low, medium or high dustiness but also by a "massive object" category.

Stoffenmanager

The web-based Stoffenmanager tool (developed in Dutch but also available in a (limited) English version) allows the assessment of inhalation and dermal exposure to solids and liquids after registration on the website. While the inhalation exposure assessment results in a quantitative estimate of the exposure concentration, dermal exposure is only addressed qualitatively with scores ranging from 1 (negligible) to 6 (extreme).

ECHA CSA 2008 (Chapter R.14.5.1) refers to a different (spreadsheet) version, which is not publicly available. The use of different percentiles including the 50th percentile (median), as described in ECHA CSA 2008, however, is not possible with the public, web-based version. Rather, the latter gives a "worst case" estimation defined as the 90th percentile.

As a higher tier tool, Stoffenmanager requires more detailed input information than e.g. the EMKG-EXPO-TOOL discussed above. In particular, it allows to select a variety of control measures, such as containment, different forms of ventilation and PPE (personal protective equipment). Figure 1-5 shows an example of the type of information required by the tool. A more extensive list of input requirements is given in appendix 4.1-4.

Figure 1-5   Print screen of one of several input screens of the Stoffenmanager tool

Stoffenmanager cannot be directly used for some very specific substances/tasks (described in more detail at https://www.stoffenmanager.nl/Public/Applicability.aspx). In addition, the inhalation model assumes a process temperature of 20°C and thus requires expert knowledge to transform input data (vapour pressure) if the process temperature is much higher or lower.

Stoffenmanager requires the user to

- first define some BASIC INFORMATION such as departments within the company and suppliers of the mixtures (called products in the tool) and

Info-Box 3

Stoffenmanager allows importing xml files and examples as well as some support is given on how to use this option. However, managing the data in xml format requires some experience and will probably only be a feasible alternative if many products have to be evaluated with this tool.

- then describe the substances in a product (called components) and the products them-
  selves (also in the basic information tab).
  For only a limited number of components, it is easier to define products and then create
  components with the "Create a new component" function available in the "risk
  assessment" section on the product information page. For many components, it is
  useful to first create all components via the "basic information – components" function.

After this basic information is entered, the RISK ASSESSMENT section serves to actually
carry out the exposure estimate for inhalation and dermal exposure. This is the main section
where detailed information on the operational conditions of use and risk management
measures is required.

The assessment results in (Figure 1-6):

- a hazard class (hc): from A (low) to E (extreme), based on the R phrase assigned in
  the basic information step,

- an exposure class (ec): from 1 (low) to 4 (very high) and

- a risk score (risk): from III (low) to I (high)

These results mirror the banding approach implemented in Stoffenmanager, which is quite
similar to the EMKG-EXPO-TOOL described above. However, Stoffenmanager also allows to
quantitatively estimate the exposure concentration in the workplace air (the "C" in the box on
the right of Figure 1-6). This exposure concentration is calculated for each component of the
product defined in the steps above.

	Name risk assessment	Product	Department	hc	ec	risk	
📝 🗑 💡	Assessment1	TEST1	RA	A	3	III	C
📝 🗑 💡	Paint A-1	Paint A	RA	B	1	III	C
📝 🗑 💡	Paint B-1	Paint B	RA	B	2	III	C

Figure 1-6   Print screen of risk assessment results in the Stoffenmanager tool: inhalation

These exposure concentrations relate to the task selected and its duration. If the duration is less than shift length (8 hrs), a time-weighted average (TWA), which is usually required for a comparison with the DNEL, can be derived (Info-Box 02).

Since Stoffenmanager was originally developed for priority setting and includes hazard information on the product (in the form of risk phrases), exposure estimation is only one of the functions of the tool. For example, selection of control measures enables the user to

> **Info-Box 4**
>
> Stoffenmanager allows calculating the "daily average concentration" (i.e. TWA). It is important to first calculate the exposure for all tasks and to calculate the daily average concentration only after all other steps have been finalised. For liquids, TWA exposure to vapours of each component is calculated, while for solids (powders) TWA exposure to the dust of the product is given. When creating a new daily average concentration calculation, it is important to be clear about what to calculate (inhalable dust or vapour) as these data cannot be altered afterwards.
>
> The calculation of daily average concentrations is located in the RISK ASSESSMENT tab.

identify measures, which can be used to control identified risks. In addition, an action plan can be developed after selection of control measures that implements the actions required in the user's company.

Discussion of adequacy/applicability

The applicability of the tool has already been described above and should always be considered in a first step.

Stoffenmanager in its current version 3.5 only allows quantitative estimation of inhalation exposure, returning what the tool describes as a "worst case" exposure concentration (defined as the 90th percentile). According ECHA CSA 2008 (Chapter R.14.5.1.2), typical input values rather than extreme ones should be used when using this exposure estimate.

It also must be emphasised that the tool represents a rough approach and it is therefore not meaningful to directly use the quantitative results that often imply a false degree of precision (e.g. 28.64 mg/m^3). Rather, it is suggested to round the result to two significant figures (e.g. 29 mg/m^3).

In its current version, some functions of Stoffenmanager (among others, the very useful reporting function and a REACH function) are limited to the Dutch language version. While these functions will be probably available in English in future version, this currently somewhat limits the applicability of the tool.

RISKOFDERM calculator

The RISKOFDERM calculator has been developed in the framework of an EU research project.[4] It evaluates dermal exposure to a mixture with a differentiation of exposure of the hands and exposure of other parts of the body (hands only in DEO unit 1 and body only in DEO unit 6; see Info-Box 5 and Table 1-2). Exposure to the constituents of the mixture has

> **Info-Box 5**
>
> The six processes of the tool are based on the so-called Dermal Exposure Operations (DEO) units, which are described in detail by Warren et al. (2006). Table 1-summarises the DEO units, provides some examples for typical tasks covered by each unit and lists the main forms of dermal exposure. Note that the titles of the processes are slightly different in the "Process" worksheet of the most recent version of the RISKOFDERM calculator (v. 2.1) but the full titles appear in the worksheets for specific processes.

to be calculated by multiplying the exposure to the product with the fraction of the constituent in the product.

Besides the spreadsheet (MS Excel®) version, ECHA CSA 2008 (Chapter R.14.5.2) refers to a web-based version of the RISKOFDERM calculator, which is currently not publicly available, and will not be discussed here.

The spreadsheet version contains separate worksheets with only the active ones appearing in the tab bar:

- The "Start" worksheet shows up when running the tool and allows users to move on to the "Process" worksheet (with the "Start" worksheet disappearing from the tab bar).

- The "Process" worksheet is the general entry screen from which to select the process most adequate for the ES under assessment. Again, this worksheet is no longer visible in the tab bar once a process is selected but can always be loaded by selecting the "Back" button in a specific process worksheet.

- The "Changes and validity" worksheet includes the validity ranges of the model but these are also included in the worksheets for the specific processes (see Figure 1-7 below).

- The brief "Explanation" worksheet is important and should be consulted before using the tool. It is also very useful to consult the RISKOFDERM calculator guidance document (see Appendix 4.1-2) as it provides details and examples on many of the processes (e.g. also activities not covered by a specific DEO unit) and also gives useful background information on all input parameters and output values.

---

[4]   RISKOFDERM: "Risk assessment for occupational dermal exposure to chemicals" (2000-2004, RTD Project: QLK4-CT-1999-01107), funded by the European Community and several national authorities and carried out by 15 partners from 11 different Member States.

Table 1-2   Processes of the RISKOFDERM calculator (from Warren et al. 2006 with adaptations from the spreadsheet version)

DEO unit	Title	Examples	Main forms of dermal exposure
1	Handling of (potentially) contaminated objects	Mixing, filling	Contact with contaminated surfaces; also deposition of aerosols and direct contact or immersion
2	Manual dispersion of products	Wiping, generally: dispersion by a tool without a handle	Immersion and some contact with contaminated surfaces
3	Dispersion of products with a hand-held tool	Brushing, dispersion with a roller or comb	Contact with contaminated surfaces and some direct contact, e.g. splashes, drops
4	Spray dispersion of a product	Spraying with equipment (with or without pressure)	Deposition of aerosols and contact with contaminated surfaces
5	Immersion of objects into a product	Mechanical immersion (using e.g. hoists but also manually)	Immersion and contact with contaminated surfaces
6	Mechanical treatment of solid objects	Grinding, sawing	Deposition of aerosols and contact with contaminated surfaces

The input requirements vary with the process chosen but the data needed are mostly qualitative in nature. Appendix 4.1-4 lists the input requirements for one process as an example.

It is useful to give the assessment a name in the "Process" worksheet to allow differentiation between different assessments. This name is automatically transferred to the worksheet of the process subsequently selected and the output worksheet (see below).

Once in the worksheet of the specific process, application of the tool is straightforward. Examples and some guidance is provided in the form of comments to the individual fields and the "Explanation" worksheet. Users generally select the appropriate answer from drop-down lists and the results are automatically updated. This allows the user to immediately assess the influence of the different parameters and their values.

A calculation (an example for DEO unit 3, this could be "painting a wall with a brush") is presented in Figure 1-7. Values were chosen to demonstrate the warning messages of the tool, so this example is not really typical.

Figure 1-7   Print screen of a DEO unit 3 calculation with the RISKOFDERM calculator (note the warning messages and comments)

As shown in Figure 1-7, the RISKOFDERM calculator first gives the resulting exposure rate (in µL/min) and then calculates the loading per shift (in µL) by multiplication with the cumulative duration during a shift. The tool presents the results as a median (50th percentile) and allows the user to set a percentile (75th percentile in Figure 1-7 but any value can be entered in this field). If the calculation leads to unreasonably high loadings per shift, a warning message in red appears at the bottom of the worksheet (see the various warnings in Figure 1-7). Also, the tool warns the user if a "unrealistic" combination of application rate and duration is used. In the example in Figure 1-7, a high application rate is combined with a long duration, which leads to a warning message in orange. Note that both input values for these parameters are within the validity range of the model (given in blue at the right side of the worksheet), it is only the combination that is not covered by the model.

Clicking on the red "Overview results" button opens a new worksheet with a new name (e.g. "Dispersion results" for a DEO unit 3 calculation), which summarises the input parameters and gives a table with preset percentiles for the results including warning messages for unrealistic estimates where appropriate. The distribution is also graphically presented in a standard diagram. The user may move back to the respective process worksheet still visible in the tab bar. If input parameters are altered, values are automatically recalculated in the "Overview results" worksheet. As a final step, the "Overview results" worksheet can be printed using the "Print" button. However, it is more convenient to use the print function from the file menu and its preview functionality in order to adjust the page layout.

In principle, calculations for other DEO units follow the same pattern and only require different input parameters.

Discussion of adequacy/applicability

It must be emphasised that the tool estimates dermal exposure to a mixture and that exposure to individual substances must be calculated separately. However, this step can be integrated in the MS EXCEL® file by creating a new worksheet in which the respective results are multiplied with the fraction of the compound in the mixture (since all cells are protected in the tool, this requires some experience in MS EXCEL® application).

The protection of the cells also leads to other problems. First, the specific worksheet returns results with 3 significant figures (e.g. 0.363 µL/min for a median and 23400 µL/min for an upper percentile). The corresponding "Overview results" worksheet formats these results as natural numbers (0 and 23374 µL/min in this example), which is not considered meaningful but cannot be altered by the user. Second, worksheets cannot be copied to the clipboard and used in other software such as MS WORD®. Again, there is a workaround by creating a new worksheet and integrating the results but this again requires some knowledge in MS EXCEL® application.

Furthermore, the RISKOFDERM calculator (even though a higher tier tool) does not take account of PPE and only estimates potential dermal exposure (Chapter 1.1.1 above). The effect of PPE in reducing exposure must therefore be evaluated separately. Since exposure both of the hands and the body is calculated in most DEO units, the differential effect of PPE can be assessed. For example, it might be sufficient to envisage protective gloves only if exposure of the hands is much higher than exposure of the body.

The tool does not allow combining estimates for separate tasks (e.g. mixing (DEO unit 1) and brush application (DEO unit 3)) to full shift estimates. Adding up the different exposure estimates would not take account of removal of contamination between tasks (e.g. by washing hands or incidentally) and might also lead to an overestimation when combining 90th percentiles.

Other tools

There are several other tools, which may be used for specific purposes. For example, the software **SprayExpo**, originally developed to assess exposure to biocidal products during spray application, can be a useful tool for these types of applications. The tool can be downloaded (together with a manual and background information) from the website of the German Federal Institute for Occupational Safety and Health[5].

1.2.6   Efficiency of risk management measures (RMMs)

The exposure estimation models discussed above at best only consider some types of risk management measures (RMMs). Therefore, results obtained from exposure estimations may have to be modified to include the efficiency of RMMs described in the exposure scenario. (In practice it is decisive that the measures are implemented with high effectivity!).

Information on efficiency of RMMs are available from various sources, but no comprehensive compilation of information exists yet. The "Library on Risk Management Measures (RMM Library)" as developed in REACH Implementation Project 3.2 (http://www.cefic.be/Templates/shwStory.asp?NID=494&HID=645) contains some information on the efficiency of individual RMMs, but needs further development. In the RMM Library typically two efficiency values are given: a "typical default value" (estimate of the 50th percentile) and a "maximum achievable value" (applying best practice). More information on how to work with the RMM library is given in ECHA CSA 2008 (Part D, Chapter 4.6.2).

Information on efficiency of <u>inhalation</u> protection measures is also available, for example, in

- BGR 190 (BG Regel 190, Rule 190 of the German Berufsgenossenschaften (Employer's Liability Insurance Associations), BGFE 2004); in this document, efficiency of inhalation protection equipment is generally expressed as the factor, by which the exposure concentration is allowed to exceed the occupational concentration limit, when wearing the equipment,

- the new "Technical Notes for Guidance" for "Human Exposure to Biocidal Products" (EC 2008) also contain the factors from BGR 190, together with British and American standards,

- Marquart et al. (2008) listed in their publication the inhalation protection factors used in the tool "Stoffenmanager",

- Fransman et al. (2008) describe systematic efforts of data collection on the efficiency of RMM and of building an „Exposure Control Efficacy Library (ECEL)".

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[5]   http://www.baua.de/nn_7554/en/Publications/Expert-Papers/Gd35.html?__nnn=true

For estimating the reduction of systemic exposure from <u>dermal</u> contact at the workplace by suitable personal protection equipment a default factor of 90% is often used (TNO 2007). Default values for dermal protection measures are also contained in the "Technical Notes for Guidance" for "Human Exposure to Biocidal Products", which provides factors expressing percentage of reduction of exposure (EC 2008). (For toxic endpoints as irritation/corrosion or sensitisation a qualitative risk characterisation has to be carried out, see the following chapter.)

1.3   Risk characterisation

As explained in chapter 3.1, Part I of the practical guide, in the risk characterisation part of the chemical safety assessment information on exposure is compared with the hazard data for a specific substance. In this step, exposure estimates are compared with the dose levels without (or with low) concern (i.e. DNELs, derived no effect levels, or DMELs, derived minimal effect levels, for substances without threshold). This process, relying heavily on expert judgement and experience, is described here only in general terms. For a more detailed description of approaches the reader is referred to ECHA CSA 2008 (Part E).

Risks for humans are considered to be adequately controlled if

the RCR (risk characterisation ratio) = exposure level / DNEL < 1,

i.e. the DNEL exceeds the exposure level.

In the case of substances with non-threshold effects, for which a DMEL has been derived, exposure levels below the DMEL characterise a low, tolerable risk. DNELs/DMELs should be derived for all critical endpoints and pathways.

When exposure to a substance in a specific setting occurs via several exposure routes, these combined exposures should be considered. This can be done either by summing up exposure doses and comparing the total exposure with an adequate DNEL or by adding up RCRs calculated for individual pathways.

In some cases, there may be information on toxic effects for some toxicological endpoints, but no data to allow derivation of a DNEL or DMEL. ECHA CSA 2008 (Part E, Chapter 3.4.1) in this regard mentions acute toxicity, irritation/corrosion (skin and eyes), sensitisation, mutagenicity and carcinogenicity. In this case, a qualitative risk characterisation has to be carried out with the aim of showing adequate control of risks. Guidance on how to carry out such an assessment can be found in ECHA CSA 2008 (Part E).

1.4   Communication of the results in exposure scenarios

The risk characterisation leads to a description of the use conditions (operational conditions of use and risk management measures), under which safe use of the substance can be shown. These use conditions form the essential part of the exposure scenario, which has to be communicated down the supply chain.

The information of the ES has to be used by the downstream user (DU) to check whether his substance use is within the conditions of use considered by the registrant ("compliance check"). The registrant can provide the DU with scaling methods as a part of the ES. Scaling methods are simple equations by which the DU can demonstrate that he operates within the conditions of the ES even if (some of) his conditions of use differ from those described by the registrant. Scaling and related tools are described in Part I of the practical guide, chapter 7.7.

Please note: application of scaling is only possible if the registrant provides the respective equations and a transparent description of his exposure estimation.

Linear correlations are the most easily applicable scaling rules. Examples for determinants linearly related to exposure can be (but may depend on the ES and the exposure model used):

- Amount used
- Concentration in mixture used
- Efficiency of different forms of local exhaust ventilation (in percent).

Scaling of non-linearly correlated determinants generally require application of more complicated exposure models or other tools, which should be clearly described and provided by the registrant, when proposing such scaling rules.

As a scaling rule the registrant may also explain how the exposure concentration has been estimated and give the model/algorithm used for the estimation. In this case the DU is able to use the same algorithm, but modify the input parameters and check, whether under his conditions the estimate is still below the DNEL given by the registrant..

1.5   References

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2   Consumer exposure estimation

2.1   Aim, basic concepts and main determinants of consumer exposure assessment and risk characterisation

This section describes the step-wise (tiered) approach for the estimation of consumer exposure to substances themselves, substances in mixtures (e.g. solvents in glues) or substances in articles (e.g. textile dyes in clothes). For the special case of articles, it is also worth consulting the "Guidance on requirements for substances in articles" (ECHA Articles 2008).

ECHA CSA 2008 (Chapter R.15.1.1) defines all mixtures and articles for which consumer exposure estimation is feasible as "consumer products" or simply products.

The general public may be exposed to substances in several ways, for example:

- to substances used by consumers;
- to substances in mixtures used by consumers;
- to substances in articles used by consumers;
- to substances at home used by professionals;
- to substances in indoor air (private and public) released from building materials;
- to substances in public areas;
- indirectly via the environment.

