ECETOC TRA version 3: Background and Rationale for the Improvements

Technical Report No. 114

EUROPEAN CENTRE FOR ECOTOXICOLOGY AND TOXICOLOGY OF CHEMICALS

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ECETOC TRA version 3: Background and Rationale for the Improvements

CONTENTS

SUMMARY

The ECETOC Targeted Risk Assessment (TRA) tool was launched in 2004. The TRA consists of 3 separate models for estimating exposures to workers, consumers and the environment that arise during a series of events ('exposure scenarios'). In order to ensure that the TRA fully aligned with the expectations contained in Chapters R12-R16 of the Technical Guidance on Information Requirements and Chemicals Safety Assessment (IRCSA), ECETOC released version 2 of the TRA in 2009. The general success of the TRA concept is witnessed by the fact that, by the end of 2011, over 10,000 downloads of TRAv2 were made from its website.

Following the completion of Phase 1 of REACH in December 2010, ECETOC approached users of the TRA to seek their ideas for how the TRA might be further improved. The aim of this exercise was to ensure that key learnings arising from the use of the TRA in 2009/10 could be captured into an updated version that would be available for use in Phase 2 of REACH. The intention was not to radically overhaul the TRA, rather to further improve its accuracy and flexibility, within its existing framework. Version 3 of the TRA incorporates a number of enhancements in each of the worker, consumer and environmental sections of the tool. The improvements are intended to increase the overall accuracy and utility of the tool, while still ensuring that the information and skill requirements necessary to develop the associated exposure predictions remain compatible with Tier 1 expectations. The rationales for these enhancements are detailed in this report.

It should be noted that the ECETOC TRA is also the basis for the worker and consumer exposure estimates used within the European Chemicals Agency's (ECHA) CHESAR (Chemical Safety Assessment and Reporting tool). In 2010, ECHA also announced its intention to significantly upgrade CHESAR. ECETOC has therefore worked concurrently with ECHA to ensure that the TRAv3 also incorporates ECHA's experiences resulting from the Phase 1 REACH registrations, as well as ensure full alignment between the TRAv3 and CHESAR v2 (planned for release in summer 2012).

Version 3 of the TRA is available in two forms: as an integrated exposure / risk assessment tool covering worker, consumer and environmental exposures; and as a standalone consumer exposure estimation tool.

1. GENERAL

1.1 Background to the TRAv3 activity

ECETOC first proposed its ideas for an integrated framework for evaluating the health and environmental risks of chemicals in 2003. Essentially, the approach advocated a basis by which chemical product risk assessment could be progressed by manufacturers and suppliers through a tiered and targeted approach. The intention was to quickly differentiate exposure situations that do not constitute a risk from those where more sophisticated approaches to risk assessment ('higher tier') are warranted. The key ideas contained in the ECETOC targeted risk assessment (TRA) approach were subsequently established in a web-based tool derived from Technical Report No. 93 (ECETOC, 2004).

The first version of the TRA was extensively reviewed as part of the REACH Implementation Project (RIP) 3.2 activity through which the Technical Guidance Documents (TGD) for Chemical Safety Assessment (CSA) under REACH (EC, 2006) were developed. These discussions also confirmed the utility of the TRA as an effective Tier 1 tool for application when evaluating both worker and consumer exposures. In parallel with the REACH activities, ECETOC continued to promote and test the value of key TRA concepts at scientific symposia and workshops.

In order to ensure that the TRA could be seen to fully align with the expectations contained in Chapters R12-R16 of the Technical Guidance on Information Requirements and Chemicals Safety Assessment (ECHA, 2010a,b,c,d), ECETOC released version 2 of the TRA in 2009.

Following the completion of Phase 1 of REACH in December 2010, ECETOC approached users of the TRA to seek their ideas for how the TRA might be further improved with the aim of ensuring that key learnings arising from the use of the TRA in 2009/10 could be captured into an updated version that would be available for use in Phase 2 of REACH. The intention was not to radically overhaul the TRA, rather to further improve its accuracy and flexibility, within its existing framework which has found widespread support across users. ECETOC also held discussions with ECHA, as the worker portion of the TRAv2 is already used as the basis for CHESAR v1 and any change to the TRA also needed to account for ECHA's experiences concerning the use of the TRAv2 (both in CHESAR and in 2010 substance CSAs).

This report details the basis for the version 3 of the TRA.

1.2 Status of the TRA under REACH

The value of the TRAv2 is explicitly recognised in Chapters R14 and R15 of the Technical Guidance on Information Requirements and Chemicals Safety Assessment (ECHA, 2010b,c) as a

preferred Tier 1 for use in the evaluation of worker and consumer health risks. Chapter R16 refers to EUSES as the preferred tool for evaluating environmental releases. However, recognising the value of the release module that was developed as part of TRAv2, ECHA incorporated it into the ECHA CHESAR CSA/ES tool.

Furthermore, Technical Report No. 107 (ECETOC, 2009) described the process by which the utility and accuracy of the TRA could be developed should users have access to specific information on exposure determinants. Appendix H described how Specific Environmental Release Classes (SpERCs) could be developed by downstream users to provide more realistic estimates of environmental release. This directly resulted in the initiation of the Cefic SpERC activity that has resulted in the creation of a library of over 150 SpERCs [http://www.cefic.org/Industry-support/Implementing-reach/Libraries/].

Similarly, Appendix F described how further refinements could be made to the consumer portion of the TRA. Subsequent to the release of v2, the European solvents industry group (ESIG) applied these suggestions into an Excel-based tool (ESIG GES Risk and Exposure Tool (EGRET): [http://www.esig.org/en/regulatory-information/reach/ges-library/consumer-gess] addressing consumer uses involving solvents i.e. introduced refined default values for those product categories relevant to solvents but using as the start point the default assumptions and algorithms (equations) described in the Technical Report No. 107 (ECETOC, 2009).