Some of the basic ideas (e.g. on routes of exposure) and main determinants have already been described in relation to occupational exposure. However, consumer exposure estimation differs in several important respects from occupational exposure. The following list describes some issues to keep in mind when assessing consumer exposure:

- Certain subpopulations (e.g. children) might specifically need to be addressed in consumer exposure estimation, as they might differ in the type and level of exposure and in their vulnerability from the average.

- Oral exposure is sometimes an important route in consumer exposure estimation, but generally not for occupational exposure.

- Adequate measured data are less often available for consumer exposure. But some data, e.g. from indoor air monitoring programmes, may serve as additional information to check the plausibility of model estimates. For example, when inhalation exposure from a volatile chemical in articles is estimated and such an article is present in many homes, then model estimates by far exceeding concentrations measured in indoor air should be checked for plausibility.

- Consumer exposure is sometimes less frequent so that short-term (acute) exposure estimates for a single event may be more meaningful (and should possibly be

addressed in the risk characterisation) than long-term (chronic) exposure levels. Sometimes, a consumer product may lead to an acute (peak) exposure during application and to a chronic exposure due to residues of the product (e.g. a carpet shampoo). Both exposures have to be assessed separately and high peak exposures (e.g. for 10 minutes) should not be averaged (over the whole day).

- Consumer exposure estimation should consider normal uses and reasonably foreseeable misuses (e.g. over-dosing a dishwasher detergent, chewing of a pen) but not deliberate abuse or accidental situations (e.g. swallowing of the dishwasher detergent).

- Annex I of REACH ("General provisions for assessing substances and preparing chemical safety reports") instructs the registrant to assume that risk management measures described in the exposure scenarios have been implemented. This includes instructions and recommendations for use of personal protection equipment by consumers. In the view of the Competent Authorities, mainly product-integrated RMMs, but not those communicated to consumers (e.g. recommendations for personal protection equipment) should be considered in the exposure estimation, as for the latter compliance cannot be assured for a high percentile of the consumers (de Bruin et al. 2007). ECHA CSA (Chapter R.15.3) also points out that "effective risk management measures for consumers are usually product-integrated measures (e.g. concentration limits, package size)."

- Substances can be emitted from articles by a variety of mechanisms, e.g. by evapo-ration, by leaching into saliva or sweat, by diffusion into skin or due to wear and tear (see Info-Box 5).

- Some of these characteristics may combine, e.g. "mouthing" of articles (toys) by a subpopulation (small children) leading to oral exposure, which does not have to be considered for other populations.

Info-Box 5

The following questions, taken from the ECHA CSA 2008, may help to identify exposure pathways from articles.

- Can the article be put in the mouth unintentionally (e.g. chewing) or is it intended to be?

- Is there skin contact with the article, e.g. textiles, belts, shoes etc.?

- Can the article or parts or particles of it be ingested?

- Can substances in the article evaporate and thus be inhaled (based on default or measured release rates)?

- Can the article release the substance, e.g. due to abrasion, sawing, handling or heating and thus lead to exposure via dust or fumes?

Eye contact with substances in articles is generally not considered a relevant pathway but may have to be addressed if eye irritants are to be intentionally released from the article.

2.2   How to estimate consumer exposure

2.2.1   Use of exposure estimation tools – Tier 0

In ECHA CSA 2008 (Chapter R 15.4), basic equations for consumer exposure estimation are given, which can be considered a Tier 0 approach to be used for spreadsheet calculations.

Generally, the same exposure equations and models can be used to estimate consumer exposure to substances from articles (ECHA CSA 2008, Chapter R.17) or consumer exposure to pure substances or substances from mixtures (Chapter R.15). Release of substances from articles will often be reduced, e.g. due to influences of a solid matrix. But this is generally not considered in a Tier 0 approach (see the following Chapter 2.2.4).

Tier 0 exposure estimation basically represents a very rough screening with worst-case assumptions (instantaneous release of the substance without any removal). If safe use can be shown under these conditions, no higher tier assessment is necessary. Currently, no models for consumer exposure estimation exist that can be considered as completely validated.

Input parameters for the following equations are generally specific for the ES under examination. This is for example the case for the amount of product used and the weight fraction of a substance in a mixture. However, default values are available for body weight and skin surface area. In addition, ECHA CSA 2008 (Appendix R.15-4) provides some values for room volumes. These data are given in Appendix 4.2-1.

Inhalation exposure

A very simple, worst case equation for Tier 0 screening purposes assumes that

- the substance in a product is completely released instantaneously (without consideration of substance-specific physico-chemical properties) and that

- there is no ventilation.

The equation can be applied to substances released from a product (i.e. a mixture or an article) as a gas or particulate and gives the concentration of the substance in air.

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

with

C_{inh} Concentration of the substance in the room [mg/m^3]
Q_{prod} Amount of the product used [kg]
Fc_{prod} Weight fraction of the substance in the product [mg/kg$_{prod}$]
V_{room} Room volume [m^3]

Note:
Units of parameters in this and the following equations deviate from those used in ECHA CSA 2008 (Chapter R.15.4.1.1) to obtain more common units for the results (e.g. mg/m3 instead of kg/m3 for inhalation exposure)

The following example demonstrates application of the above equation.

Example:

The scenario is brushing an object with 500 mL of a paint that contains 20% (w/w) of the volatile substance X. In this case (liquid mixture), the density of the paint has to be taken into account, which is 1.43 g/mL according to the SDS. The amount of paint used (Q_{prod}) is therefore (500 mL x 1.43 g/mL =) 0.715 kg. The weight fraction of substance X in the paint is (20 g /100 g =) 200 000 mg/kg$_{prod}$.

Application will be carried out in a hobby room. While Appendix 4.2-2 (and Appendix R. 15-4 in ECHA CSA 2008) do not contain a specific value for this room type, the value of 16 m^3 (sleeping room) appears to be reasonable (5.3 m^2 with a height of 3 m).

Exposure to substance X can thus be estimated as:

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

$$C_{inh} = \frac{0.715 \text{ kg} \times 200\,000 \text{ mg/kg}}{16 \text{ m}^3}$$

$$C_{inh} \quad = \quad\quad\quad\quad\quad\quad\quad\quad\quad\quad 8938 \text{ mg/m}^3$$

This value will be rounded to 8900 mg/m^3.

The product-specific input parameters Q_{prod} and Fc_{prod} will be available to the assessor and room volumes can be taken from Appendix 4.2-2 if the ES refers to application in a particular setting (e.g. in a kitchen or bathroom).

In some cases (e.g. when acute respiratory effects are of concern), the type of exposure is better represented by a short-term peak exposure (for a few minutes) in the im-

Info-Box 6

If the inhalable or respirable fraction is know, it should be taken into account. The Guidance (ECHA CSA 2008, Chapter R.15) provides an equation (Equation 15-2) to calculate the body dose resulting from inhalation of the respirable fraction and gives advice how to calculate the oral exposure resulting from swallowing the non-respirable fraction as well on how to estimate the overall systemic exposure from inhalation and oral exposure.

mediate vicinity of the user. In this case, the room volume can be reduced to e.g. 1 or 2 m^3.

The calculated concentration of the substance is compared to the long-term DNEL in the standard case and to the short-term DNEL in the latter case (peak exposure).

Dermal exposure

The Tier 0 dermal exposure estimation differentiates two distinct scenarios:

- Dermal scenario A: instant application of a substance contained in a <u>mixture.</u>
- Dermal scenario B: a non-volatile substance migrating from an <u>article.</u>

It is important to realise that dermal exposure estimation can lead to a dermal <u>load</u> (expressed in mg/cm^2 skin) relevant for local effects (e.g. irritation) or a dermal <u>dose</u> (expressed in mg/kg body weight and day) relevant for systemic effects. Both are calculated as external exposure values, i.e. percutaneous absorption – although important for an evaluation of systemic effects – is not considered in this step.

As already described for occupational exposure, some substances predominantly exert local effects such as skin or eye irritation and corrosion and skin sensitisation. In these cases, it may be difficult to quantify these effects and to derive DNELs. Dermal exposure estimation may then not be meaningful and a qualitative risk characterisation should be carried out to identify suitable risk management measures.

Dermal scenario A: instant application of a substance contained in a <u>mixture</u>

The equation used for this scenario is very similar to the one for inhalation exposure (see above). This calculation assumes that all of the substance in the mixture is applied to the skin, which clearly represents a worst case assumption.

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

with

L_{der}	Dermal load: amount of substance on skin area per event [mg/cm^2]
Q_{prod}	Amount of the product used [mg]
Fc_{prod}	Weight fraction of the substance in the product [-]
A_{skin}	Surface area of the exposed skin [cm^2]

Again, the product-specific input parameters will be available to the assessor. The skin surface area exposed requires:

- a judgement on the body parts exposed: this should be evident from the type of mixture in many cases (e.g. fingertips when using tube glue).

- data for the surface area of these body parts: see Appendix 4.2-1.

Application of the above equation is illustrated by the following example.

Example:

The scenario is use of a glue marketed in a tube. Exposure to an additive Z contained in the glue at a concentration of 0.5% (w/w; Fc_{prod} = 0.005) has to be assessed. The amount of product (Q_{prod}) used should be available from the ES. If specific values are unavailable, the respective ConsExpo fact sheets may provide relevant data. For this example, the ConsExpo fact sheet for do-it-yourself products (ter Berg et al. 2007) assumes a value of 0.08 g (80 mg) for tube glue and this value is used here.

It is further assumed that exposure occurs only to the fingertips. The skin surface area of the fingertips (A_{skin}) is not included in Appendix 4.2-1, and Appendix R. 15-4 ("Data references") of ECHA CSA 2008 also contains no data. Again, the ConsExpo fact sheet is a useful source and the value of 2 cm^2 reported by ter Berg et al. (2007) for fingertips in the tube glue scenario is used.

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

$$L_{der} = \frac{80 \text{ mg} \times 0.005}{2 \text{ cm}^2}$$

$$L_{der} = 0.2 \text{ mg/cm}^2$$

For other scenarios the dermal load per day (and not per event) may be required. For example, Api et al. (2008) recently proposed a quantitative risk characterisation framework for skin sensitizers, in which consumer exposure levels are expressed as mass per cm^2 of skin per day. These daily dermal loads can easily be obtained from the equation above by multiplication with the number of events per day if there is more than one event per day.

If systemic effects need to be considered, the dermal dose has to be calculated according to the following equation:

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

with

D_{der}	Dermal dose: amount of substance potentially taken up [mg/kg body weight and day]
Q_{prod}	Amount of the product used [mg]
Fc_{prod}	Weight fraction of the substance in the product [-]
n	Mean number of events per day [1/d]
BW	Body weight [kg]

Example:

The above example is extended to calculate the dermal dose. The body weight (BW) is taken from Appendix-Chapter 4.2.1 (65 kg). The only other parameter missing is the mean number of events (n). This may be available from the ES. An alternative source are the ConsExpo fact sheets with the one for do-it-yourself products (ter Berg et al. 2007) giving 1 event/week (0.14 events per day) for the use of tube glue (the result is the daily dose averaged over 1 week).

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

$$D_{der} = \frac{80 \text{ mg} \times 0.005 \times 0.14/d}{65 \text{ kg}}$$

D_{der}	=	0.0009 mg/kg x d

The mean number of events per day will be available from the specific ES under examination but can sometimes also be derived from other sources (see example in the box 7 above).

Info-Box 7

ECHA CSA 2008 (Chapter R.15.4.1.2) contains instructions on how to calculate exposure if the substance is contained in a liquid mixture that is further diluted. The respective equations can also be used for some other specific cases, e.g. a non-volatile substance in a volatile medium.

Dermal scenario B: a non-volatile substance migrating from an <u>article</u>

The fundamental difference between this scenario and dermal scenario A discussed above is that *articles* are considered here and, as such, not all of the substance will be in contact with the skin. The main task then is to estimate the amount of substance that will migrate from an article (e.g. textiles) in contact with the skin during 24 hours (default for Tier 0 screening). Compared to the scenarios discussed so far, the calculations are more complex and require more parameters.

Dermal load for this scenario is calculated with the following equation:

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

with

L_{der}	Dermal load: amount of substance on skin area per event [mg/cm^2]
Q_{prod}	Amount of the product used [mg]
Fc_{prod}	Weight fraction of the substance in the product [-]
Fc_{migr}	Migration rate: Fraction of substance migrating to skin per hour [mg/mg and hour]
$F_{contact}$	Fraction of contact area for skin: article is only in partial contact with skin [m^2/m^2]
$T_{contact}$	Contact duration [hours]
A_{skin}	Surface area of the exposed skin [cm^2]

As a default, $F_{contact}$ is set to 1 (ECHA CSA 2008, Chapter R.15.4.1.2) and will not considered here further. Of the two other parameters not previously addressed (Fc_{migr} and $T_{contact}$), information on the contact duration $T_{contact}$ may be available from the ES. The migration rate Fc_{migr} depends on a variety of factors (e.g. the matrix of the article). A worst-case estimate should be derived for Fc_{migr} based on known properties of the article and used in the assessment. Alternatively, higher tier models may be used.

The following example illustrates application of the above equation by using a model calculation carried out by BfR (2007).

Example:

The scenario considered is exposure to a textile dye contained in a textile at a concentration of 10 g/kg. All input values were taken from BfR (2007).

Q_{prod} and Fc_{prod} are not separately available but are calculated as follows: the textile mass (100 g/m^2) and the skin area (1 m^2) result in 100 g of textile, which contain 10 g/kg of the dye, i.e. 1 g of dye in the textile. Please note that the term Q_{prod} x Fc_{prod} is useful in many cases to calculate the amount of substance contained in an article but that this term can be substituted if the amount of substance is known or can be calculated by other means as in this example.

The migration rate is given as 0.5% for the contact duration ($T_{contact}$) of 16 hours (0.5 mg/100 mg x 16 h). $F_{contact}$ is set to 1 (see above).

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

$$L_{der} = \frac{1000 \text{ mg} \times 0.5 \text{ mg} \times F_{contact} \times 16 \text{ h}}{100 \text{ mg} \times 16 \text{ h} \times 1 \text{ m}^2}$$

$$L_{der} = \frac{5 \text{ mg}}{\text{m}^2}$$

The result can be converted to:

$$L_{der} = 0.5 \text{ µg/cm}^2$$

The dermal dose is calculated from the dermal load:

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

with

D_{der} Dermal dose: amount of substance that can potentially be taken up [mg/kg body weight and day]

L_{der} Dermal load: amount of substance on skin area per event [mg/cm^2]

A_{skin} Surface area of the exposed skin [cm^2]

n   Mean number of events per day [1/d]

BW   Body weight [kg]

For both dermal scenarios it is important to realise that the <u>dermal load</u> (in mg/cm^2 skin) is calculated for one event and will generally be compared with the acute DNEL for local effects expressed in the same unit (see ECHA CSA 2008, Chapter R.8.1).

The <u>dermal dose</u> will usually be compared with the long-term DNEL for systemic effects since an acute DNEL for systemic effects is typically not derived for the dermal route (see ECHA CSA 2008, Chapter R.8.1).

Oral exposure

ECHA CSA 2008 (Chapter R.15.4.1.3) presents only one scenario for oral exposure.

Oral scenario A: unintentional swallowing of a substance in a product during normal use

At the very basic level, the oral intake is calculated with the equation:

$$D_{oral} = \frac{Q_{prod} \times Fc_{prod} \times n}{BW}$$

with

D_{oral} Intake of the substance [mg/kg body weight and day]

Q_{prod} Amount of the product used [mg]

Fc_{prod} Weight fraction of the substance in the product [-]

n   Mean number of events per day [1/d]

BW   Body weight [kg]

This equation is intended to be used both for mixtures and articles or, more realistically, parts of articles. Typical examples are the swallowing of (parts of) articles by small children (e.g. parts breaking away from a toy car) and scraped off product material due to chewing on a pen by older children and adults.

Example:

The scenario is the unintentional swallowing of modelling clay by a child and the resulting exposure to substance A contained in the clay at a concentration of 1% (Fc_{prod} = 0.01). ECHA CSA 2008 (Appendix R. 15-4) does not give body weight data for children. Again, the respective ConsExpo fact sheet (Bremmer and van Veen 2002) provides important data for input parameters. The age of the children playing with modelling clay is assumed to be 4.5 years by default and the respective body weight (BW) is 16.3 kg. The mean number of events (n) for playing with modelling clay is 52/year (0.14/d) and this figure is used here, assuming the worst-case that modelling clay is swallowed each time the child plays with it. The product amount ingested (Q_{prod}) is given as 1 g (1000 mg, derived from product volume and density), although this is a poorly documented estimate (Bremmer and van Veen 2002).

$$D_{oral} = \frac{Q_{prod} \times Fc_{prod} \times n}{BW}$$

$$D_{oral} = \frac{1000 \text{ mg} \times 0.01 \times 0.14/d}{16.3 \text{ kg}}$$

$$D_{oral} = 0.086 \text{ mg/kg} \times d$$

Info-Box 8

Besides the swallowing scenario, some articles might be put into the mouth without actually being swallowed (mouthing). In this case, a substance may migrate into saliva and subsequently be ingested. ECHA CSA 2008 (Chapter R.17) proposes to use the equation above for screening purposes (the equation above assumes complete release of the substance) or to use data provided by van Engelen et al. (2006) specifically for the mouthing behaviour of children. Bremmer and van Veen (2002) also give useful values for several parameters both for the direct swallowing and the migration scenario.

ECHA CSA 2008 provides another equation that can be used if the substance is diluted before swallowing takes place. In addition, the equation may also be used if oral intake of the non-respirable fraction of inhaled particles has to be considered (see section "inhalation exposure" above).

In most cases, the exposure estimation for oral intake will be compared with the long-term DNEL for systemic effects since an acute DNEL for systemic effects is usually not derived for the oral route (see ECHA CSA 2008, Chapter R.8.1).

Please note that the scenarios and formulas above do not cover all possible consumer exposure situations. For example, for substances accumulating in house dust, ECHA CSA 2008 (Chapter R.15.4.1.3) recommends to measure actual concentrations in house dust, which then may be used for estimating inhalation, oral and dermal exposure. More generic scenarios for consumer exposure can be expected to be available in the future.

Info-Box 9

If specific information is missing on some of the parameters required in the equations above (e.g. frequency of use, room volume for specific applications, or product amount used), it is useful to consult the defaults database of the ConsExpo 4.1 software (described in detail below). It contains several values for these parameters (e.g. amount of dishwashing powder used, adapted "room volumes" modelling the immediate vicinity of the user for some applications). Useful background information is available in the form of "fact sheets", which e.g. describe the origin and nature (e.g. 75th or 90th percentile) of these values. Fact sheets are available at the website: www.consexpo.nl.

2.2.2   Use of exposure estimation tools – Tier 1

As already noted for occupational exposure estimation (chapter 1.2.4.1), ECETOC TRA is now implemented as a Microsoft Excel® tool and includes many changes, which are described in more detail in the Technical Report (ECETOC, 2009). While consumer exposure can also be estimated with the integrated version briefly alluded to above (see Info-Box 1, Chapter 1.2.4.1), the stand-alone version of the ECETOC TRA Consumer tool is discussed here in more detail. Similar to the Worker tool, the Consumer tool comes as a single MS Excel® file, a back-up copy of which should be retained before entering data.

Compared to the previous version, the ECETOC TRA Consumer tool now fully implements the REACH product categories (PC) and article categories (AC). Many of these categories are further divided into sub-categories with different scenarios (which may differ in target populations, exposure routes and default input values). For example, PC31 ("Polishes and wax blends") has the sub-categories

- „Polishes, wax / cream (floor, furniture, shoes)" and
- „Polishes, spray (furniture, shoes)".

Note that while the ECETOC TRA Worker tool uses process categories (PROCs, see Chapter 9.3), the Consumer tool uses PCs and ACs, i.e. the product or article in which the substance is finally used is crucial for the exposure estimation.

In addition, the algorithms used in the calculations have been revised to a minor extent and the values of parameters used in these algorithms have been changed, sometimes substantially (see ECETOC 2009 for details). However, many basic concepts of the original version remain in place, for example:

- The tool automatically assigns the relevant exposure routes to each PC and AC

- The bioavailability of a substance is assumed to be 100% for all routes of exposure

- The values of default parameters are fixed except for two key parameters per route of exposure (e.g. the amount of substance used per event for inhalation exposure)

- Systemic exposure from all routes can be added for each sub-category but exposure from different sub-categories is not added up.

Upon starting the tool and after enabling macros at the security warning, the tool opens the first ("user input") of eight worksheets, between which the user can navigate by using the tabs. It is helpful to divide the eight worksheets in three groups:

- Input (one worksheet)
  The worksheet "User Input" contains the sections where actual user input is required and, in fact, it is the only one where user input is allowed.

- Results (five worksheets)
  The worksheets "Results by Sentinel Prod" and "Results by Prod Subcat" contain the results depending on what has been chosen in the "user input" (sentinel products/ articles, product/article sub-categories or both). These two worksheets also show the risk characterisation results (when reference values have been entered). The worksheets "Dermal (Prod Subcat)", "Oral (Prod Subcat)" and "Inhalation (Prod Subcat)" contain details on the estimation per sub-category, differentiated by route of exposure (see Info-Box 10).

- Defaults (two worksheets)
  The "Defaults" and "Defaults2" worksheets contain several defaults, e.g. the route of exposure considered relevant for a particular PC or AC sub-category, and underlying anthropometric parameters (e.g. body surface areas).

Info-Box 10

The tool allows estimating exposure for a specific sub-category and/or a sentinel product (i.e. at the PC or AC level). If sentinel product calculation is chosen, the output is for the sub-category giving the highest exposure estimate. For example, one may choose "sentinel product" for PC1 ("Adhesives, sealants") and the sub-category resulting in the highest exposure estimate is displayed in the "Results by Sentinel Prod" worksheet. If the exposure estimated for the sentinel product demonstrates safe use (when compared with the reference value), then safe use is also demonstrated for the respective sub-categories. It must be stressed that the sentinel product can be different for different routes of exposure. For example, oral exposure for PC 9 is only assessed for children for the sub-categories "finger paints" (PC9c) and "modelling clay" (PC9b-3), which are therefore the sentinel products for oral exposure. A different sub-category may be the most relevant one for another route.

Also note that the ECETOC TRA Consumer tool differentiates between children and adults. Generally, exposure is estimated either for adults <u>or</u> children for a particular sub-category (e.g. exposure to finger paint is calculated for children only). In some sub-categories, however, both groups are considered, but with different exposure routes. For example, oral exposure is considered relevant for children, while dermal and inhalation exposure is considered relevant for adults in AC 5-1 ("Clothing"; see "Defaults" worksheet of the tool for more details).

Data input in the tool is straightforward due to the colour-coding employed. Cells requiring user input are in green while fields that automatically calculate a value are in pink. Grey cells can be populated with values chosen by the user, which must be documented and explained (default values are used if these fields are left empty). However, only some parameters are open to user input and are shown under the heading "optional" in the "user input" worksheet:

- amount of product used,
- fraction of the substance in the product/article and
- skin contact area.

User-specific input for these parameters is only possible if the parameter is needed for exposure estimation in the specific sub-category. For example, if only inhalation exposure is considered relevant by the tool, the skin contact area cannot be altered in the "user input" worksheet.

Generally, exposure estimation is carried out in the following sequence in the "user input" worksheet (Figure 2-1):

- Enter a value for the vapour pressure (the respective default fraction released to air is automatically assigned).

- Enter all reference values (e.g. DNELs) in the correct units, with the inhalation reference value given either in mg/m^3 or in mg/kg x d.[6] The worst-case reference value is generally the lowest of the reference values (but see below).

- Select the relevant sentinel products and/or sub-categories (see Info Box 10) by inserting an "x". There is no limit as to the number of sentinel products or sub-categories being evaluated at the same time.

- Select if product is a spray if not already selected by default and if the respective cell is grey (i.e. open to user input). For example, "spray" may be chosen for water-borne latex wall paints (PC 9a-1), but not for finger paints (PC 9c). The fraction released to air for a spray is always 1. It cannot be altered and overwrites the fraction released to air based on the vapour pressure of the substance.

- As a last step, change default values in columns F to K if applicable (see below). Changing default values is only allowed for some of the parameters such as the product ingredient fraction (i.e. the fraction of the substance being evaluated in the product/article) and the amount of product used per application. In fact, these two parameters will often require product-specific data since the default values are very general. For example, a default product ingredient fraction of 0.6 (60%) for dish-washing products (PC 35-1) may only be correct for some ingredients.

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[6] Technically, it is only necessary to enter reference values for the pathway, for which exposure estimation is carried out in the PC/AC chosen (this can be checked in the "Defaults" worksheet). For example, only inhalation exposure is considered relevant for PC 3-1 (Aircare, instant action (aerosol sprays)), so that only an inhalation reference value has to be entered. However, to avoid error messages and to be able to evaluate different products for the same substance, it is easier to enter all reference values at the start (if available).
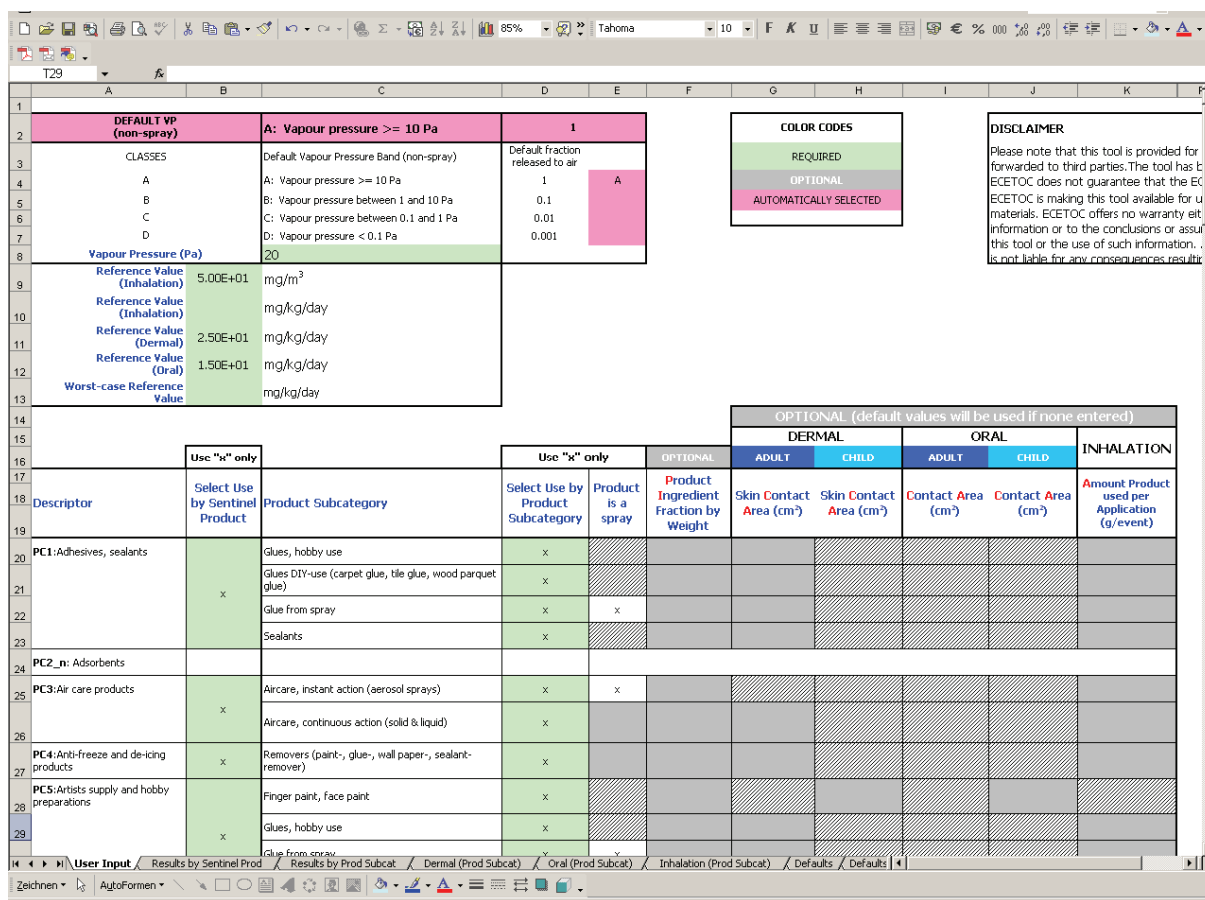
Figure 2-1   Printscreen of the "user input" worksheet (only first PCs shown with all sentinels and all sub-categories selected)

The results are automatically calculated upon user input and can be accessed by choosing one of the five results tabs (see above). The presentation of the results and the level of detail vary somewhat between the different worksheets. For example, results by sentinel product provide an overall view with exposure estimates and RCRs (the latter in red if they are above 1) for the PC/AC resulting in the highest estimate (worst-case scenario). Very helpful is the functionality at the top of the worksheet, where users can display ("unhide") and hide details of the calculations.

The results by product sub-category also mark RCRs above 1 in red. In contrast to the results by sentinel product, this worksheet not only displays results for all sub-categories chosen for calculation but also gives the additional information whether the worst-case scenario is based on exposure of adults, children or both. This overview by sub-category does not display any details of the calculation but is helpful, e.g. in judging whether only the one sub-category in the PC/AC shows high RCRs, while safe use can be demonstrated for all other sub-categories.

The three worksheets containing the route-specific results per sub-category, finally, are different from the result presentations mentioned above in that only the exposure estimate is presented (with all details), but not the risk characterisation. They are essential in comprehending the calculations, which is facilitated by the algorithm shown in the header (this information is also accessible in the sentinel products results via the "unhide" function (see above), but only for the worst-case scenario and not all sub-categories selected). This can be very useful in identifying the parameters that have an important impact on the exposure estimate. The following figure 2-2, for example, shows that the default value for the amount of PC 1 product used is the most crucial parameter for the inhalation exposure estimate (for the concentration, the default amount alone is responsible for the differences).

Info-Box 11

It is not the intention of this guide to review and discuss the algorithms and default values used in the tool. These are documented in the Technical Report (ECETOC 2009). Generally, the default input parameters are based on ConsExpo fact sheets (see chapter 2.2.3) or expert judgement. However, the source/rationale of some of the default values is not immediately evident. For example, a default frequency of 1 event/day has been chosen for almost all sub-categories, although the ConsExpo fact sheets given as a source generally contain more specific data. While this default is certainly conservative for most uses, a few products (e.g. dishwashing liquids) may be used more often. The user should discuss the frequency in the context of comparison with reference values (see below).

The new algorithm for dermal exposure estimation does not require a migration factor (see dermal scenario B in Chapter 2.2.1.2). This is achieved by assuming an (imaginary) layer of a product/article in contact with the skin, for which the thickness is included in the tool. The tool assumes complete transfer of the substance contained in this layer.

Descriptor	Product Subcategory	Parameter:	Product Ingredient (g/g)	Amount Product Used per Application (g/event)	FreQuency of Use (events / day)	Fraction Released to Air (g/g)	Exposure Time (hr)	Inhalation Rate (m³/hr)	Conversion Factor	Room Volume (m³)	Body Weight (kg)	Exposure (mg/kg/day)	Exposure (mg/m³)
		Algorithm:	(PI x	A x	FQ x	F x	ET x	IR x	1000)	/ x (V	BW)		
PC1: Adhesives, sealants	Glues, hobby use		0.3	9	1	1	4.0	1.4	1000	20	60	1.23E+01	1.35E+02
	Glues DIY-use (carpet glue, tile glue, wood parquet glue)		0.3	15000	1	1	6.0	1.4	1000	20	60	3.08E+04	2.25E+05
	Glue from spray		0.3	255	1	1	4.0	1.4	1000	20	60	3.50E+02	3.83E+03
	Sealants		0.3	390	1	1	4.0	1.4	1000	20	60	5.35E+02	5.85E+03

Figure 2-2   Screenshot for inhalation exposure results for PC 1 products (default values used for input; partly reformatted for better display).

Note that in this result presentation red values have nothing to do with risk characterisation but highlight those parameters that are open to user input.

If a substance in several products has to be assessed, it is helpful to run the tool for all PCs/ACs and all sub-categories. This approach is also useful if a particular product might not be directly matched by one of the sub-categories available but may be represented by a surrogate sub-category (obviously, this requires review and, if applicable, changes in the default values). In addition, estimates for similar sub-categories can be compared and add confidence in the exposure estimation.

For this purpose, it appears to be a good idea, to generate a "default file" with all sentinel products and all sub-categories selected. This can then form the basis for exposure estimation for various substances. At the end, the user will have several files (one each per substance) containing all exposure estimations and RCRs. However, if this procedure has to be applied to many substances, the Integrated tool should be considered as an alternative.[7]

Discussion of adequacy/applicability

The ECETOC TRA Consumer tool does not provide exposure estimates for several PCs and ACs. These are assigned an "n" in the descriptor code and cannot be selected for the estimation (i.e. the respective cells are not green and inserting an "x" is impossible). While some of these PCs and ACs are obviously not relevant for consumer exposure estimation (e.g. PC 19 (intermediates)) or outside the scope of REACH (e.g. PC 29 (pharmaceuticals)),

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[7]   It is impossible to give a „cut-off" value for the number of substances above which application of the Integrated tool is indicated. As an orientation, it appears that screening 5-10 substances across all sub-categories is not very time-consuming with the stand-alone ECETOC TRA Consumer tool.

this does not apply to all PCs/ACs concerned. For example, anti-freeze and de-icing products (PC4) clearly have the potential for consumer exposure but these cannot be assessed with the tool. One workaround is to select a surrogate PC/AC or sub-category and to adapt the input parameters. The ECHA Guidance (ECHA CSA 2010, Chapter R.12) gives some advice in Appendix R.12-7 on surrogate categories. If surrogate categories are used, the following should be considered:

- Review the routes of exposure and input parameters in the "Defaults" worksheet
- Adapt input parameters to actual use (e.g. with sector-specific data)
- Document changes and discuss similarities and differences between use (actual use vs. PC/AC selected)

Similar to the ECETOC TRA Worker tool, total exposure from all three routes of exposure can be calculated in the Consumer tool. In the risk characterisation part (various columns in the "Results by Sentinel Prod" and "Results by Prod Subcat" worksheets), total exposure is divided by the worst-case reference value (defined in the User Guide as "generally the lowest of the pathway-specific reference values") to give an overall RCR. As the following (fictitious) example shows, this approach might be completely misleading because it is possible that the overall RCR is well above 1 even when all route-specific RCRs are below 1. This is due to the possibility that an oral reference value (which will probably be the one most often available) may be the lowest of all reference values (i.e. taken for comparison with total exposure), while oral exposure itself is not expected to occur. The latter is not an exception but rather the rule in the ECETOC TRA Consumer tool, since oral consumer exposure is by and large restricted to small children's mouthing behaviour (oral exposure of adults is only expected to occur in one out of 46 sub-categories).

Exposure (mg/kg x d)			
Dermal	Oral	Inhalation	Total
10		15	25
Reference value (mg/kg x d)			
Dermal	Oral	Inhalation	Worst-case
50	10	20	10
RCR			
Dermal	Oral	Inhalation	Total / Worst-case
0.2		**0.75**	**2.5**

It is therefore not recommended to use the overall RCR based on total exposure without scrutiny. In some cases, expert evaluation of the route-specific RCRs might be more appropriate.

Appendix F of the Technical Report (ECETOC 2009) describes several options for refinement, which ultimately increase the accuracy of the estimates. When many of these are

applied (e.g. inclusion of air exchange rates and application of specific rather than default values), the tool virtually becomes a "Tier 1.5" (ECETOC 2009) model, situated somewhere between Tier 1 and higher tier models, such as ConsExpo. Many of these refinements cannot be implemented in the tool but have to be calculated separately. For example, the tool does not offer the possibility to enter air exchange rates (which makes sense since it is a Tier 1 tool).

Finally, a word of caution is in place. With only one exception, the frequency of use is set to 1 event per day (i.e. no average over 1 week or 1 year is taken). The exposure estimates of the tool thus basically refer to the exposure during this event on one day (e.g. during application of a paint or while a child plays with a toy). The estimated exposure thus has to be compared with an acute reference value, especially in cases in which daily use cannot be expected. For example, it is highly unlikely that a consumer applies 15 kg of carpet glue per day over an extended period of time (PC 1-2; this is the default value used in the tool). Alternatively, for an intermittent exposure regime exposure can be averaged from the one-day value and compared with chronic reference values. This requires knowledge and documentation of the frequency of use for the respective product.