The TRA is now widely used as witnessed by more than 10,000 downloads by the end of 2011, and it has been used in many 2010 substance registration dossiers.

1.3 Main differences between version 2 and version 3

The new version of the TRA does not significantly differ from version 2. The primary reasons for this are twofold:

1. The overwhelming feedback from TRA users was to retain the existing structure and functionality, as the tool was considered easy-to-use and delivered reasonable inter-user consistency. Users found a standalone (albeit locked) model to be preferred due to a variety of reasons, not least the security it offered for confidential business information. They also considered the ability to readily iterate different exposure control options to be critical in adopting an efficient CSA process that ensures that the exposure scenario (ES) is described in a manner that is understandable and relevant for downstream users.
2. The European Chemical Agency (ECHA) developed a CSA/CSR tool (CHESAR) that incorporated the worker and consumer TRA exposure estimation models, as well as many of the features of the original (v2) TRA. The utility of the TRA as a sufficiently conservative

and simple-to-use 'exposure engine' within CHESAR has been verified. If, however, CHESAR is to retain the TRA at its core, then no profound changes to the structure of the TRA can be made without a consequential major re-programming of CHESAR.

The consequence of this is that version 3 of the TRA focuses on organic improvements to the basis of the exposure assessments for workers, consumers and the environment. However, the TRA continues to maintain its key features of usability across all groups; integrity and transparency of the supporting science; and provision of output reports that are capable of incorporation in the process for exposure scenario development throughout the Chemical Safety Assessment. The key technical features of version 3 are summarised in sections 1.3.1 to 1.3.4.

1.3.1 Workers

The structure of the worker exposure predictions remains the same as that of TRAv2 i.e. worker exposures (inhalation and dermal) can be predicted across the range of REACH Process Categories (PROC), with an ability to differentiate between the exposures that might be anticipated under circumstances of industrial and professional use. Version 3 eliminates a number of anomalies that were identified in TRAv2, particularly relating to the need for an equivalency of ventilation effectiveness when applied to inhalation and dermal exposures. Version 3 now introduces the ability to predict short-term inhalation exposures and to account for the presence of different forms of general ventilation. An initial prediction of the local dermal exposure is also introduced in TRAv3. It also clarifies areas that were included in version 2 but which were not universally clear for users e.g. the treatment of liquid substances with very low volatility. As with previous versions of the TRA (and consistent with the expectations of Tier 1 models), the ability of users to iterate remains limited.

1.3.2 Consumers

The basis for the version 2 consumer exposure models underwent extensive discussion across stakeholders. These discussions shaped both the form of the algorithms and defined certain default conditions. In TRAv3, ECETOC has retained the basis of the TRAv2 algorithms used to describe exposures, but has introduced the ability to better account for (limited types of) consumer habits and practices (H&P) data where these are available, in order that the predictions are more realistic than those in TRAv2. TRAv3 contains improved functionality to allow users to generate new use scenarios where no suitable scenario is contained in the TRA tool. It does this by offering the capability of building additional new sub-categories within the product and article categories (PCs/ACs) already existing in the tool. At the same time, using the SpERC experiences as a reference point, ECETOC has developed a format to facilitate the collection and communication of relevant H&P information for identified consumer uses (termed SCED,

specific consumer exposure determinants). As a consequence of these developments, predicted exposures are expected to be less conservative than those suggested by version 2.

1.3.3 Environment

With the TRA version 3 (TRAv3), ECETOC has implemented several improvements to the TRAv2. Most notable for the tool users is that there is increased flexibility in the emission estimation via SpERCs and that risk management measures and their efficiencies are specified separately for controlling emissions to water and air. Besides, ECETOC TRAv3 contains updated SpERC information and allows a structured output of environmental assessment information such that this information can seamlessly be used as input for Tier two environmental scaling tools.

In addition to the modifications in the ECETOC TRAv3 tool, this report provides additional guidance on refining the emission estimation. It is to aid the user in applying the flexibility the tool provides.

1.3.4 User interface and datasheets

All three elements of the TRA (workers, consumers and the environment) are incorporated into an integrated version 3 tool with a common user interface and common datasheets. The user interface allows a user to perform assessments of a single substance for different settings (e.g. different processes, consumer articles and environmental release classes). It is also used to manage various steps / activities of the assessment process via macro buttons, such as running a single substance assessment from the user interface, clearing all inputs to the user interface, running a batch of substances from the datasheets, etc.

The data entered into the user interface can be stored in Excel tables, the datasheets, and further processed. The datasheets can store up to 80 substances and more scenarios per substance than the user interface. While the user interface is limited to ERC and SpERC based environmental assessments, the datasheets allow significant refinements of substance data and release estimation approaches (higher Tier assessments).

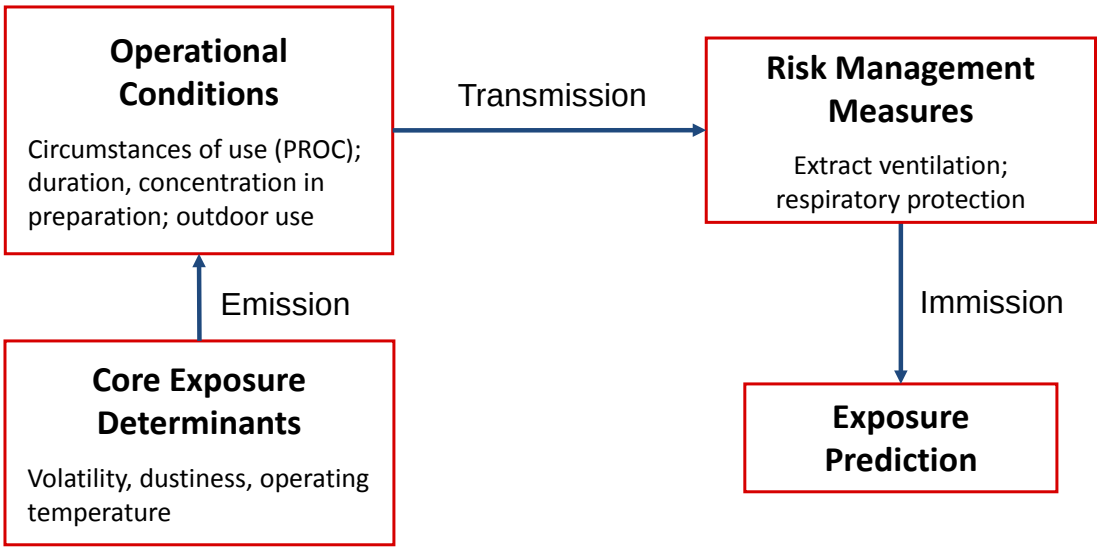
In addition, a standalone version of the consumer portion of the TRA is available in version 3. Version 3 no longer supports a standalone version of the worker portion of the TRA.

2. WORKER REVISIONS

2.1 Background

Worker exposure is estimated using, as its basis, a scenario-based source receptor type model. The main components of the model that has been applied to the TRAv2 are schematically described in Figure 1. The use of the source receptor model in this manner ensures that the structure of the TRA can not only be seen to align with the expectations of REACH Chapter R14 (i.e. worker exposure estimation), but that the TRA is also amenable to be readily adapted as part of the process for creating ESs within CSAs (i.e. the evaluation of the impact and effectiveness of different risk management strategies as required by Part D of the Technical Guidance).

Figure 1: Principle elements of TRAv2 worker inhalation exposure prediction



Key learnings arising from the use of the TRA in 2009/10 were identified and then reviewed concerning the utility of their wider application in version 3 i.e. whether they were capable of being applied across a range of substances and uses. By definition, improvements which were only considered relevant to a narrow range of substance properties or use types were not considered as being appropriate for inclusion within a general model: the intention was not to radically overhaul the TRA, rather to further improve its accuracy and flexibility, within its existing framework.

The feedback received from users was universally supportive of how the broad operating structure is executed in the TRA as it provides potential flexibility to apply OCs and RMMs beyond those incorporated into the TRA.

The structure of the worker exposure predictions remains the same as that used for version 2 i.e. worker exposures (inhalation and dermal) can be predicted across the range of REACH Process Categories (PROC), with an ability to differentiate between the exposures that might be anticipated under circumstances of industrial and professional use. The initial (8 hour) exposure prediction is a function of the fugacity of the substance and its circumstances of use (PROC). Then, depending on the extent to which additional Operational Conditions (OCs) and/or Risk Management Measures (RMMs) apply, the initial prediction is modified using simple multipliers (described more fully in ECETOC, 2009).

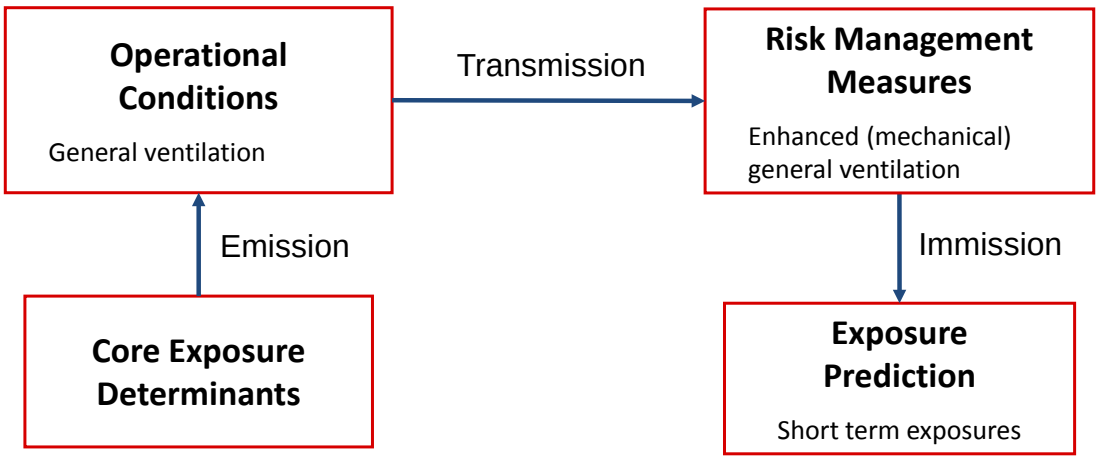
Although a range of suggested improvements and enhancements were put forward by users of v2 of the TRA, most were discounted due to the fact that the scientific basis was either limited or only applicable for a limited range of conditions (i.e. something that is more appropriately progressed at the substance and/or use level). For example, certain exposure control devices which were suggested as being included are only relevant for very volatile substances (vapour recycle and recovery) or only encountered in a few industrial sectors (film isolators and laminar downflow booths).

The number of revisions implemented in version 3 is therefore limited.

Inhalation exposures

Version 3 of the TRA now includes general ventilation as a default assumption with the ability to select good or enhanced (mechanical) ventilation as risk management measure. Furthermore the tool now also offers the functionality to provide short-term (15 minute average) inhalatory exposure predictions. Figure 2 summarises the changes that have been introduced into version 3 for inhalatory exposure and which are described in further detail in the following sections.