As already mentioned, dermal exposure is calculated with a new algorithm, which avoids inclusion of a migration factor. This algorithm calculates exposure by assuming a skin contact area and a thickness of the layer of the product in contact with the skin. Together with the default density of 1 g product/cm^3, this results in the amount of product contributing to exposure. Using the example of AC 8-3 (Tissues, paper towels, wet tissues, toilet paper; default input values), it can be shown that this figure can deviate somewhat from the total amount of product assumed in inhalation exposure estimation:

Dermal exposure		Inhalation exposure
Contact area	857.5 cm^2	
Thickness of layer	0.01 cm	
Density of product	1 g/cm^3	
Amount of product	**8.572 g**	**5.7 g**

While the deviation in the amount of product is not very large for a comparatively rough Tier 1 tool, the user should be clear about this difference resulting from the different algorithms employed. In consequence, a mass balance check is clearly helpful in this context, especially

▪ when default input values are altered by the user (e.g. the amount of product used for inhalation exposure) and

▪ for total exposure estimates (see discussion above) since the algorithms generally assume 100% release of the substance, thus potentially resulting in "double counting" in the total exposure estimate.

In summary, the ECETOC TRA Consumer tool is very valuable in screening the exposure of consumers and allows identifying exposure associated with a high risk. It contains many default values and is easier to handle than the equations introduced in Chapter 2.2.1, especially if many scenarios have to be assessed. In some cases, it leads to identical results than the equations if the same input values are used (e.g. for inhalation exposure to substances with a high vapour pressure, fraction released to air = 1). In other cases, results are quite different, e.g. for substances with a low vapour pressure (fraction released to air e.g. 0.01) since this factor is not considered in the simple equations.

2.2.3   Use of exposure estimation tools – higher tier

Users of exposure estimation tools should keep in mind that most tools are of a very conservative nature (i.e. in most cases they tend to the cautious, higher side of exposure estimates) and that they are only validated to a limited extend and/or for some uses. Application of higher tier models in particular will in many situations require in-depth understanding of exposure estimation and expertise in handling the tools to avoid highly inaccurate estimates.

The higher tier tool discussed in this section can, in principle, be used for substances as such, substances in mixtures and substances in articles.

The software ConsExpo (version 4.1, available from: http://www.consexpo.nl, the manual (Delmaar et al. 2005) is also available but has not yet been updated from version 4.0 to 4.1) will be discussed here in more detail since it is widely used and provides several product-specific input data (available via the defaults database), the origin of which can traced back in the "fact sheets" (see box above). It is therefore possible to assess, whether a ConsExpo default value is conservative enough or overly conservative for the ES under examination (a quality category is also assigned to each value). However, as will be shown below, the complexity of the software and of consumer exposure itself make it difficult to perform assessments without a certain level of experience and expertise in exposure assessment.

After starting the software, it is helpful to go through the four different sections of ConsExpo from the top down:

- Product & compound: basic data input (e.g. Molecular weight, P_{OW} and vapour pressure for the substance);
- Exposure scenario: selection from defaults database (see below);
- Exposure Routes: input of missing data (i.e. not provided by defaults database);
- Output: Results, reporting and analysing function.

The defaults database contains the following product databases:

- Painting products;
- Cosmetics;
- Pest control products;
- Cleaning and washing;
- Disinfectants;
- Do-it-yourself products.

For each product database, there are several product categories, and for each product category there are several default products, for which one or more scenarios are defined (i.e. many default input values are already included). This tree-like approach is for a machine dishwashing powder:

- Cleaning and washing (product database);
    - Dishwashing products (product category);
        - Machine dishwashing powder (default product);
            - Loading (scenario).

One of the main advantages of ConsExpo is that default values are included for many scenarios (see below) and that the route to consider and the most appropriate model is selected once the scenario is chosen. For example, once the loading scenario is selected in this example, the input screen identifies inhalation exposure as the route (indicated by question marks, i.e. data entry is required) and states the model (Exposure to vapour: instantaneous release) (Figure 2-3, left).

If, on the other hand, the post-application scenario is chosen for the same default product, the input screen indicates that oral exposure needs to be considered with the model "Oral exposure to product: direct intake" (Figure 2-3, right).
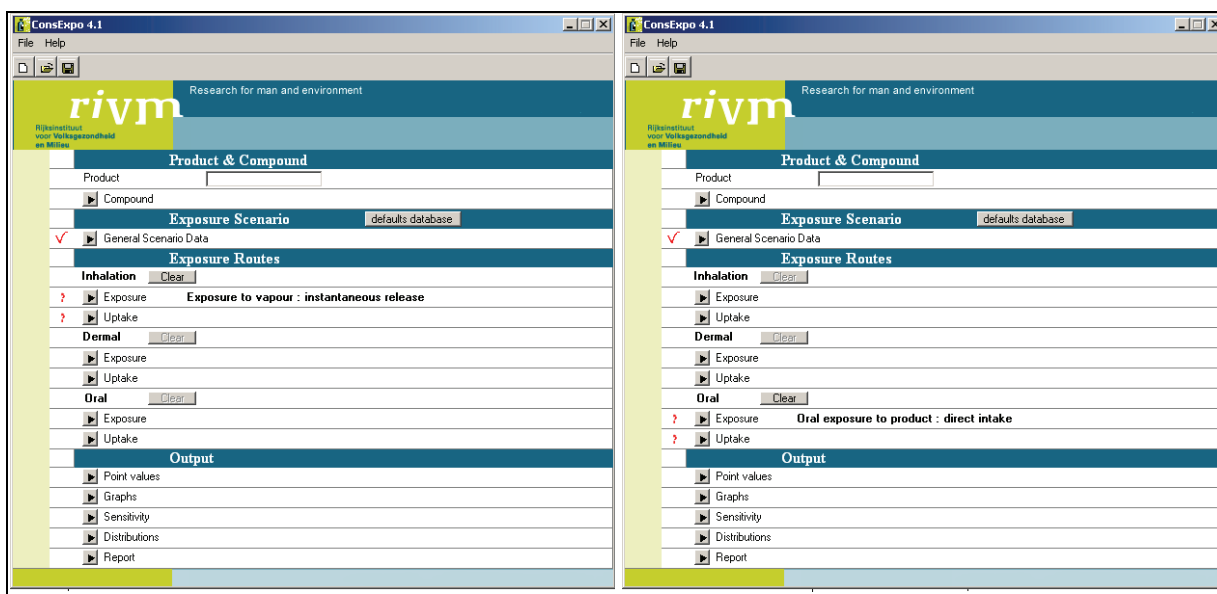
Figure 2-3   Print screen showing route of exposure to be considered and model applied in ConsExpo: machine dishwasher powder, loading (left) and post-application (right)

The following Table 2-1 shows the input parameters for the example of loading the machine dishwashing powder (substance-specific data have been omitted) with values to be chosen by the user in italics. Of these,

- the uptake fraction refers to the fraction available for systemic uptake and is set to 1 since an external exposure should be calculated,

- the weight fraction of the compound (substance) is known from product-specific data.

This example also shows the type of default data that users can expect in Cons-Expo, e.g. the exposure frequency (252 uses of machine dishwashing powder per year), duration (0.25 min. for loading the powder in the dishwasher) and the room volume (1 m^3 set as default to model inhalation exposure in the immediate vicinity of the source).

Info-Box 12

A closer look at the default input values in Table 2-1 identifies a very small applied amount of only 0.27 µg. An inexperienced user would probably overwrite this with a higher value. However, this is the amount of dust generated by 200 g of powder (derived from laundry powder; Proud'homme et al. 2006). This demonstrates that information from the "fact sheets" (in this example: Proud'homme et al. 2006) is often required when using ConsExpo. More generally, it shows that expertise in exposure assessment and an understanding of the parameters and models involved is necessary to use ConsExpo.

Table 2-1:   Example of data input for ConsExpo: loading of a machine dishwashing powder containing 1% of the substance under assessment (values to be chosen by the user are in italics)

Input parameter	Value	Unit
General Exposure Data		
Exposure frequency	252	1/year
Body weight	65	kilogram
Inhalation model	Exposure to vapour: instantaneous release	
Weight fraction compound	*0.01*	*fraction*
Exposure duration	0.25	minute
Room volume	1	m^3
Ventilation rate	2.5	1/hr
Applied amount	2.7E-7	gram
Uptake model	Fraction	
Uptake fraction	*1*	*fraction*
Inhalation rate	24.1	litre/min

Note:
the model also calculates the dose and therefore requires data (e.g. inhalation rate), which are not necessary for estimation of the substance concentration in air.

The example shown above is a more sophisticated Tier 0 model (instant release assumed as in Tier 0, but now with room ventilation).

It is another strength of ConsExpo, that input values (including the ones set as defaults in the database) can be changed. In this respect, the sensitivity function in the output section may also be helpful. For example, it allows users to model the concentration of the substance in the air in dependence of the room volume.

The above example refers to a mixture but ConsExpo can also be used to model exposure to a substance from an article. For example, dermal exposure in the post-application scenario for the default product "detergent powder" (laundry powder) can be estimated using the "Direct dermal contact with product: migration" model. While some default values are set in this model, the important parameter of the leachable fraction requires consultation of the respective "fact sheet" (Proud'homme et al. 2006).

In principle, ConsExpo may also be used for modelling exposure without using the defaults database (e.g. dermal exposure to a substance used in textile finishing with the migration model mentioned above). However, this requires a very clear understanding of the models, the influence of the different parameters and the user must identify adequate values for all input parameters.

Info-Box 13

ConsExpo allows the user to use distributions rather than point values for many input parameters (e.g. if the mean and standard deviation of a parameter is known). The software can then perform probabilistic (Monte Carlo) calculations.

A special case is the particle size distribution of a product, which has an important influence on inhalation exposure to spray and can be entered in the respective model. This, however, is not a distribution in the above sense and does not allow Monte Carlo calculations.

Industry has developed several default values, which could be used in addition to the ConsExpo default values. For example, AISE (International Association for Soaps, Detergents and Maintenance Products; http://www.aise.eu) provides detailed "habits and practices" default values for consumers (e.g. on the amount of household product used and the duration and frequency of use).

Other tools

The European Union System for the Evaluation of Substances (EUSES) software (version 2.1, available from: http://ecb.jrc.it/euses/) is another software package that allows to estimate exposure for almost all impact areas, including consumers. If more complex models are required for consumer exposure assessment, EUSES is referring to ConsExpo.

ECHA CSA 2008 mentions several software tools provided by the U.S. Environmental Protection Agency; (e.g. E-FAST (Exposure and Fate Assessment Screening Tool, which includes CEM, Consumer Exposure Model), MCCEM (Multi- Chamber Concentration and Exposure Model) or WPEM (Wall Paint Exposure Assessment Model), available at http://www.epa.gov/opptintr/exposure/index.htm, see also Appendix R.15-3 "Computer tools for estimation of consumer exposure" in ECHA CSA 2008) that might be useful for higher tier exposure estimation. These models require the same or even more experience than ConsExpo.

Also, the British Aerosol Manufacturers' Association (BAMA; http://www.bama.co.uk/) has developed a tool (BAMA Indoor Air Model) to estimate aerosol exposure from sprays under a wide range of conditions of use. The user guide contains generic examples as well as advice on model application and use of the estimates in Chemical Safety Assessments.

2.2.4   Refinement of consumer exposure estimation

If safe use cannot be demonstrated with the higher tier tools discussed in the previous section, a refinement of the exposure estimation will become necessary. This may take several forms, for example:

- consideration of (product-integrated) RMMs (if not already considered when drawing up the ES), e.g. if a product is placed on the market in pellet or granular form, inhalation exposure may be assumed to be lower than the one to dust generated by handling powders

- substitution of the default input values in ConsExpo with more product-specific or ES-specific data (if it can be justified): consult the respective ConsExpo "fact sheet", if available, and assess input parameters,

- use of specialised modelling tools, e.g. for estimating the migration of a substance from an article (e.g. for migration from plastic and polymer food contact materials: http://www.inra.fr/Internet/Produits/securite-emballage),

- use of measured exposure data (check e.g. data in the EIS-ChemRisks project: http://web.jrc.ec.europa.eu/eis-chemrisks/),

- generation of measured data, especially for critical input parameters, such as

    – the particle size distribution for inhalation exposure to sprays: an extensive list of available methods can be found in Chapter R.7.1.14 ("granulometry") of ECHA CSA 2008.

    – the release of a substance from an article for the dermal migration models: consult BfR (2007) for a brief discussion of methods used to determine migration of chemicals from textiles (this paper also contains default values for textile dyes and auxiliaries),

    – the release of a substance from an article (leachable fraction) for mouthing scenarios: consult van Engelen et al. (2006, Chapter 4) for a detailed discussion of the different methods available.

    – There are several norms for the determination of migration from articles (partly discussed in the overviews mentioned above), e.g.

        - "DIN EN 71-10: Safety of toys – Part 10: Organic chemical compounds - Sample preparation and extraction",

        - "DIN EN ISO 105-E04 (draft standard): "Textiles – Tests for colour fastness - Part E04: Colour fastness to perspiration" and

        - "DIN EN 1186-3: Materials and articles in contact with foodstuffs – Plastics – Part 3: Test methods for overall migration into aqueous simulants by total immersion"; available e.g. from http://www.beuth.de.

The approach taken for a refinement of the exposure estimation ultimately depends on the nature of the ES under examination and requires expert knowledge in exposure assessment (and other disciplines) both to choose the most meaningful strategy and in the interpretation of results.

2.2.5   Combined uptake

As a final step in the exposure estimation, combined uptake (usually separately for acute and long-term exposure) should be assessed. This involves two cases:

- If consumers are exposed to <u>one particular product</u> via different routes of exposure (e.g. inhalation and dermal), the combined uptake has to be determined (summation of doses).

- If consumers are exposed to <u>different products</u> containing the same substance and if these products are likely to be used in parallel, the uptake of the substance from these different products may be summed up. (In practical terms, this can be achieved only in those cases, in which the registrant is aware of this situation, for example where known downstream users prepare several products, which can in principal be used in parallel, and he receives respective up-stream information.)

More advice on this step is given in ECHA CSA 2008 (Part E, Chapter 3.5; "Step 5: combined exposures").

2.2.6   Special case: Humans exposed indirectly via the environment

Exposure of humans via the environment results from the consumption of food and drinking water, inhalation and soil ingestion (only relevant in specific situations). It is estimated on the basis of predicted environmental concentrations (PECs) of the substance in (surface) water, groundwater, air and soil. Methods to estimate PECs are described in the chapter on environmental exposure estimation (Chapter 3).

2.3   Risk characterisation

According to REACH, Annex I, the risk characterisation should assume that risk management measures as described in the exposure scenarios are implemented. In this respect the REACH text does not discriminate between consumers and workers. This approach has been criticised (de Bruin et al. 2007), as compliance with instructions and recommendations for use of personal protection measures may be limited, thus leading to risks for relevant parts of the population. As it is undisputable that severe health risks for consumers should be avoided, adequate control of risks should not rely on risk management measures in those cases, in which non-compliance with risk management measures may give rise to severe health effects such as corrosion or respiratory sensitisation. For such a differentiation according to severity of effects, methodological proposals in ECHA CSA 2008

(Part E, Chapter 3.4) may give some guidance: for qualitative risk assessment substances are assigned to groups of "high", "moderate" or "low" hazard according to their classification.

As explained in Chapter 3.1, Part I of the practical guide, in the risk characterisation part of the chemical safety assessment information on exposure is compared with the hazard data for a specific substance. In this step, exposure estimates are compared to the dose levels without (or with low) concern (i.e. DNELs, derived no effect levels, or DMELs, derived minimal effect levels, for substances without threshold). This process, relying heavily on expert judgement and experience, is described here only in general terms. For a more detailed description of approaches the reader is referred to ECHA CSA 2008 (Part E).

Risks for humans are considered to be adequately controlled if

the RCR (risk characterisation ratio) = exposure level / DNEL < 1,

i.e. the DNEL exceeds the exposure level.

Tier 0 models as explained in Chapter 2.2.1 result in various types of exposure estimates. The following table contrasts these types of estimates with the corresponding types of DNELs (for types of DNELs see also ECHA CSA 2008, Chapter R.8).

Table 2-2   Types of exposure estimates (Tier 0) and corresponding types of DNELs for the general population

Exposure estimate	DNEL
C_{inh}: concentration of the substance in the room [mg/m^3] (either acute or long-term)	DNEL acute inhalation DNEL long-term inhalation
L_{der}: dermal load: amount of substance on skin area per event [mg/cm^2]	DNEL acute dermal local (presumably rarely available)
D_{der}: dermal dose: amount of substance that can potentially be taken up [mg/kg body weight and day]	DNEL long-term dermal
D_{oral}: intake of the substance [mg/kg body weight and day] (either acute or long-term)	DNEL acute oral DNEL long-term oral

In the case of substances with non-threshold effects, for which a DMEL has been derived, exposure levels below the DMEL characterise a low, tolerable risk. DNELs/DMELs should be derived for all critical endpoints and pathways.

When exposure to a substance in a specific setting occurs via several exposure routes or when different products contain this substance, leading to exposure of humans, these combined exposures should be considered. This can be done either by summing up exposure doses and comparing the total exposure with an adequate DNEL or by adding up RCRs calculated for individual pathways or situations.

In some cases, there may be information on toxic effects for some endpoints, but no data to allow derivation of a DNEL or DMEL. ECHA CSA 2008 (Part E, Chapter 3.4.1) in this regard

mentions acute toxicity, irritation/corrosion (skin and eyes), sensitisation, mutagenicity and carcinogenicity. In this case, a qualitative risk characterisation has to be carried out with the aim to show adequate control of risks. Guidance on how to carry out such an assessment can be found in ECHA CSA 2008 (Part E, and Chapter R.8).

2.4   Communication of the results in exposure scenarios and scaling

The risk characterisation leads to a description of the use conditions (operational conditions of use and risk management measures), under which safe use of the substance can be shown. These use conditions form the essential part of the exposure scenario, which is communicated down the supply chain.

The information of the ES has to be used by the downstream user (DU), e.g. a company using a substance to produce a consumer product, to check whether his substance use is within the conditions of use considered by the registrant ("compliance check"). The registrant can provide the DU with scaling methods as a part of the ES. Scaling methods are simple equations by which the DU can demonstrate that he operates within the conditions of the ES even if (some of) his conditions of use differ from those described by the registrant. Scaling and related tools are described in Part I of the practical guide, chapter 7.7.

Please note: application of scaling is only possible if the registrant provides the respective equations and a transparent description of his exposure estimation.