Figure 2: New elements of TRAv3 worker inhalation exposure prediction

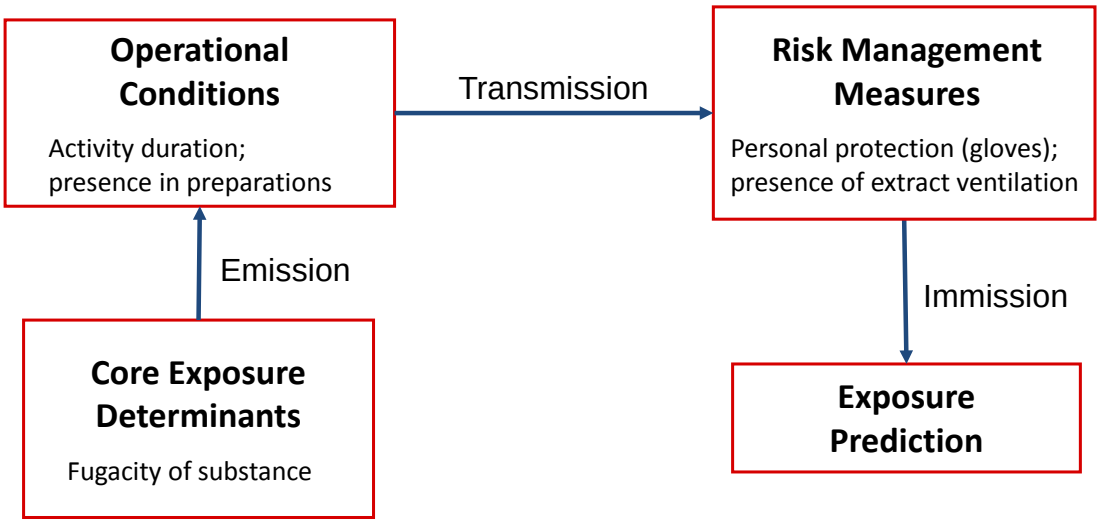


Dermal exposures

The basis for exposure prediction of the TRAv2 was limited to a single value per PROC that did not differ between industrial or professional use and where the only exposure modifier which was accounted for was the presence / absence of extract ventilation. Version 3 of the TRA now aligns the basis for dermal exposure prediction with that adopted for inhalation exposures i.e. a range of modifying conditions are now considered, including the use of personal protection (gloves). Furthermore, the anomaly that existed in version 2 between the differences in ventilation effectiveness when applied to common inhalation and dermal estimates has now been removed and a common value is now applied in most instances.

Figure 3 summarises the changes that have been introduced into version 3 for dermal exposure and which are described in further detail in the following sections.

Figure 3: New elements of TRAv3 worker dermal exposure prediction



2.2 Inhalation exposures

Version 3 of the TRA resolves a number of issues that were identified in the basic look-up table of version 2 (Appendix A of Technical Report No. 107 (ECETOC, 2009)).

2.2.1 Elimination of anomalies

For inhalation exposures, these relate to two observations:

1. A need to ensure that differences in exposure that are likely to be experienced are adequately reflected in how the TRA addresses different substance / PROC combinations.

2. A need to ensure that an appropriate distinction is made between industrial and professional exposures, where such exposures are likely to be materially different.

These observations led ECETOC to undertake a complete review of the original version 2 data with the aim of eliminating 'anomalies'. A number of specific points had been highlighted by users, particularly relating to how exposure was estimated for PROCs 2, 3, 8a, 8b, 12, 17 and 18. These have now been remedied and the revised values, together with an indication of the direction of the change, are shown in Appendix A. In order to improve the transparency of the TRA for substances with 'very low vapour pressures' (< 0.01 Pa), Appendix A now also incorporates the exposure estimates for these materials.

2.2.2 Short-term inhalation exposure prediction

Chapter R14 of the REACH Technical Guidance indicates that short-term (15 min) exposure values might be calculated by multiplying by 4x the (8 hour) TRAv2 exposure estimate. R14 cites the work of Kumagai and Matsunaga (1994) in support of this advice. The work of Kumagai and Matsunaga describes the relationship between shift average and peak exposures for a restricted range (n=10) of job types, mostly concerned with formulating and using solvent-based products. The paper found that for the identified jobs, the peak exposures were typically no greater than two times the shift average concentration. But the paper only described the experiences in a limited population. Furthermore, no details are provided in the paper on the relationship between job title and the different tasks / activities (where short-term exposures are likely to occur) that it covers.

It can be argued that a 95th% short-term value can be derived for all the 'process-based' PROCs [e.g. 1-4, 12, 16 and 20] by the application of a modification factor of 4x (consistent with R14) based on the work of Kumagai and Matsunaga and the fact that the TRA is intended to reflect the 75th percentile value of the 8hour value. For all PROCs which are predominantly task-related, the estimated short-term value will be largely independent of time i.e. the exposure modifier would be 1x the 8 hour value, or 2x the 8 hour value if a 95th% is required. If the initial estimate is based on the saturated vapour concentration, which cannot be exceeded, then the short-term estimate will also be equal to the shift average estimate.

In the case of PROCs 21-25, which have been derived from (the upper end of) measured data from the metals industry, then no such simple relationship can be derived. Indeed, the available information is such that for these mainly 'activity-based' PROCs, a multiplier of 2x is sufficient to predict the short-term exposure value.

Having described the state and limitations of the current science, ECETOC has chosen to apply a factor of 4 to derive the 95th% of the 15 min average (short-term) for all PROCs as a pragmatic

and conservative solution. However, users may wish to note that this relationship is heavily influenced by the nature of the work activity (task) being undertaken and should TRA users have available information that suggest that the application of a reduced multiplier is more appropriate for a specific task-related PROC then, provided suitable justification is available, they may wish to consider this as a Tier 1.5 refinement.