Example:

Consumer exposure to a volatile substance from use in a mixture has been calculated. The registrant assumed complete evaporation of the substance contained in the mixture and homogeneous distribution in room air to calculate the inhalation exposure concentration. Both room size and the amount of substance in the mixture are linearly correlated with the exposure concentration. This has been made transparent by the registrant who also gave the following scaling rules in the ES:

1. Exposure concentration inversely linearly correlated to room size;

2. Exposure concentration linearly correlated to concentration of substance in mixture;

3. Exposure concentration linearly correlated to amount of mixture used.

A manufacturer (downstream user) of an adhesive mixture for consumer uses the substance in higher concentrations. But the amount of mixture used is substantially lower. By applying scaling rules 2 and 3 he is able to show that his use is compliant with the ES, even when some conditions of use are not met:

Values given by the registrant in the exposure scenario:

- Concentration of substance Y up to 20% (w/w), amount to be used: up to 10 g

---

> (single application).
>
> Conditions of use for the adhesives consumer product:
>
> - Concentration of substance Y in product is 40% (w/w), amount to be used per single application 1 g (single application).
>
> To show compliance with the exposure scenario the manufacturer of the adhesives product may
>
> 1. either use the algorithms, if provided by the registrant with his own input values to recalculate the exposure under his own conditions of use, or
>
> 2. (based on linearity of the associations stated by the registrant) argue that the 2-times higher concentration of Y in the product is outweighed by the 10-times lower amount used per application.

Linear correlations are the most easily applicable scaling rules. Examples for determinants linearly related to exposure can be (but may depend on the ES and the exposure model used):

- Room volume (up to a certain limit, as long as homogenous distribution can be assumed);
- Amount used;
- Concentration in the mixture;
- Exposure duration;
- Application area for coatings.

Scaling of non-linearly correlated determinants generally requires application of more complicated exposure models or other tools, which should be clearly described and provided by the registrant, when proposing such scaling rules.

2.5   References

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3 Environmental exposure estimation

3.1 Aim of the environmental exposure estimation and risk characterisation

The purpose of carrying out environmental exposure estimation is to derive the predicted environmental concentration (PEC) for environmental compartments of interest, i.e. water, sediment, soil, air and top-predators, which are then compared with the Predicted No Effect Concentrations (PNEC).

The first step in environmental exposure assessment is to estimate the quantities of the substance released to the environmental compartments water, sediment, air, soil and top predators during all life cycle stages of the substance. These emissions result in an exposure of the environment. Release estimations may be based on measurements, on pre-defined environmental release classes, on expert judgement or on IT based calculations. The second step is the exposure estimation in order to derive predicted environmental concentrations (PECs) for all environmental compartments. PECs are derived either by measurement (monitoring data) or by model predictions taking into consideration distribution and fate processes after the chemical has entered the environment.

Environmental exposure assessment encompasses the following targets:

- Fresh surface water (including sediment);
- Marine surface water (including sediment);[8]
- Terrestrial ecosystem;
- Top predators via the food chain (secondary poisoning);
- Micro-organisms in sewage treatment systems;
- Atmosphere – mainly considered for chemical with a potential for ozone depletion, global warming, ozone formation in the troposphere, acidification;
- Man indirect, i.e. man exposed via the environment.

In the subsequent risk characterisation, the PEC values are then compared with the Predicted No Effect Concentrations (PNEC). The PNEC for a specific environmental compartment is regarded as a concentration below which adverse effects on ecosystems will not occur. The PNEC is derived from toxicity test endpoints (e.g. LC50s or NOECs) using appropriate assessment factors.

For some substances (e.g. inorganic substances & metals), the standard environmental exposure assessment including risk characterisation by PEC/PNEC ratios and the guidance materials on these methods may not be applicable as these guidance materials are mainly

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[8] Risk assessments for the marine environment are only required for specific industrial sites that release wastewater directly into the sea.

focussed on organic chemicals[9]. A "Metals Environmental Risk Assessment Guidance" (MERAG) has been developed presenting scientific concepts for assessing the risk posed by the presence of metals and inorganic metal compounds in the environment.[10]

Other substances may exhaustively be removed from the wastewater by chemical processes like oxidation, neutralisation, precipitation, etc. Environmental exposure assessments for these substances could be done on basis of measured release and exposure data.

3.2   Approaches to environmental exposure assessment

The environmental exposure assessment follows the following workflow:

1. Release estimation (measured or calculated data) taking into account applied risk management measures (e.g. biological / chemical waste water treatment)

2. Consideration of distribution and fate processes (e.g. degradation) in the environment

3. Exposure estimation including derivation of PECs

4. Risk characterisation by comparing PEC/PNEC

The workflow for an environmental exposure assessment with a subsequent risk characterisation is illustrated in Figure 3-1.

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[9] For several inorganic substances / metals (i.e. ZnO, CdO, etc), EU Risk Assessments on the basis of PEC/PNEC ratios are already available, thus indicating that the PEC/PNEC approach is not only applicable for organic substances but also for inorganic substances and metals. The available RAR (see http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=ora) can give guidance how to perform risk assessments for inorganic substances / metals.

[10] http://www.icmm.com/page/1185/metals-environmental-risk-assessment-guidance-merag
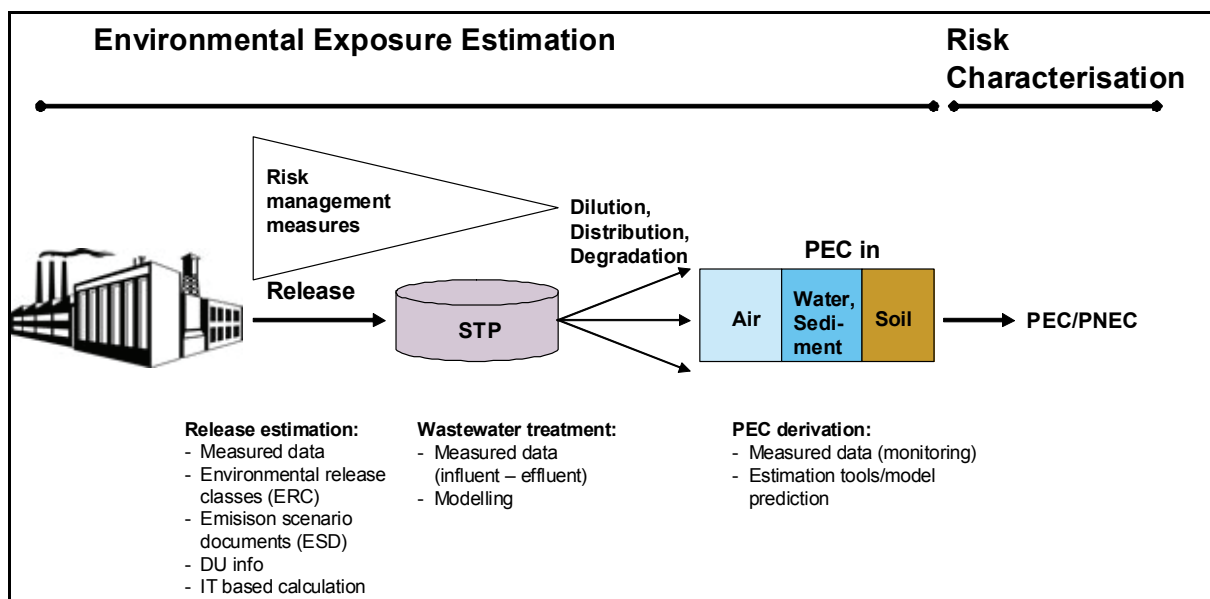
Abbreviations: STP: sewage treatment plant; DU: downstream user

Figure 3-1   Environmental exposure assessment and risk characterisation

3.2.1   Release estimation

As mentioned above release estimation is the first step in environmental exposure assessment. Emissions into the environment may occur as a result of any process or activity during the life cycle of a chemical i.e. manufacture, formulation, industrial/professional/private use, service life & waste treatment.

Concerning the emission pattern it needs to be distinguished between distribution on the local and on the regional scale. Local emissions are assessed in the vicinity of point sources and are expressed as daily average concentrations. Regional emissions are not calculated for single emission sources, but for larger areas over a longer time period, thus representing background concentrations of a substance. Regional exposure estimation is based on year-averaged emissions to water, air and soil. The relationship between regional and local scale emissions is illustrated in Figure 3-2.
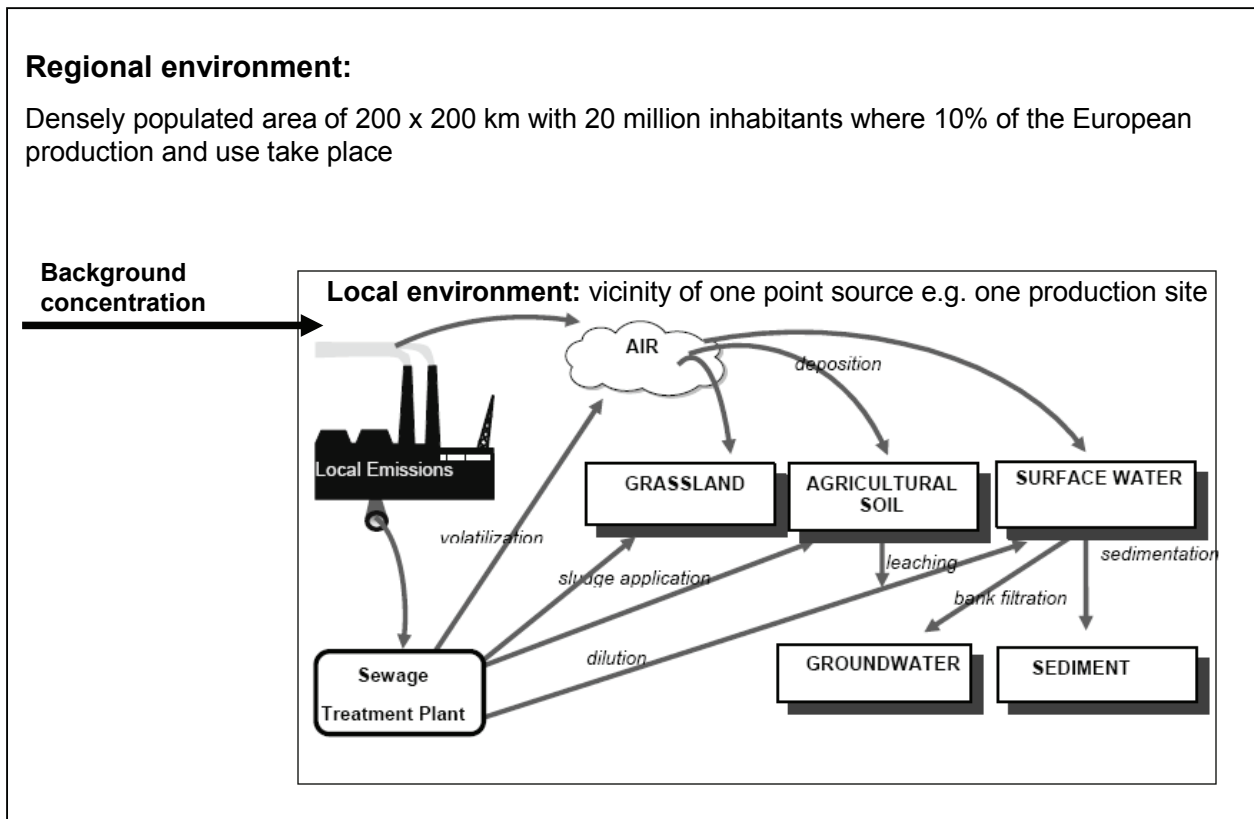
Figure 3-2   Relationship between regional and local scale

Determinants of release

Key determinants of substance release resulting in environmental exposure are:

- Quantity of substance applied in a use or a process per time;

- Emission pathways (i.e. emission to water, air, soil, or (solid) waste);

- Release / emission factors from processes and products (before abatement);[11]

- Efficiency of any abatement or control technology that reduces the emission to air, water, soil or (solid) waste;

- Spatial dispersion of emission sources (local or regional emissions);

- Duration of emission (e.g. working days per year).

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[11] Release / emission factors: the fraction of the substance emitted from the process or use to (waste) water, (waste) air, soil, or (solid) waste before onsite or offsite abatement measures.

How to assess release / emissions to the environment

Measured release information of substances might be easily obtained for the first three life cycle stages (LCSs): (i) Production, (ii) Formulation, and (iii) Industrial Use because this information often is laid down in the licence(s) supplied by the authorities. Before using measured data, it needs, however, to be considered if they cover the use(s) described in the exposure scenario (ES). Measured data are not preferable per se but have to meet certain criteria, as it is the case for modelling. For general criteria on measured data please refer to Chapter 1.2.1 above. Additional criteria to be fulfilled by measured data are listed in the subsequent chapter "Use of measured data".

For the remaining LCSs the availability of measured data is expected to be quite limited and consequently the emissions to the environment need to be estimated with appropriate methods. Several release estimation methods are available. As already discussed in Chapter 1.2.1, the level of differentiation, and thus the input requirements, increase from a lower tier (level 1) to a higher tier (level 2). This step-wise approach ensures that a more detailed, labour-intensive assessment is not carried out for situations, in which negligible exposure is expected.

The following methods are suitable for Tier 1 assessments:

1. Calculation (either manual or IT-based e.g. with the tool EUSES) of the environmental release using given basic equations (Guidance document Chapter R.16, equations R.16-1 and R.16-2).

   a) Key input parameters to these equations are listed above as "determinants of release".

   b) For an initial Tier 1 assessment, pre-defined release/emission factors can be taken from the newly developed Environmental Release Categories (ERC) presented in the Guidance document Chapter R.16 (Appendix R.16-1, Tables R.16-20 until R.16-23). These ERCs specify default emission factors for different life cycle stages of chemicals i.e. the fraction of a substance emitted from the process or use considered to (waste) water, (waste) air, soil, or (solid) waste before abatement measures (for a more detailed description see below). The ERC method does not require any explicit substance information. The concept of ERCs within the Use Descriptor System is described in Part R.12 of the ECHA Guidance (Section R.12.3.4, Appendices R.12.4.1 and R.12.4.2).)

2. Branch-specific OECD and EU Emission Scenario Documents (ESDs) including generic scenarios by US EPA (US EPA OPPT Generic Scenarios (http://www.epa.gov/oppt/exposure) might be used instead of ERCs but are not yet available for all industrial uses.

3. Generic exposure scenarios (GES) and further branch-specific information as developed by sector groups (see Chapters 9.7 and 10 of the practical guide).

4. Use specific information on emission; either based on measurements or downstream user (DU) information, expert judgement or more precise process descriptions.

Use of Environmental Release Categories (ERC)

Environmental Release Categories (ERC) have been established to facilitate the derivation of release/emission factors for an initial Tier 1 assessment (Guidance document Chapter R.16, Tables R.16-22 and R.16-23). For each ERC default emission / release factors to air, water and soil have been defined based on the assumption that no risk management measures are in place. These release/emission factors are then used as input into equations R.16-1 and R.16-2 for the calculation of the environmental release. The selection of the appropriate ERCs needs basic information on the operational conditions of use of the substance under consideration. In detail, knowledge on the following parameters is required for the selection of the adequate ERC:

- lifecycle stage of the substance i.e. production, formulation or use;
- level of containment i.e. application in open or closed systems;
- type of use in life cycle stages i.e. inclusion into/onto matrix, processing aid, inter-mediate, monomer etc.;
- dispersion of emission sources i.e. industrial use or wide disperse use;
- indoor use (connection to sewage treatment given) or outdoor use (no connection to sewage treatment assumed).

For the selection of the adequate ERC and the derivation of the pre-defined release/emission factors, no substance specific properties are required.

In addition to the release/emission factors, the ERCs include also pre-set values for the percentage of the substance used as input to the emission calculation, the release time in days per year assumed for the calculation as well as the dilution factor to be applied for the subsequent PEC derivation (see Table R.16-23 of Guidance Chapter R.16).

Release estimation based on ERC can be regarded as a first conservative approach used for a Tier 1 assessment under REACH.

If a risk is indicated in this Tier 1 assessment based on conservative release estimates, the assessment of the release rates may be refined by using more precise data on risk management measures. Furthermore, if detailed information on the identified uses is available, a higher Tier assessment may be performed by using specific information on marketing, use, release days or exposure of the substance. To refine the default emission

factors, branch-specific Emission Scenario Documents (ESDs), generic exposure scenarios (GES) or other data sources like downstream user information are needed to improve the initial exposure estimate.

Industrial sector groups can define more specific environmental release categories which describe more precise the emission situation for specific processes. These categories are called "specific Environmental Release Categories" (spERCs) (see section R.16.3.5 of the ECHA Guidance on information requirements and the chemical safety assessment).

The present version of ECETOC TRA provides the option to use spERCs. The updated integrated tool can be found at http://www.ecetoc.org/tra (last update: April 26, 2010).

Waste water treatment

One of the critical questions in the environmental exposure estimation (especially for the aquatic environment) is whether or not the substance will pass through a wastewater treatment plant before being discharged into the environment.

Many of the larger industrial installations are usually connected to a municipal wastewater treatment plant or have treatment facilities on site. These treatment plants are not always biological treatment plants but often physico-chemical treatment plants in which organic matter is flocculated by auxiliary agents e.g. by iron salts followed by a sedimentation process resulting in a reduction of organic matter (measured as COD[12]) of about 25-50%. The above-described situation is taken into account as follows in the environmental exposure assessment:

On a local scale, wastewater may or may not pass through an STP before being discharged into the environment. Depending on the exposure scenarios, an aquatic PEClocal with or without STP can be calculated. In some cases, both may be needed if it cannot be ascertained that local emissions will pass through the STP. The PEC without considering an STP-treatment will only be used in the exposure estimation, when the substance considered has a specific identified use where direct discharge to water is widely practised;

For a standard regional scale environment it is assumed that 80% of the wastewater is treated in a biological STP and the remaining 20% released directly into surface waters.

The degree of removal in a wastewater treatment plant is determined by the physico-chemical and biological properties of the substance (biodegradation, adsorption onto sludge, sedimentation of insoluble material, volatilisation) and the operating conditions of the plant. As the type and amount of data available on degree of removal may vary, the following order of preference should be considered:

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[12] COD: chemical oxygen demand

- Measured data in full scale STP:

  The percentage removal should preferably be based upon the difference of measured influent and effluent concentrations. As with measured data from the environment, the measured data from STPs should be assessed with respect to their adequacy and representativeness.

- Simulation test data

  Simulation testing is the examination of the potential of a substance to biodegrade in a laboratory system designated to represent either the activated sludge-based aerobic treatment stage of a wastewater treatment plant or other environmental situations, for example a river.

  The most common simulation tests on biodegradability of substances are "Inherent biodegradability test" according to OECD Guideline 301 and "Ready biodegradability tests" according to OECD Guideline 302.