It should be noted than when short-term exposure estimates are being derived for liquid substances with 'very low' volatility, then the saturated vapour concentration is calculated to be 0.1 ppm as a maximum (this level cannot be exceeded for the vapour phase). In these situations the short-term inhalation exposure estimate is equal to the long-term exposure estimate i.e. it is independent of the duration. The exception is for those situations where aerosols are generated (PROCs 7, 11, 17, 18) or for PROCs 10 and 19 (where no LEV is present). In these situations, vapour exposure is calculated consistent with the values shown in Appendix A.

2.2.3 General ventilation and combination with LEV

General ventilation of the workplace can contribute to reduction of exposure levels although not to the same level of effectiveness as local exhaust ventilation. ECETOC has become aware that there is a lack of clarity about how general ventilation (GV) in its different forms is addressed within the TRA. For example, it is often incorrectly assumed that 'good' general ventilation is already covered in the TRA initial inhalation estimates. In terms of exposure modifiers, TRAv2 included the ability to consider work outdoors (where a 30% exposure reduction was assigned) and the presence of local extract ventilation (where the level of exposure reduction differed by PROC and industrial / professional setting). But no other forms of ventilation were accounted for.

The TRA estimates derive from those originally proposed by the UK Health and Safety Executive EASE model (Tickner *et al*, 2005). EASE presented its estimates as concentration bands with a difference of a factor 5-10 between the minimum and maximum figures (representing approximately the lower and higher quartiles of the distributions). The TRA presents single figures (point estimates) and has generally incorporated the top end of the EASE bands. The EASE estimates are based upon measurements obtained from (predominantly) enforcement activities in the 1980s (and earlier). They are accepted to be conservative in nature. Part of the reason for this conservatism is the fact that because many of the higher end exposures resulted from workplaces that operated to poor standards of exposure control. These can be assumed to be related to the absence of good general ventilation and while some form of basic natural ventilation may exist, its effectiveness is limited. By way of comparison, the advanced research tool (ART) model (TNO, 2009) uses 0.3 to 3 acph (air exchanges per hour) (good natural ventilation) and the TRA suggestion of 1-3 acph is consistent with this.

When good general ventilation is selected as being present in the tool, then this is associated with an effectiveness of 30% (corresponding to an air exchange rate of 3-5 acph). This is consistent with the level of reduction resulting from work outdoors. By comparison, EASE does not specify a number of acph for general ventilation, although it applies a reduction factor of between 2 and 3 when 'dilution ventilation' (which is not further defined) is applied. The UK COSHH Essentials approach (HSE, 1999) describes 'good general ventilation' as equating to 5-15 acph). The ventilation modifying factors applied in the ART model have been derived from simulations following the work of Cherrie *et al*, 2011. When 'good natural ventilation' is selected for a room size of 300 m^3, then the exposure reduction is approximately 45%. When the results for all room sizes are accounted for, then the average reduction amounts to almost 40%. This is higher than the TRA assumption of 30%. When engineered forms of general ventilation are available (such as mechanical or enhanced general ventilation, corresponding to general ventilation with an air exchange rate of at least 5 but preferably 10 acph), then an exposure reduction of 70% is applied.

In the implementation of this control option in the TRAv3, it should be noted that it cannot be used in combination with 'use outdoors'. On the other hand, in some workplace situations the presence of good general ventilation and LEV will both have a positive impact on exposures. For those who handle highly volatile substances, it is common practice to have both good general ventilation and LEV in industrial settings. Since use of additional mechanical ventilation may be more variable in professional settings, consistent with Tier 1 tool principles, the TRA allows for the combination of enhanced general ventilation and LEV only for industrial settings. A summary of how the TRA now treats general ventilation, both in the presence or absence of LEV, is shown in Table 1 below.

Table 1: Treatment of different forms of general ventilation within the TRA

Type of general ventilation	**Application**	**Ventilation effectiveness (modifier to initial inhalation estimate)**
'Basic' general ventilation is assumed in the base TRAv1 and TRAv2 estimates	Corresponds to: • Basic natural ventilation (i.e. normal GV arising from incidental activities within a workplace) • Typically 1-3 air exchange per hour	0% (1.0 x)
'Good' general ventilation is not assumed in the TRA estimates and can be applied as an exposure modifier for indoor activities (exposure reduction consistent with 'use outdoors')	Corresponds to: • Good natural (e.g. intentional opening of doors and windows) and/or 'non-engineered' mechanical ventilation • Typically 3-5 air exchange per hour • TRA does not support use in combination with 'use outdoors'	30% (0.7 x)
Enhanced general ventilation	Corresponds to: • Engineered mechanical ventilation for the workplace • At least 5-10 air exchanges per hour • TRA does not support use in combination with 'use outdoors' • TRA does not support use in combination with LEV for professional settings	70% (0.3 x)

2.2.4 Substances with very low vapour pressures

Appendix D of Technical Report No. 107 (ECETOC, 2009) described how exposure to substances with very low vapour pressures is determined in the TRAv2 i.e. for non-aerosol applications the saturated vapour concentration can replace the TRA estimation. In the TRA, a cut off value of 0.01 Pa (corresponding with an estimate based on the saturated vapour concentration of 0.1 ppm) has been be used to address these situations.

Although the application of this logic successfully addresses exposures to the vapour phase of the substance, there are several PROCs that are associated with use conditions where the predominant exposure would be to liquid aerosols (mists). To ensure that TRA users did not underestimate the risks posed by such exposures, the logic within Technical Report No. 107 (ECETOC, 2009) Appendix D was further extended to include additional considerations for those PROCs which are most associated with mist exposures (PROCs 7, 11, 12, 17 and 18). These considerations included the use of 'enlarged' exposure predictions for the affected PROCs for the vapour phase (i.e. beyond those capable of being achieved as a saturated vapour for a substance of very low volatility).