- Modelling STP:

  If there are no measured or simulation test data available, the degree of removal can be estimated by means of a wastewater treatment plant model. For the calculation the following substance specific input data are required:

  - octanol/water partitioning coefficient (log Kow);
  - Henry's Law constant;
  - results of biodegradation tests.

  A wastewater treatment plant model (SimpleTreat) is implanted in exposure estimation tool EUSES which is presented below.

3.2.2 Distribution and fate processes in the environment

As a second step of the environmental exposure estimation, the distribution and fate processes of the substance in the environment are considered.[13]

After the release of a chemical into the environment, various partitioning, transformation and/or degradation processes might take place resulting in that the chemical will be distributed in the various environmental compartments (air, soil, water, sediment, biota) at certain concentration levels.

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[13] From a practical point of view, distribution and fate processes are mainly important for those cases where initial exposure estimations show that the predicted environmental concentrations (PECs) exceed the predicted no-effect concentrations (PNEC) indicating that the use is not safe. Consideration of distribution and fate processes of a substance in the environment will result in lower PEC values and thus, in lower PEC/PNEC ratios.

To assess the environmental exposure, the following main distribution processes are considered:[14]

- Volatilisation of substances with high vapour pressure;

- Adsorption to soil, sediment and suspended matter;

- Bioconcentration and biomagnification in humans and animals;

- Transformation and degradation processes in the environment. Both biodegradation[15] and abiotic degradation (i.e. hydrolysis and photolysis) should be considered. If stable and/or toxic degradation products (metabolites) are formed, these should be assessed as well, at least to the extent information on the degradation products is available.

In order to assess the partitioning and degradation behaviour of a substance in the environment, the following minimum information is required: molecular weight, water solubility, vapour pressure, octanol-water partition coefficient and information on ready biodegradability for the substance. For an inorganic substance, it is also advised to provide information on the abiotic degradation, and solid-water partition coefficients and the water-biota partition coefficients.

3.2.3   Exposure estimation including derivation of PECs

Exposure of the environment is the result of the release of substances, which may partly be degraded/removed due to treatment facilities, subsequent distribution and degradation within the environment. As output from the distribution and exposure calculations predicted environmental concentrations (PECs) for the environmental compartments water/sediments, soil and air are derived. In addition, secondary poisoning of predators and intake of man via the environment is calculated based on the environmental exposure concentrations in water, air, soil.

Use of measured data

For some substances measured concentrations will be available for the environmental compartments air, fresh or saline water, sediment, biota and/or soil. These data may have been collected by environmental monitoring. They have to be carefully evaluated for their adequacy and representativeness according to the criteria below before they are used for the enrvironmental risk assessment. They are used together with calculated environmental concentrations for the exposure estimation.

The evaluation of measured data should follow a stepwise procedure:

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[14]   These processes are considered automatically by the exposure estimation tool EUSES.

[15]   Biodegradation takes place in the sewage treatment plant, in surface water, sediment and soil as well as in the marine environment.

- ▪ The reliability of the measured data should be checked by evaluation of the sampling and analytical methods employed. A quality check of the applied measuring techniques is necessary to decide whether the measured data are valid without restriction and may be used for the exposure estimation or are only valid with restrictions any thus may only be used to support the calculated exposure estimation. Chapter R.16 (Table R.16-4) lists quality criteria for the use of existing data.

- ▪ The data should be representative for the environmental compartment of concern meaning that the sampling frequency and sampling pattern should be sufficient to adequately represent the concentration at the selected site. If the measured data are results of sporadic examinations they are less representative than measurements of a substance at the same site over a certain period of time. Measured concentrations caused by an accidental spillage or malfunction should not be considered in the exposure estimation.

- ▪ Measured data should be assigned to local or regional scenarios by taking into account the sources of exposure. Samples taken at sites directly influenced by an emission should be used to describe the local scenario (PEClocal), while samples taken at larger distances from emissions may represent the regional concentrations.

Both the mean concentration and the concentration range should be presented. If only maximum concentrations are reported, they should be considered as a worst-case assumption, providing they do not correspond to an accident or spillage. However, the use of only mean concentrations can result in an underestimation of the existing risk, because temporal and/or spatial average concentrations do not reflect periods and/or locations of high exposure.

The measured data should be compared to the corresponding calculated PEC. For naturally occurring substances background concentrations have to be taken into account. For risk characterisation, a representative PEC should be decided upon based on measured data and a calculated PEC (see subsequent paragraph on "Calculated versus measured PEC values").

Calculated PEC values

PEC values for the aquatic and soil compartment as well as for the atmosphere are calculated both for the local and for the regional scale. As mentioned before, the local scale accounts for local emissions and the regional background concentration which is added to this, whereas the regional scale accounts for overall emissions into a region.

The local concentration (PEClocal) close to a point source emission is calculated as the sum of the concentration from the point source and the background concentration. The background concentration or the regional concentration (PECregional) is calculated by accounting for all releases over a wider, regional area and by accounting for the distribution

and fate of the chemical after the release to the environment. In obtaining the regional concentration, the manufacturer/importer (M/I) has to account for all releases into the environment for his supply chain. However, it can be useful on a voluntary basis to consider exposure resulting from emissions of the same substance manufactured or imported by other registrants (e.g. the overall estimated market volume).

In addition to predicted concentrations in environmental compartments, **predicted concentrations in the food for predators**, i.e. the concentration in worms and fish, may need to be calculated (PECoral, predator) in order to estimate the potential of a substance for secondary poisoning. Secondary poisoning is concerned with toxic effects in organisms in higher trophic levels of the food web, either living in the aquatic or terrestrial environment, which result from ingestion of organisms from lower trophic levels that contain accumulated substances. This exposure route is relevant when there are indications for a potential bioaccumulation:

If, at production/import volumes between 1–100 tonnes[16] per year, a substance:

- has a log Kow ≥ 3 and a molecular weight below 700 g/mol; or
- is highly adsorptive; or
- belongs to a class of substances known to have a potential to accumulate in living organisms; or
- there are indications from structural features;
- and there is no mitigating property such as of hydrolysis (half-life less than 12 hours);

then there is an indication of bioaccumulation potential.

For the assessment whether secondary poisoning is a relevant exposure route, it is further necessary to consider whether the substance has a potential to cause toxic effects if accumulated in higher organisms. This assessment is based on classifications on the basis of mammalian toxicity data, i.e. the classification Very Toxic (T+) or Toxic (T) or harmful (Xn) with at least one of the risk phrases R48 "Danger of serious damage to health by prolonged exposure", R60 "May impair fertility", R61 "May cause harm to the unborn child", R62 "Possible risk of impaired fertility", R63 "Possible risk of harm to the unborn child", R64 "May cause harm to breastfed babies". Here it is assumed that the available mammalian toxicity data can give an indication on the possible risks of the chemical to higher organisms in the environment.

If a substance is classified accordingly or if there are other indications (e.g. endocrine disruption), an assessment of secondary poisoning should be performed.

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[16] REACH Annex IX indicates that information on bioaccumulation in aquatic species is required for substances manufactured or imported in quantities of 100t/y or more.

As mentioned before, secondary poisoning describes the risk to (fish or worm eating) predators and is calculated as the ratio between the concentration in their food (PECoral-predator) and the no-effect concentration for oral intake (PNECoral). The concentration of a substance in food (fish or worm) is calculated on basis of its predicted environmental concentrations in water or soil considering the bioconcentration factors (BCF[17]) in fish or earthworms as well as the respective biomagnification factor (BMF[18]).

The **indirect exposure of humans via the environment** may also be determined in the course of the environmental exposure assessment. An indirect exposure may occur by consumption of food (e.g. fish, crops, mean or milk) and drinking water or by inhalation of air. The output of the calculation is regional and local total human doses of the substance via the environment.

An assessment of indirect exposure is generally only conducted if:

- the tonnage >1,000 t/y; or
- the tonnage >100 t/y and the substance is classified
    - as "Toxic" with a risk phrase "R48"; or
    - as a carcinogen or mutagen (of any category); or
    - as toxic to reproduction (category 1 or 2).

Calculated versus measured PEC values

When PECs have been derived from both measured data and calculations, they should be compared. If they are not of the same order of magnitude, analysis and critical discussion of divergences are important steps for developing an environmental risk assessment. The following cases can be distinguished:

- Calculated PEC ≈ PEC based on measured concentrations
  The result indicates that the most relevant sources of exposure were taken into account. For risk characterisation, the value with the highest confidence should be used;
- Calculated PEC > PEC based on measured concentrations
  This result might indicate that relevant elimination processes were not considered in the PEC calculation or that the employed model was not suitable to simulate the real environmental conditions for the regarded substance. On the other hand measured

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[17] BCF describes the bioaccumulation in aquatic species and is the ratio between the concentration in the organisms and the concentration in the surrounding water. BCF is either measured or estimated on basis of the logKow (n-octanol/water partition coefficient) using QSAR methods (see Guidance document Chapter R.7c, Section R.7.10.3.2).

[18] BMF is defined as the relative concentration in a predatory animal compared to the concentration in its prey (BMF = Cpredator/Cprey).

data may not be reliable or represent only the background concentration or PECregional in the regarded environmental compartment. If the PEC based on measured data has been derived from a sufficient number of reliable and representative samples then they should override the model predictions.

- Calculated PEC < PEC based on measured concentrations
  This relation between calculated PEC and PEC based on measured concentrations can be caused by the fact that relevant sources of emission were not taken into account when calculating the PEC, or that the used models were not suitable. Similarly, an overestimation of degradation of the compound may be the explanation. Alternative causes may be spillage, a recent change in use pattern or emission reducing measures that are not yet reflected in the samples.

If the measured values have passed the procedure of critical statistical and geographical evaluation, a high degree of confidence can be attributed to those data and they shall override the calculated PECs.

3.2.4   Risk characterisation by comparing PEC/PNEC

Quantitative risk characterisation

A quantitative risk characterisation is carried out by comparing the PEC with the PNEC[19] values deriving the so-called risk characterisation ration (RCR). This is done separately for each of the following environmental protection targets:

Inland environmental protection targets:

- aquatic ecosystem including sediment;
- terrestrial ecosystem;
- atmosphere;[20]
- micro-organisms in sewage treatment plants
- fish- and worm-eating predators (secondary poisoning).[21]

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[19] PNEC: Predicted no-effect concentration; methods for PNEC derivation from ecotoxicological tests can be found in Chapter R.10: Characterisation of dose [concentration]-response for environment.

[20] PECair cannot be compared with the PNEC for air because the latter is usually not available. However, PECair is used as input for the calculation of the intake of substances through inhalation in the indirect exposure of humans (PECair / DNELinhalation).

[21] Exposure of predators is only relevant if the substance shows indications for bioaccumulation and has a potential to cause toxic effects if accumulated in higher organisms (see paragraph "Calculated PEC values").

For specific industrial sites that release wastewater directly into the sea, an additional risk assessment for the marine environment is required. For inland industrial sites, however, discharging their wastewater to rivers, marine risk assessments are not required.

Marine environmental protection targets comprise:

- aquatic ecosystem including sediment;
- predators and top predators (secondary poisoning).

A list of the different PEC/PNEC ratios (= RCR) that should be considered for the inland and marine environments is given in Table 3-1 and Table 3-2, respectively.

Table 3-1   Overview of PEC/PNEC ratios considered for inland risk assessment[a)]

Local		Regional	
Water:	PEClocalwater / PNECwater	Water:	PECregionalwater / PNECwater
Sediment:	PEClocalsediment / PNECsediment	Sediment:	PECregionalsediment / PNECsediment
Soil:	PEClocalsoil / PNECsoil	Soil:	PECregionalagr.soil / PNECsoil
Microorganisms:	PECstp / PNECmicroorganisms	-	
Predators, fish eating:	(0.5 x PEClocal,oralfish + 0.5 x PECregional,oralfish) / PNECoral		
Predators, worm-eating:	(0.5 x PEClocal,oralworm + 0.5 x PECregional,oralworm) / PNECoral		

[a)]   *These ratios are derived for all stages of the life-cycle of a compound. The regional risk characterisation for each compartment is based on the sum of regional PNECs for all life-cycle stages. The PEC-local for each life-cycle stage and compartment is based on the sum of the local concentration and the PEC-regional (sum).*

Table 3-2   Overview of PEC/PNEC ratios considered for marine risk assessment[a)]

Local		Regional	
Water:	PEClocalseawater / PNECsaltwater	Water:	PECregionalseawater / PNECsaltwater
Sediment:	PEClocalsediment / PNECmarine sediment	Sediment:	PECregionalsediment / PNECmarine sediment
Predators:	[(PEClocalseawater,ann + PECregionalseawater) x 0.5 x BCFfish x BMF1] / PNECoralpredator		
Top predators:	[(0.1 x PEClocalseawater,ann + 0.9 x PECregionalseawater) x BCFfish x BMF1 x BMF2] / PNECoraltop predator		

[a)]   *These ratios are derived for all stages of the life-cycle of a compound. The regional risk characterisation for each compartment is based on the sum of regional RCRs for all life-cycle stages. The PEC-local is based on the sum of the local concentration and the PEC-regional (sum).*

For the air compartment usually only a qualitative assessment of abiotic effects is carried out.

As mentioned before, the indirect exposure of humans via the environment is also determined in the course of the environmental exposure assessment. The output of the calculation is regional and local total human doses of the substance via the environment. These values are to be compared with the DNEL values for external exposure.

In case control of risks cannot be demonstrated the input parameters for the environmental exposure estimation may be refined. If the necessary data are not available, further information and/or testing may be required. A decision must be taken as to whether both the PEC and PNEC will be iterated or only one of them. If additional information needs to be generated, it should be based on the principles of lowest cost and effort, highest gain of information and the avoidance of unnecessary testing on animals.

The following possibilities for refinement should be investigated:

- Get more exact knowledge on the actual number of emission days and fraction of main source by contacting the DU or the branch organisation of the DU

- Get more exact knowledge on the actual emission fractions by contact to the DU or the branch organisation of the DU

- If the water solubility in the waste water is exceeded in the initial emission estimation, then modify the emission fraction to waste water accordingly.

- If the substance has a low Henry constant (< 1 Pa·m3/mol), then consider the emission to air as of no importance.

- Consider the introduction of (additional) RMMs to lower the releases to the environment. When introducing the impact of an RMM, make sure that the RMM was not already included in the applied emission factors. Quantify the effectiveness of additional RMMs that decrease the overall emitted or released amounts.

Both, the release calculation and the exposure prediction can be further refined by measured data, e.g. waste water concentrations or monitoring data for surface water. However, the assessor should make sure that the CSR includes sufficient documentation that the operational conditions and the RMMs described in the exposure scenario match the conditions under which the measured data were obtained.

Qualitative risk characterisation

When no quantitative risk characterisation can be carried out, for example for remote marine areas or when either PEC or PNEC cannot be properly derived, a qualitative risk charac-terisation should be conducted.

An environmental hazard assessment in accordance with REACH, Annex I, and the estimation of the long-term exposure of the environment (Annex I, Section 5) cannot be

carried out with sufficient reliability for substances satisfying the PBT and vPvB criteria. This necessitates a separate PBT and vPvB assessment (Guidance document Chapter R.11). For a qualitative assessment of risks for PBT and vPvB substances, the approach should be used as described in Section R.11.2.2.

For some substances it may not be possible to undertake a full quantitative risk assessment, using a PECwater/PNECwater ratio because of the inability to calculate a PNECwater. This can occur when no effects are observed in short-term tests. However, an absence of short-term toxicity does not necessarily mean that a substance has no long-term toxicity, particularly when it has low water solubility and/or high hydrophobicity. For such substances, the concentration in water (at the solubility limit) may not be sufficient to cause short-term effects because the time to reach a steady-state between the organism and the water is longer than the test duration. This is also the case for non-polar organic substances with a high potential to bioaccumulate.

In summary it is recommended to conduct a qualitative risk assessment in order to decide if further long-term testing is required in the following cases: for substances with log Kow > 3 (or BCF > 100) and a PEClocal or PECregional > 1/100th of the water solubility.

Also in cases where the logKow is not a good indicator of bioconcentration, or where there are other indications of a potential to bioconcentrate (see ECHA Guidance Section R.7.10), a case-by-case assessment of the presumable long-term effects will be necessary.

3.2.5   Exposure estimation tools – Tier 1

Environmental exposure estimation including release estimation, PEC calculation and risk characterisation can be done with the software program EUSES or with the TGD excel sheet which has been revised by ECETOC. It is the basis for the new ECETOC TRA tool (see below).[22]

EUSES (2.1) and a manual to the program can freely be downloaded from the internet (http://ecb.jrc.it/euses). EUSES can be run on a normal PC.

For Tier 1 assessments, the information described in Appendix 4.3-1 should be collected (more information on fate may be needed for inorganic substances).

EUSES has built-in models for conservative release/emission estimation. Instead of using the standard EUSES release estimation, the newly developed ERCs (see chapter on "Environmental Exposure Categories") can be manually entered into EUSES. Alternatively, release estimation can be done separately as indicated in Chapter 3.2.1 above, and the calculated release estimates can then entered into EUSES for subsequent PEC calculations.

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[22] The TGD excel sheet has been revised by ECETOC together with Radboud University Nijmegen. The new version of ECETOC TRA is available since autumn 2009. The old TGD is not state of the art anymore.

The output of the Tier 1 exposure estimation consists of the predicted environmental concentrations (PECs) for the different environmental compartments (see Appendix 4.3-2). An example of environmental exposure calculation with EUSES is given in Appendix 4.3-2.

Environmental exposure estimations can also be made using the new version of ECETOC TRA. For access and documentation of ECETOC TRA see Appendix 4.1-2, first line of the table. The environmental exposure part of ECETOC TRA is based on the EUSES excel tool which has been described above.

Environmental exposure calculations are in ECETOC TRA part of the so-called "integrated tool" (for worker exposure and consumer exposure, stand-alone-versions are available within ECETOC TRA in addition to the integrated tool.).

The new version of the exposure assessment tool ECETOC TRA (version 2) uses the same input parameters as EUSES. It already contains the newly developed ERCs and offers the possibility to use specific environmental release categories (spERCS). ECETOC TRA provides the same output as EUSES.

The environmental tool of ECETOC TRA consists of two modules: release estimation and calculation of the predicted environmental concentration (PEC). The release estimation module starts with the environmental release categories (ERCs, see chapter chapter 9.3, Part II of the Practical Guide). It offers four different alternatives to the ERCs: specific environmental release categories, default values from the A tables and B tables of the earlier Technical Guidance Document on Risk Characterisation of existing and new substances (http://ecb.jrc.ec.europa.eu/tgd/), data from the OECD Emission Scenario Documents and measured data (site specific emission data).