Furthermore, in TRAv2, for low volatility substances (VP < 0.00001 kPa), the initial exposure estimate for PROCs 10 and 19 is dependent on whether LEV is indicated or not (10ppm where no LEV is indicated and 0.1ppm where LEV is chosen). This results in an 'apparent LEV efficiency' of 99%, which can be confusing because LEV efficiency is in effect not used to derive the exposure estimate for low volatility substances. This 'logic' (i.e. difference in exposure estimate based on whether LEV is selected) was implemented to flag the likely need to adopt LEV to cover the aerosol exposures associated with these uses (and which the TRA is not intended to address). Version 3 clearly states that only vapour exposures are being assessed and that when LEV is selected, then the final estimate will be derived from the 80 and 90% values for professional / industrial. A message in the lookup table reinforces this ('Note that the TRA predicts vapour phase exposure; exposure by aerosols is not taken into account; if aerosol formation is relevant, refer to other information or models'). This message is also returned when PROCs 10 or 19 are selected for liquids (negligible, low, medium or high volatility) in the absence of LEV. It should also be noted that for PROC 1 (Use in closed process, no likelihood of exposure), where no likelihood of exposure is foreseen, the TRA cut off value is set to 0.01ppm. A summary of how the TRA now treats substances with very low vapour pressure is shown in Table 2 below.

Table 2: Treatment of 'very low vapour pressure' substances in version 3

Cut-off value applies (i.e. TRA exposure estimate replaced by 0.1 ppm)	Cut-off value does not apply (i.e. initial TRA exposure estimate applies)
PROC 1 (0.01 ppm used as cut-off value)	PROCs 7, 11, 12, 17, 18
PROCs 2, 3, 5, 5, 6, 8a, 8b, 9, 13, 14, 15, 16, 20	PROC 10 (without LEV)
PROC 10 (with LEV)	PROC 19 (without LEV)
PROC 19 (with LEV)	PROCs 21-25

2.2.5 Operations at elevated temperature

For volatiles, TRA version 2 used the vapour pressure of the substance as entered in the physicalo-chemical properties section to assign to fugacity bands (very low / low / medium / high). This VP refers typically to ambient temperature (15-25°C), but does not allow operating temperatures of different activities to be specified. Therefore, TRA version 3 allows the input of the vapour pressure of the substance at the actual operating temperature (in Pa) for each (contributing) scenario. The TRA does not provide the facility to derive vapour pressure at different temperature, so the user will need to obtain this value from other sources. If users are unable to derive the VP at elevated temperatures, then a conservative approach is to set VP to a value > 10000 Pa which will return the exposure prediction for the highest fugacity band (conservative default approach).

2.2.6 Other forms of exposure control

For exposure modification, version 2 of the TRA includes a limited range of RMMs (presence of local exhaust ventilation, respiratory protection, outdoor activity), in addition to the identified OCs (exposure duration; concentration in a preparation). However, the number of RMMs and OCs that are potentially relevant for predicting exposure is, in practice, far more extensive and embraces various technical and software strategies for reducing exposure. One of the outcomes of the 2010/11 user consultation was the suggestion to incorporate a number of additional inhalation RMMs and OCs into the TRA.

Apart from the need for any new exposure modifier to be scientifically supportable, for a new modifier to be integrated into the TRA, it is also necessary to have universal application. The user consultation exercise identified a number of different RMMs and/or OCs that have been applied by various groups to refine TRA exposure predictions e.g. general ventilation; specific working training; specific work procedures; specific work equipment; enhanced respiratory protective equipment (RPE); and high efficiency extraction ventilation (beyond the 95% level). These suggestions have been reviewed and only those considered to have both universal

application and a robust scientific basis (i.e. demonstration of their effectiveness across a representative range of uses) have been considered suitable for incorporation into TRAv3. This is not to say, however, that those exposure modifiers that have not been included have no scientific merit or justification. Rather, the data that are currently available to support them are currently too limited (confined to a small range of sectors / uses or PROCs) to justify their wider application at this time. When TRA users consider that they have sufficient confidence to apply such measures then they will need to implement these at the Tier 1.5 level.

2.2.7 Substances in mixtures

In addition to assessing exposure to the 'pure' (100%) substance, the TRA also considers how exposure may differ from the use of mixtures containing the substance. Section 2.1.6 of Technical Report No. 107 (ECETOC, 2009) describes how approaches such as Raoult's and Dalton's laws can be applied to assess the contribution of volatile substances (i.e. liquids in liquids). Technical Report No. 107 (ECETOC, 2009) did not specifically address the impact of solid / solid mixtures on exposure, but in the absence of any major differences in the dustiness of solid components, it is reasonable to assume that changes in exposure are likely to be related to the proportion of the substance in the mixture. As the multipliers implemented in TRAv2 (Technical Report No. 107 (ECETOC, 2009), Table 2) for mixtures are significantly more conservative than any 'proportionate approach', the TRA can also be considered suitable for Tier 1 use for solid / solid mixtures. The solids PROC estimates reflect the fact that there are activities that use such materials and that, because the particle size of these substances is not homogeneous (e.g. the inclusion of 'fines'), it is appropriate to make exposure estimates for low / moderate / high dustiness.