Discussion of adequacy/applicability

EUSES enables the user to perform all steps of the environmental exposure assessment (including release estimation and refinement of risk management measures) as well as the subsequent risk characterisation within the same software tool. For a conservative Tier 1 assessment only few input data are actually required. For many required parameters default values are incorporated in the tool that may be overwritten if substance or process specific data are available.

However, it is not easy to work with the current user-interface of EUSES as an un-experienced user, in particular where tonnage and use information data is to be specified. The impact of information inputs on the overall results are not always transparent and easy to understand. Also, it is not possible to trace to which extent risk management measures are already assumed in the default emission factors. Thus iteration may lead for example to a duplication of RMMs already included in the default emission factor.

These limitations are the reasons for introducing the Environmental Release Categories (ERCs). The ERCs can be entered manually in EUSES. To introduce RMMs and changes in the conditions of use, the presets for the ERCs can be replaced with own estimates, information from downstream users, expert judgements or measured data.

The correlations used for the derivation of substance parameters, i.e. mainly partition data, are not valid for inorganics and surfactants. Whenever measured partition and degradation data are available, these should be used in the calculations. This is of very high importance for metals, inorganic compounds and surfactants.

With regard to the default values used in EUSES it needs to stressed that these should critically be checked on their suitability to represent the actual situation of the M/I and/or DU. If reliable and representative substance or process or site-specific data are available these should be used to replace the given default values. For example, the discharge volume of a sewage treatment plant (i.e. the outflow from a standard STP) is standardised in EUSES to a volume of 2,000 m³/day. The effluent of the sewage treatment plant is discharged into surface water (e.g. a river). By mixing processes the effluent is diluted in the surface water assuming a default dilution factor of 10, i.e. the 2,000 m³/day are discharged in a river with a flow rate of 18,000 m³/day resulting in a total surface water volume of 20,000 m³/day. Experiences from the textile industry showed, however, that in reality the receiving water bodies vary significantly, thus influencing the resulting PEC value significantly. In these cases, site specific data should be used for the environmental exposure assessment.

In order to enable to relate to the calculation, all parameters and default values used for the environmental exposure calculations must be documented. EUSES can prepare an electronic report of all the input and output data in a Word or Excel format automatically.

CHESAR, the ECHA IT tool for preparation of chemical safety assessments and chemical safety reports, will contain a tool for the environmental exposure estimation. It consists of a specific release module and the EUSES fate model. The defaults in the release module come from the earlier Technical Guidance Documents on risk assessment of existing and new substances (http://ecb.jrc.ec.europa.eu/tgd/) (for a description of CHESAR see Part I of this practical guide, chapter 3.5).

3.2.6   Use of exposure estimation tools – higher tier

EUSES and TGD excel sheet calculations may be improved by refining some of the input data.

Both, the release calculation and the exposure prediction can be further refined by measured data, e.g. waste water concentrations or monitoring data for surface water. However, the assessor should make sure that the chemicals safety report includes sufficient documentation that the operational conditions and the RMMs described in the exposure scenario match the conditions under which the measured data were obtained.

Furthermore, at a higher tier in the risk assessment process more specific information on the biodegradation behaviour of a chemical may be available that can be used to refine the assumptions for the STP. Similar to EUSES; also in the environmental exposure part of ECETOC TRA version 2 higher tier calculations can be made by using additional and more specific input data.

3.2.7   Other tools for environmental exposure estimation

Other tools for environmental exposure estimation may be used for substances which are applied in a way similar to a pesticide, for example as a fertilizer, or for substances which are applied in offshore installations. For these substances, models recommended by FOCUS[23] or the CHARM model,[24] respectively, can be an alternative to EUSES/TGD excel sheet.

3.3   Scaling related to environmental exposure

A downstream user (DU) who receives the exposure scenario (ES) from his supplier needs to check if his use is in compliance with the received ES. If several of his conditions of use differ from the ES it is not always apparent whether or not his use is covered by the ES. In order to allow this compliance check the supplier of the ES should communicate scaling rules or assessment instruments to enable the DU to assess the coverage of his use by scaling[25] the determinants of exposure. Scaling and related tools are described in Part I of the practical guide, chapter 7.7.

In the following example the scaling procedure related to environmental exposure is illustrated:

A manufacturer/registrant calculates the predicted environmental concentration of his substances in surface water for the following operational conditions (OC) and risk management measures using the subsequent equation:

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[23] FOCUS: Forum for the Co-ordination of pesticide fate models and their USe (http://viso.jrc.it/focus/)

[24] https://www.ogp.org.uk/pubs/CHARMManualFeb05.pdf

[25] Scaling in this context means the use of simple equations in the ES by which the DU can demonstrate that he operates within the conditions of the ES provided by the registrant.

Quantity of product, in which the substance of concern is processed or used per year and site	M_{ES}	1000 kg/day
Concentration or fraction of the substance in the product	C_{ES}	0,1
Emission factor: the fraction of the substance emitted from the process or use to wastewater (before abatement)	f_{water}	0,3
Efficiency of an abatement or control technology that reduces the emission to air, surface water or land	$f_{abatement}$	0,95
Removal of the substance in the STP	F_{STP}	0,95
Duration of emission (e.g. working days per year)	$T_{emission}$	200 days/year
Water treated in the sewage treatment plant	CAPACITY	2,000 m^3/day
Dilution factor in the receiving water body	DILUTION	10

$$\text{PEC}_{local} = \text{PEC}_{regional} + \frac{\dfrac{M_{ES} * C_{ES} * f_{water} * (1 - f_{abatement})}{T_{emission}} * (1 - F_{STP})}{CAPACITY * DILUTION}$$ (see also Example R.16.2)

The registrant calculates a risk characterisation ratio[26] (RCR_{ES}) for surface water for his use situation at 0.3, i.e. below 1, and concludes that the use is safe.

From the above given relevant determinants (i.e. OC and RMM) the registrant considers the following determinants likely to vary in other similar uses of DUs:

M_{ES}, C_{ES}, f_{water}, $f_{abatement}$, and $T_{emission}$

All of the above determinants are considered to be mutually independent.

As all determinants are linear with respect to exposure level, the following **equation for scaling** is proposed by the registrant to be used by DUs:

$$RCR_{DU} = RCR_{ES} * \frac{M_{DU}}{M_{ES}} * \frac{C_{DU}}{C_{ES}} * \frac{f_{water,DU}}{f_{water,ES}} * \frac{(1 - f_{abatement,DU})}{(1 - f_{abatement,ES})} * \frac{T_{emission,ES}}{T_{emission,DU}}$$

The DU uses the same substance but with different OCs/RMMs for his use:

M_{DU}: 750kg/day

C_{DU}: 0,1

$f_{water, DU}$: 0,35

$f_{abatement, DU}$: 0,98

$T_{emission, DU}$: 150 days/year

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[26] Risk characterisation ration (RCR) = PEC/PNEC

Using the equation for scaling given above, the DU checks whether he is in compliance with the received ES and whether his use is safe with regard to environmental exposure:

$$RCR_{DU} = RCR_{ES} * \frac{750}{1000} * \frac{0,1}{0,1} * \frac{0,35}{0,3} * \frac{(1-0,98)}{(1-0,95)} * \frac{200}{150} = 0,3 * 0,75 * 1 * 1,17 * 0,4 * 1,3 = \mathbf{0,14}$$

The calculated RCR for the use of the DU is < 1. Hence, scaling showed that the specific conditions of use of the DU are considered safe.

3.4   References

EUSES European Union System for the Evaluation of Substances; Version 2.1 (2008);
http://ecb.jrc.ec.europa.eu/euses/

EU TGD 2003 Risk Assessment Spreadsheet Model;
http://www.envsci.science.ru.nl/cem-nl/products.html

OECD Chemicals Testing – Guidelines;
http://www.oecd.org/department/0,3355,en_2649_34377_1_1_1_1_1,00.html

US EPA OPPT Generic Scenarios;
http://www.epa.gov/oppt/exposure

4   Appendices

4.1   Appendix to Chapter 1: Occupational exposure estimation

Appendix 4.1-1   Examples of publicly available sources for measurement data

Sources	Data quality*	Comments
EU Risk Assessment Reports http://ecb.jrc.it/esis/	High	Limited number of substances
BGAA-Report 1/99e: Existing commercial chemicals – Exposure at the workplace http://www.hvbg.de/d/bia/pub/rep/rep01/pdf_datei/bgar0199/gesamt.pdf	High	Limited number of substances
Environmental Health Criteria http://www.inchem.org/pages/ehc.html	Low	Limited number of substances
SIDS – "Screening Information Data Sets" AND/OR SIDS Initial Assessment Reports (SIAR) http://www.chem.unep.ch/irptc/sids/oecdsids/indexcasnumb.htm	Low	Limited number of substances
CICAD – "Concise International Chemical Assessment Documents" http://www.inchem.org/pages/cicads.html	Low	Limited number of substances

Data quality:

High: Data are likely to satisfy most of the criteria for exposure estimation and might be sufficient to be used on their own.

Low: Data are likely to satisfy some of the criteria for exposure estimation but are probably insufficient to be used on their own.

Appendix 4.1-2   Overview of tier 1 and higher tier estimation tools

Tier	Tool	Route of exposure	Resources	Status
1	ECETOC TRA	Inhalation and dermal exposure: quantitative estimates (single point values)	Internet: http://www.ecetoc.org/tra (registration required), tool (MS Excel® spreadsheet) and user guide. Print: ECETOC 2004, ECETOC 2009TR	New version published August 2009
	EMKG	Inhalation exposure only Banding approach	MS Excel® spreadsheet available at: http://www.reachhelpdesk.de/en/Exposure/Exposure.html?__nnn=true. Print: Packroff et al. 2006 (for EMKG in general, doesn't address the more recent MS Excel® spreadsheet)	Unknown

Tier	Tool	Route of exposure	Resources	Status
Higher	**RISKOF-DERM calculat or**	Dermal exposure only: quantitative estimates (median and percentiles)	Calculator (MS Excel® spreadsheet) available at: http://www.tno.nl/content.cfm?&context=markten&content=product&laag1=177&laag2=333&item_id=1155&Taal=2. A guidance document can be downloaded from the same website. Print: e.g. Marquart et al. 2006; Warren et al. 2006	Version 2.1
	Stoffen-manager	Quantitative estima-tes currently only for inhalation exposure	Internet: https://www.stoffenmanager.nl/ (registration required). Report and REACH-related output currently in Dutch only. Brief online guide at: https://www.stoffenmanager.nl/Public/Explanation.aspx. Print: Marquart et al. 2008; Tielemans et al. 2008	Version 3.5 (June 2006)4.0 now available

For the occupational exposure assessment of metals and inorganic substances the MEASE tool was developed (online available at: http://www.ebrc.de/ebrc/ebrc-mease.php), based on the exposure estimation model EASE (see http://www.hse.gov.uk/research/rrhtm/rr136.htm) and some measured data (see also chapter 1.2.5).

Appendix 4.1-3   Input information needed for tier 1 tools: occupational exposure estimation

Parameter	Required in		Available from
	ECETOC TRA	**EMKG**	
Physical state: substance	☑		Substance-specific data
Physical state: product			Product-specific data
Operating temperature (liquids)	☑[5]	☑[5]	ES-specific
Vapour pressure (liquids)	☑	☑	Substance-specific data
Boiling point (liquids)		☑	Substance-specific data
Dustiness (solids)	☑	☑	SDS/Substance-/product-specific data and Tables R.14-2 and R.14-8 in ECHA CSA 2008 (Chapter R.14)
Duration of activity	☑[1]	☑[1]	ES-specific but only very basic data required
Amount of substance/product used		☑[2]	ES-specific but only very basic data required
Information on use	☑[3]	☑[3]	ES-specific but only very basic data required
Information on RMM	☑[4]	☑[4]	ES-specific but only very basic data required
Reference values (e.g. DNELs)	optional		

Notes:

Substance-specific data should usually be available within the framework of the registration process, i.e. these data are also required for the IUCLID5 datasets.

Product-specific data should usually be available

1   *Four duration "bands"in ECETOC TRA and consideration of short-term exposure only (activity < 15 min. during a full 8 h shift? (yes/no)) in EMKG*

2   *Only information of the scale is required: small, medium or large and for liquids if more than 1 L/shift is applied to surfaces.*

3   *Only information on application on surfaces > 1m^2 (yes/no) is required in EMKG, while more information is required in ECETOC TRA (indoor/outdoor use, use in mixtures with concentration, industrial vs. professional activity).*

4   *LEV (yes/no) and respiratory protection (no, 90% protection or 95% protection) in ECETOC TRA, three different options in EMKG: general ventilation, engineering controls (e.g. LEV) or containment in EMKG.*

5   *The operating temperature needs to be known since volatility has to be assessed at the operating temperature.*

Appendix 4.1-4   Input information needed for higher tier tools: occupational exposure estimation

Parameter	Required in		Available from
	Stoffen-manager	RISKOFDERM calculator[1]	
Substance information			
CAS number	☑		Substance-specific data
Physical state			
Vapour pressure	☑		Substance-specific data
Molecular weight	☑		Substance-specific data
Percentage in product	☑		SDS
Product information			
Physical state	☑		SDS
Vapour pressure (liquids)	☑		SDS
Dustiness (solids)	☑		SDS/Substance-/product-specific data and Tables R.14-2 and R.14-8 in ECHA CSA 2008 (Chapter R.14)
Viscosity		☑	Product-specific data
Dilution with water	☑		ES
Contamination of objects with product	☑		ES
R and S phrases	☑		SDS
Application rate [L/min]		☑	Product-specific data, may also depend on the ES
Other information			
Level of containment	☑		ES
Information on ventilation	☑		ES
Information on control measures	☑		ES
Duration of activity/task	☑		ES
Frequency of activity/task	☑		ES
Information on use/task	☑		ES
Distance worker-source	☑		ES
Further detailed information	☑		ES
Body parts exposed	☑		ES
Room volume	☑		ES
Direction of application		☑	ES
Length of handle of the tool		☑	ES

Notes:

Substance-specific data should usually be available within the framework of the registration process, i.e. these data are also required for the IUCLID5 datasets.

Product-specific data should usually be available.

ES: information on these parameters may be available in the exposure scenario.

[1]   *For the process "Dispersion hand-held tools" (DEO unit 3) as an example (requirements for other processes differ)*

4.2   Appendix to Chapter 2: Consumer exposure estimation

4.2.1   Default values

Body weight

The body weight can be assumed to be 70 kg for adult males and 60 kg for adult females (see also Appendix R.15-4 ("Data references") of ECHA CSA 2008). Bremmer et al. (2006) derive slightly different values of 74 kg for males and 61 kg for females with 65 kg taken as the default value for adults in general in the ConsExpo software (see Chapter 2.2.3 for details). ConsExpo uses a default body weight for children of 8.69 kg (age 10.5 months) in a specific post-application scenario of pest-control products. Default body weight values for children of different age groups are given in Bremmer et al. (2006).

Skin surface area

Appendix R.15-4 ("Data references") of ECHA CSA 2008 contains detailed data for the skin surface area of men and women. The following table summarises the values for some body parts and the total skin surface area (mean of values for men and women). Values for other body parts, total skin surface area data for children or sex-specific values can be taken from Appendix R.15-4 of ECHA CSA 2008. If more detailed information is needed, e.g. data for specific body parts of children, the references cited in Appendix R.15-4 of ECHA CSA 2008 provide a good starting point.

Appendix 4.2-1   Skin surface areas for adults (Source: ECHA CSA 2008 R15-4)

Body part	Skin surface area (in cm^2) for adults
Arms	2 132
Forearms	1 337
Hands (fronts and backs)	786
Total	**18 150**

Room volume

Appendix R.15-4 ("Data references") of ECHA CSA 2008 provides data on the volume of different room types in the Netherlands (25th percentiles) with some additional data for Germany (not worst-case).

Appendix 4.2-2   Default values for various room volumes (Source: ECHA CSA 2008 R15-4)

Room type	Room volume (in m^3)
Living room	58 (64 in German data)
Unspecified room	30 and 40 (43 for children's rooms in German data)
Sleeping room	16
Kitchen	15
Toilet	2.5
Bathroom	10*

A value of 4 ^{3} is given in Appendix R.15-4 ("Data references") of ECHA CSA 2008. The most recent version of the source (the ConsExpo "General Fact Sheet"; Bremmer et al. 2006) contains the value used here, which is also considered more meaningful.

If more detailed information is needed, the report by Bremmer et al. (2006) provides a good starting point with some additional values.

4.3   Appendix to Chapter 3: Environmental exposure estimation

Appendix 4.3-1   Information requirements for Tier 1 assessment of environmental distribution

Parameter	Description	Source
MOLW	Molecular weight	Technical dossier – Chapter 2
MP	Melting point of substance	Technical dossier – Chapter 7
BP	Boiling point of substance	Technical dossier – Chapter 7
VP	Vapour pressure of substance	Technical dossier – Chapter 7
SOL	Water solubility of substance	Technical dossier – Chapter 7
KOW	Octanol water partition coefficient of substance	Technical dossier – Chapter 7 (not inorganics)
Kpsoil	Soil-water partition coefficient. As a default, EUSES calculates the parameter on the basis of KOW. For inorganic substances however, Kpsoil should be measured directly, because other sorption mechanisms, like sorption to mineral surfaces play in important role.	Technical dossier –adsorption-desorption screening – Chapter 9 See also Section R.16.4.3.3
Kpsed	Sediment-water partition coefficient. As a default, EUSES calculates the parameter on the basis of KOW. For inorganic substances however, Kpsed should be measured directly, because other sorption mechanisms, like sorption to mineral surfaces play in important role.	Technical dossier – adsorption-desorption screening – Chapter 9 See also Section R.16.4.3.3

Kpsusp	Solids-water partition coefficient in suspended matter. As a default, EUSES calculates the parameter on the basis of KOW. For inorganic substances however, Kpsusp should be measured directly, because other sorption mechanisms, like sorption to mineral surfaces play in important role.	Technical dossier – adsorption-desorption screening – Chapter 9 See also Section R.16.4.3.3
Biode-gradability	Results of screening test on biodegradability. Not relevant for inorganic substances.	Technical dossier – Chapter 9 See also Section R.16.4.4.4, R.16.4.4.5, R.16.4.4.7
Ej,local	Local emission to compartment j (j: water, air, soil). May be based on fraction of main source (Fmainsource) and number of emission days (Temission), M/I_volume, and release fractions	Release estimation based on use scenario See Section R.16.2
Eij,regional	Regional emission from source i to compartment j (j: water, air, soil)}	Release estimation based on exposure scenario See Section R.16.2
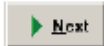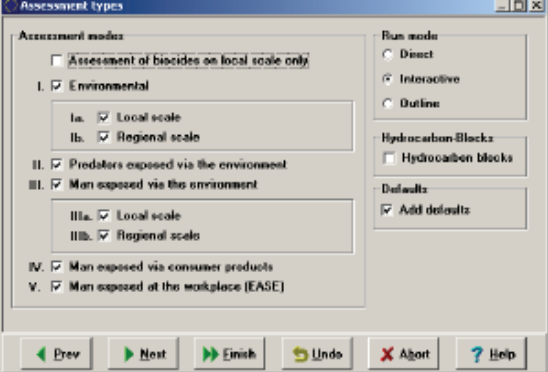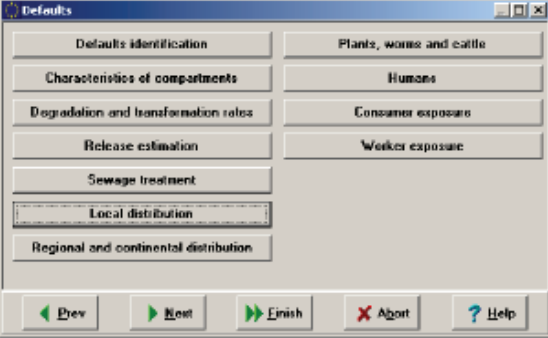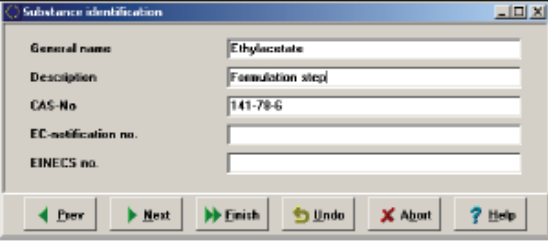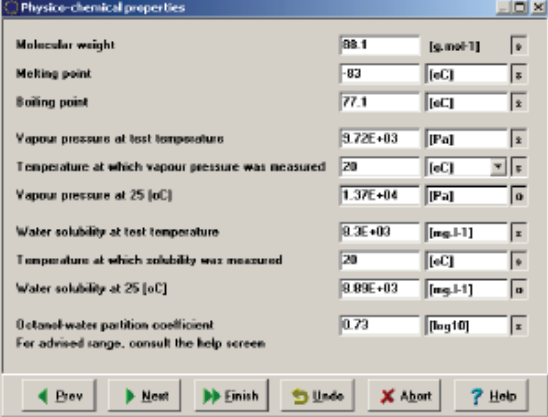
Appendix 4.3-2   Output EUSES: Predicted environmental concentrations (PECs)
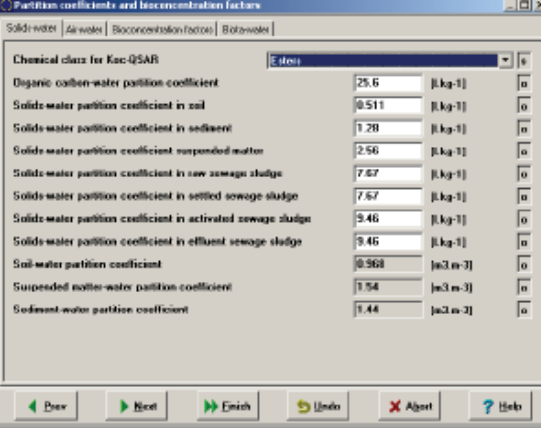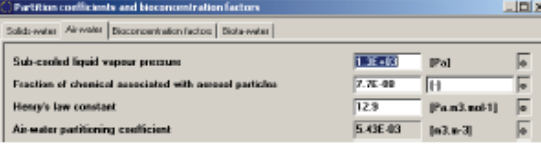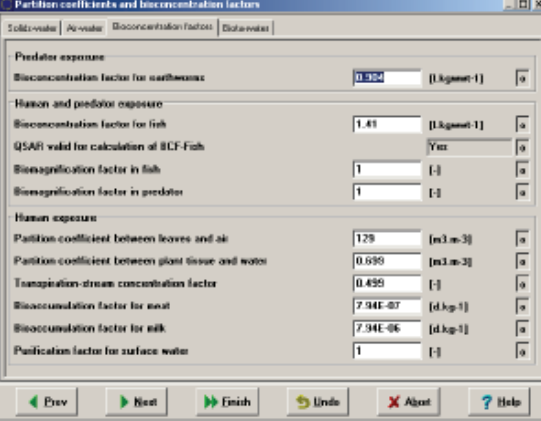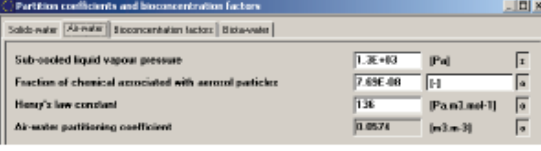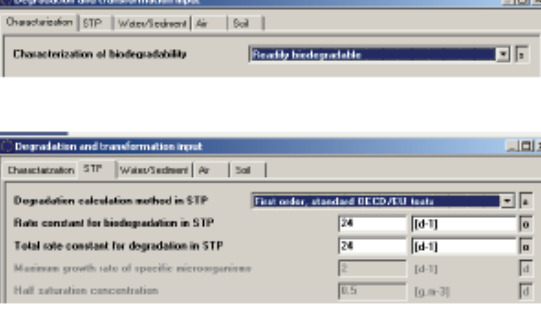
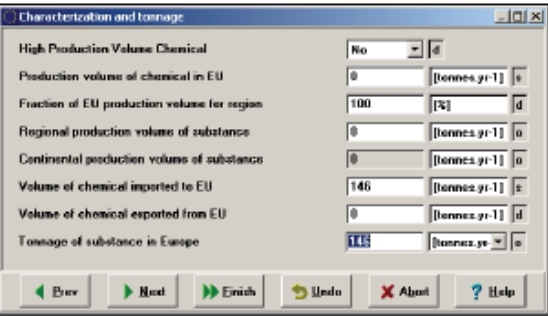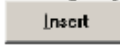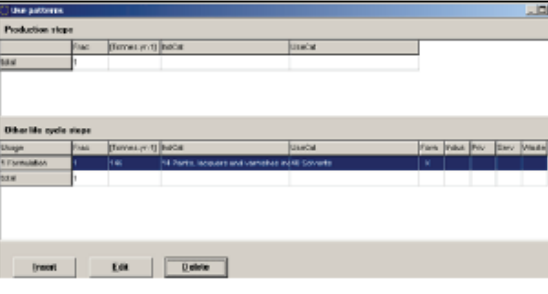| PEC	Parameter	Destination
PECstp	Concentration in the aeration tank of the sewage treatment plant	Assessment of whether the substance may inhibit processes in the STP
PEClocal.air,ann	Annual average local PEC in air (total)	–
PEClocal.water	PEC in surface water during episode	Risk assessment fresh water
PEClocal.water,ann	Annual average local PEC (dissolved)	Secondary poisoning
PEClocal.water,marine	PEC in marine water during episode	Risk assessment marine water
PEClocal.water,ann, marine	Annual average local PEC in marine surface water (dissolved)	Secondary poisoning
PEClocal.sed	PEC in sediment	Risk assessment fresh water Secondary poisoning
PEClocal.sed,marine	PEC in marine sediment	Risk assessment marine water
PEClocal.agric,30	Local PEC in agricultural soil (total) averaged over 30 days	Risk assessment terrestrial environment
PEClocal.agric,180	Local PEC in agricultural soil (total) averaged over 180 days (to calculate concentration in crops)	Secondary poisoning Indirect exposure of humans
PEClocal.grass,180	Local PEC in grassland (total) averaged over 180 days	Secondary poisoning Indirect exposure of humans
PECreg.water,tot	Regional PEC in surface water (total)	Risk assessment fresh water Secondary poisoning Indirect exposure of humans
PECreg.seawater,tot	Regional PEC in seawater (total)	Risk assessment marine water Secondary poisoning Indirect exposure of humans
PECreg.air	Regional PEC in air (total)	–
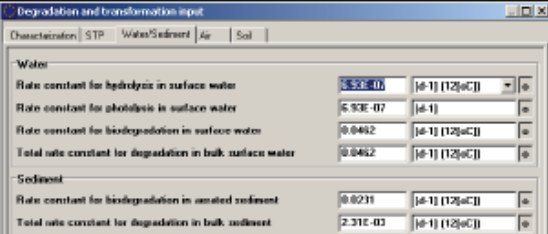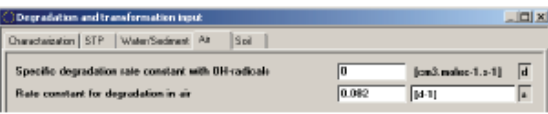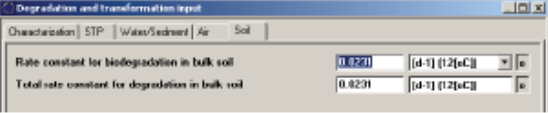
PECreg.agric	Regional PEC in agricultural soil (total)	Risk assessment terrestrial environment Secondary poisoning Indirect exposure to man
PECreg.natural	Regional PEC in natural soil (total)	Risk assessment terrestrial environment Secondary poisoning
PECreg.ind	Regional PEC in industrial soil (total)	–
PECreg.sed	Regional PEC in sediment (total)	Risk assessment fresh water
PECreg.seased	Regional PEC in seawater sedim. (total)	Risk assessment marine water

Appendix 4.3-3   Example of an environmental exposure calculation with EUSES (taken from RIP 3.2.2 REFER-
ENCE TGD – PART D)
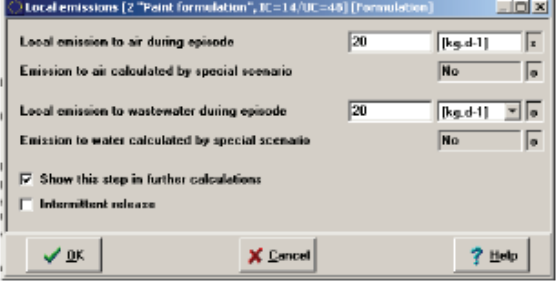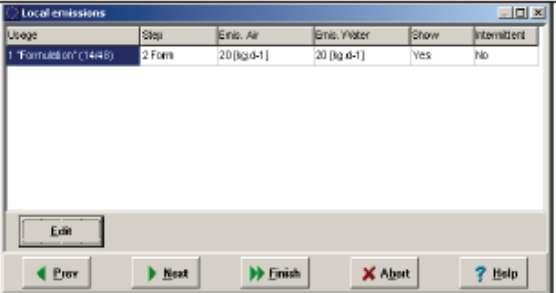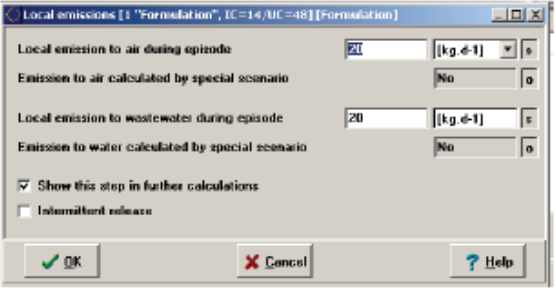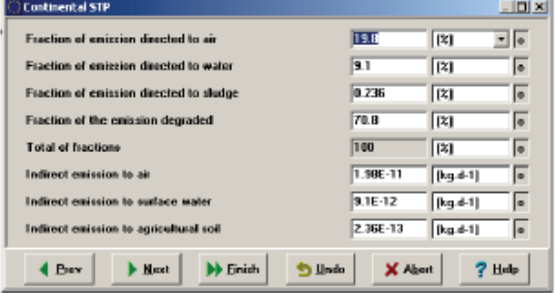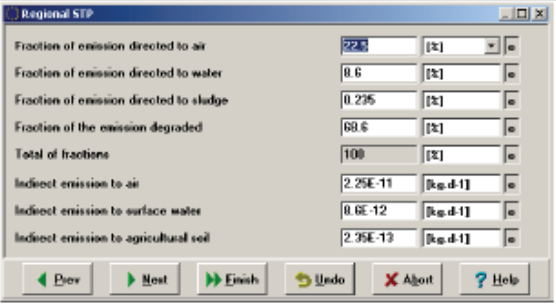
Tier 1 assessment

A paint formulator produces a decorative paint. Ethylacetate is present in the paint at a concentration of 5%. The formulator has obtained the following information via the eSDS for etahylacetate, which was obtained from the supplier:

Molar mass	g/mol	88.1
LogKow	-	0.73
Vapour Pressure at 20oC	Pa	9720
Water solubility at 20oC	mg/L	8300
Biodegradability	-	Readily biodegradable
Melting point	K	-83
Boiling point	K	77.1
Half-life in air	d	8.45
PNEC water	µg/L	96.5
PNEC air	mg/m^3	Not determined
PNEC sediment	mg/kg ww	0.1
PNEC soil	mg/kg ww	0.05
PEC regional, supply chain	µg/L	<<0.1

The paint formulator knows that at maximum 5% of the raw material ends in wastewater, which is discharged to a municipal STP. It is estimated that 5% of the consumption is released to the air on the basis of VOC emissions.

The formulator uses approx. 400 kg/d of ethylacetate, or 80 approx. tonnes/yr as the production runs 200 days per year.

In order to assess if the use of ethylacetate is environmentally safe the formulator performs an EUSES calculation.

The formulater opens the EUSES and from the **select** button and defines the type of assessment: – Interactive mode – Environmental, local and regional scale – Predators exposed via the environment, local and regional scale – Man exposed via the environment, local and regional scale The formulator presses the **Next**-button to proceed	Assessment types screen showing Assessment modes: Assessment of biocides on local scale only; I. Environmental (Ia. Local scale, Ib. Regional scale); II. Predators exposed via the environment; III. Man exposed via the environment (IIIa. Local scale, IIIb. Regional scale); IV. Man exposed via consumer products; V. Man exposed at the workplace (EASE). Run mode: Direct, Interactive, Outline. Hydrocarbon-Blocks: Hydrocarbon blocks. Defaults: Add defaults. Buttons: Prev, Next, Finish, Undo, Abort, Help
Via this screen it possible to see and change some of the defaults used in the calculations factors, e.g. the dilution factors (local distribution)	Defaults screen with buttons: Defaults identification; Plants, worms and cattle; Characteristics of compartments; Humans; Degradation and transformation rates; Consumer exposure; Release estimation; Worker exposure; Sewage treatment; Local distribution; Regional and continental distribution. Buttons: Prev, Next, Finish, Abort, Help
The formulator fills in the general information for the substance	Substance identification screen: General name: Ethylacetate; Description: Formulation step; CAS-No: 141-78-6; EC-notification no.; EINECS no. Buttons: Prev, Next, Finish, Undo, Abort, Help
.. and the information obtained from the eSDS To proceed the formulator presses the **Next** button	Physico-chemical properties screen: Molecular weight 88.1 [g.mol-1]; Melting point -83 [oC]; Boiling point 77.1 [oC]; Vapour pressure at test temperature 9.72E+03 [Pa]; Temperature at which vapour pressure was measured 20 [oC]; Vapour pressure at 25 [oC] 1.37E+04 [Pa]; Water solubility at test temperature 8.3E+03 [mg.l-1]; Temperature at which solubility was measured 20 [oC]; Water solubility at 25 [oC] 8.89E+03 [mg.l-1]; Octanol-water partition coefficient 0.73 [log10]. For advised range, consult the help screen. Buttons: Prev, Next, Finish, Undo, Abort, Help

"Esters" is selected as the chemical class for calculation of Koc (organic carbon water partition coefficient). The remaining partition coefficients are calculated from the Koc.

If actual values are available, these can be entered directly into the relevant fields.

The Henry's law constant is calculated from the vapour pressure and water solubility.

If actual values are available, these can be entered directly into the relevant fields.

The bioconcentration factors are calculated from log Kow.

To proceed the formulator presses the **Next** button

The information on degradation is filled in:

Characterisation of biodegradability (readily biodegradable)

For the STP part the default values are used (estimated on the basis of that the substance is readily biodegradable)

For the water/sediment part default values are also applied (estimated on the basis of that the substance is readily biodegradable)	
The formulator fills in the degradation rate in air (=ln(2)/halflife in air = 0.082 d^{-1}	
For the soil part default biodegradation values are applied (estimated on the basis of that the substance is readily biodegradable) To proceed the formulator presses the ▶ Next button	
The next screen is an update of the removal rates from soil. These are estimated from biodegradation rate in soil, soil-water partition coefficient.	
The formulator has been informed that the regional concentrations for the supply chain are negligible (PEC regional <<0.1ug/L). The formulator specifies an import valume corresponding to the company's own usage. The formulator presses the ▶ Next button to proceed.	
For the specification of the company's own use the formulator presses the Insert button By use of the Edit -button the formulator specifies the use of ethylacetate in paint. The formulator ticks the Formulation life cycle stage.	

Via the next screen the formulator specifies the emission data: 5% to air and 5% to wastewater. As the formulator has only entered his own tonnage (146 tonnes/yr), the fraction of main source is 1. The number of emission days is 200 days/yr.	
In order eliminate the background concentration, the formulator sets all regional and continental releases to 0 kg/d.	
.. and also the total regional and continental releases to 0 kg/d	

The formulator then enters the actual emission rate (200 kg/d) and the emission fractions to air and wastewater (both 5% = 20 kg/d)	
The emission rates (20 kg/d) are specified in the window – <u>E</u>dit	
Intermittent results are shown	
Intermittent results are shown	

Intermittent results are shown	
A possibility to specify actual site-specific dilution factor exist under "Configuration"	
Intermittent results	
Intermittent results	

Fresh water

The concentration in water is estimated at 0.0841 mg/L. The Risk Characterisation Ratio (RCR) for surface water is then 0.0841/0.0965 = 0.9, i.e. below 1.

Sediment

The concentration in sediment = 0.113 mg/kg ww.

The Risk Characterisation Ratio (RCR) for sediment is then 0.113/0.1 = 1.

Soil

The concentration in soil (30 d. average) = 0.0175 mg/kg ww.

The Risk Characterisation Ratio (RCR) for soil is then 0.0175/0.05 = 0.4, i.e. below 1.

Even though the RCR for sediment is very close to 1, safe use is demonstrated. DISKUSSION – RCR >1