In contrast, the TRA does not provide exposure estimates for solid substances that have been blended into liquid products (e.g. of inorganic pigments in paints, etc.). Depending on the circumstances of use, then exposures to such products can be a combination of solid, vapour and liquid / solid phases. The proportion of these phases will vary with product and use characteristics. Modelling such exposures is beyond the abilities of Tier 1 tool. It should also be noted that while the TRA assesses exposure arising from the presence of the substance in a mixture, it does not undertake any form of 'mixtures risk assessment' i.e. either co-exposures to other substances or the risks that this may present. Such assessments are outside the domain of the TRA.

2.2.8 Other aspects

The TRA worker estimates link directly to the current REACH Use Descriptor system (ECHA, 2010a). The estimates are reliable as far as the description of any PROC is able to

reasonably reflect the characteristics of the activity being assessed. But the 'matching' of uses with PROCs is not intuitive and requires understanding and judgement. TRA users should therefore consult the advice contained in Ch R12 when assigning PROCs as the TRA may not provide a reliable estimate of exposure for such uses. For example, many abrasive spraying processes are not directly covered by PROCs 7 or 11, whereas on the other hand these PROCs can be used to consider exposures arising from powder coating applications.

2.2.9 Domain of reliable application

Although Technical Report No. 93 and Technical Report No. 107 (ECETOC 2004;2009) describe the circumstances under which the TRA can be reliably applied, these boundaries are not always clear to users. Indeed it has become clear that despite the documentation, some users have been applying the TRA in situations where it was never intended to be used. Table 3 summarises those circumstances where the use of the TRA is advised against.

Table 3: Domain of reliable application of the TRAv3

Domain Boundary	Comments
Gases	The TRA does not predict exposure to gases. The reason for this is that the EASE model did not extend to gases. However the TRA does allow exposures to very volatile liquids (with no upper bound set on vapour pressure) to be estimated. As these very volatile liquids might be assumed to be the equivalents of gases for many circumstances of use (PROCs), then provided users are able to assure themselves of such equivalencies, then it is reasonable to assume that the high volatility exposure prediction can also be used to predict exposures to gases in certain scenarios.
Aerosol mists	Although exposures aerosol mists might be expected to be associated with certain uses which are open and associated with the release of significant amounts of energy (e.g. spraying, machining, etc.), the TRA does not address such exposures. However, in circumstances where users have available representative measured exposure data on mists, then these may be able to be used to 'calibrate' and read across to relevant PROCs e.g. by assessing whether medium dustiness values might offer a conservative approximation of actual data (but where consideration also needs to be given to the vapour component of such exposures).
Process fumes	Although exposures to process fumes might be expected to be associated with certain uses which are undertaken at elevated temperatures (e.g. handling hot materials when their melting point lies at or above ambient temperatures), the TRA does not address such exposures. Appendix E addresses this aspect in further detail.
Fibrous materials	The TRA does not predict exposure to fibrous solids.
Exposures above ambient temperature	The TRA predicts exposure at 20^{o}C. Where a liquid substance is handled at temperatures significantly in excess of this, then users should apply the vapour pressure calculated at the operating temperature. The exception to this 'rule' is PROC6 (calendaring) where the TRA predictions already account for the elevated temperatures applied in this activity (see also 'process fumes' above when solid substances are handled).
Solids in liquids	The TRA cannot predict exposures to solids suspended or dissolved in liquids. If such exposures are considered relevant, then in circumstances where users have available representative measured exposure data, then these may be able to be used to 'calibrate' and read across to relevant PROCs, or alternatively users are referred to other tools capable of estimating such exposures.
CMRs and 'very high hazard' substances e.g. respiratory sensitisers	Although the TRA is a Tier 1 model and hence is conservative in the nature of its predictions, it requires judicious application to CMRs and other high hazard substances, largely because several of these materials can present exposures via means not covered by the TRA (and described elsewhere in this section). However, for 'simple' substances such as readily volatile liquids (e.g. toluene, benzene, n-hexane), then provided users can assure themselves that the exposures lie within the domain boundaries, the TRA will be capable of offering valid predictions.
UVCBs	The TRA estimates have been developed for mono-constituent substances. Where UVCB substances are being assessed using the TRA (in particular those substances having a range of volatilities) then users should apply the nominal VP for the substance (or the VP of most volatile component present at >1% when this is known). If an UVCB material is handled at elevated temperatures, then further correction will need to be applied consistent with the guidance contained elsewhere in this section.
Mixtures	The concentration modifier enables the TRA to predict exposures to a single substance within a (simple) mixture. However, the TRA is not intended to be applied to calculate combined exposures to different substances in a mixture beyond the 'concentration banding' that already exists.
Fractions of airborne solids	The TRA exposure predictions for solids do not differentiate between total inhalable exposure (respirable and non-respirable) and respirable exposures fractions. Users should therefore assume that any output for solids describes the inhalable fraction.
Out of scope PROCs	The TRA does not cover certain PROCs, specifically PROC 25 (handling of solid inorganic substances at ambient temperature); PROC 27a (production of metal powders using hot processes) and PROC 27b (production of metal powders using wet processes). If these PROCs are considered relevant, then users are referred to other tools capable of estimating exposure in these circumstances (e.g. MEASE).

2.2.10 TRAv2 vs TRAv3 comparison

Table 4 below summarises the changes introduced in version 3 with the functionality incorporated into version 2. It will be observed that, for inhalation exposures, although version 3 now includes new features, it also retains the basic structure of version 2.

Table 4: Comparison of features of TRAv2 and TRAv3 (inhalation exposure)

Applicability		**ECETOC TRAv2**	**ECETOC TRAv3**
Route		Inhalation	Inhalation
PROC Code		Yes	Yes
Task / Process		Yes	Yes
Covered physical state		Solid liquid = volatile	Solid liquid = volatile
Beyond Scope		Fibres, liquid aerosols or emissions from hot processes (e.g. fumes). Caution also needs to be exercised when applying to CMRs	
Type of enterprises		Industrial & professional: separate base estimates for each type	Industrial and professional: revised base estimates for some PROCs
Substance emission potential Volatility / Dustiness		3 categories for solids (low / medium / high) 4 categories for liquids (very low / low / medium / high)	
Amount of substance		Not included	Not included
Concentration of the substance		Modifying factors (4 bands) for liquids and solids	Modifying factors (4 bands) for liquids and solids
Duration		Modifying factors (4 bands)	Modifying factors (4 bands)
			Ability to calculate peak exposure
Frequency / Contact level		Not included	Not included
Farfield factors		Not explicitly included but are implicit in the PROC estimates	
Background factors		Exposure estimates are intended to be reflective of the application of basic occupational hygiene considerations (such as regularly laundered workwear; basic employee training on chemical hazards and exposure control; suitable washing and changing facilities; etc.) and are not representative of 'worst case' conditions	
RMM	**Operational conditions (OC)**	PROC-inherent OC	PROC-inherent OC
		Local Exhaust Ventilation	Local Exhaust Ventilation
		Outdoor uses	Outdoor uses
			General ventilation (2 levels)
	PPE	Yes (APFs of 10 and 20. Higher forms are not considered)	Yes (APFs of 10 and 20. Higher forms are not considered)

2.3 Dermal exposures

The structure of the worker dermal exposure predictions has been revised in order that worker exposures (inhalation and dermal) can now be predicted across the range of REACH Process Categories (PROC), with an ability to differentiate between the exposures that might be anticipated under circumstances of industrial and professional use.

The basis for dermal exposure prediction in v2 of the TRA was limited to a single value per PROC that did not differentiate between industrial or professional use and where the only exposure modifier which was accounted for was the presence / absence of extract ventilation. Version 3 of the TRA now aligns the basis for dermal exposure prediction with that adopted for inhalation exposures i.e. distinguishing between industrial and professional uses, with the ability to account for a range of modifying conditions, including the use of personal protection (gloves). Furthermore, the situation that existed in version 2 concerning the fact that different ventilation efficiencies were applied to the inhalation and dermal estimates for the same PROC has now been rectified and a common value is now applied in all instances.

Note that the TRA version 3 provides the functionality for the user to decide to benefit from the reduction of initial dermal exposure estimate by applying LEV or not. Although applying LEV reduction factors to the initial dermal exposure estimate is justifiable from a scientific point of view, the user may want to take a more conservative approach in estimating Tier 1 dermal exposure by not using the LEV reduction factors for dermal exposure.

2.3.1 Elimination of anomalies

In version 2 of the TRA, the choice (magnitude) of local exhaust ventilation (LEV) effectiveness was related to how dermal exposure was derived in the EASE model (Tickner *et al*, 2005). The resulting 'apparent LEV effectiveness' ranged from 50 to 99.5% depending on the circumstance of use (i.e. PROC) and this value was applied equally to industrial and professional settings. This approach to estimating exposure differed to that applied to inhalation exposures where (with certain exceptions) the ventilation effectiveness was set at 90% for industrial settings and 80% for professional uses. This lack of consistency meant that where extract ventilation was considered to be an essential risk management measure for controlling inhalation and dermal exposure, then TRA users were not always sure which extract efficiency to cite in CSAs and ESs. Moreover, the upper end efficiencies seemed somewhat optimistic for many potential circumstances of use.

Version 3 eliminates these anomalies; where extract ventilation is identified as a risk management measure, then a common value is applied to both inhalation and dermal exposures and this value differs according to whether the use is industrial or professional. Appendix A details the full basis of the extract ventilation efficiencies assigned to each PROC for industrial and professional uses respectively. It should be noted that for PROC 24 that address high energy exposures to metals and metal powders, as the exposure estimates are based upon actual measured exposure data rather than EASE predictions, the reduction efficiencies differ from the more usual 90/80% value (see also Appendix B of Technical Report No. 107 (ECETOC, 2009) for fuller explanation). It should also be noted that regardless of what form of general ventilation is

applied, then it has no consequence for predicted dermal exposures i.e. only engineered local extract ventilation can be expected to have a positive impact.

TRAv3 predicts the local shift average (8 hour) concentration expressed in µg/cm^2. This value is based on the modifications to the EASE predictions as described in Technical Report No. 107 (ECETOC, 2009). The dermal estimate is influenced by the presence of local extraction ventilation and the concentration of the substance, as well as the presence of dermal PPE. The ability to assess exposure durations of less than 8 hours (but not short-term exposure events) is addressed via the inclusion of the duration modifiers. The TRA is also capable of displaying the RCR for this exposure route if a suitable DNEL (local, long-term) has been selected.

Finally, certain PROCs imply some form of direct substance handling and in those cases the presence of LEV is unlikely to influence the dermal exposure level. For these PROCs (10 and 19) the option of LEV as RMM has been discontinued in TRAv3. Equally, for PROC1 exposure reduction from the presence of LEV is not foreseen.

2.3.2 Short-term ('peak') exposure prediction

Unlike for inhalation, the TRAv3 does not predict short-term ('peak') dermal exposures i.e. the likely maximal exposure that might reasonably be expected to occur during a task / activity. Neither the scientific literature nor ChR14 Technical Guidance offers any guidance on the numerical relationship between either the shift average or event characteristics (PROC) and short-term dermal exposures. Moreover, few substances might be expected to have a relevant dose metric (such as a DNEL) that relates to short-term local skin loading (expressed in µg/cm^2).

It should be noted that while the initial (long-term) estimates can be adjusted for time duration (taking into account the limitations for fugacity of the substance, see next section), the choice of the modifying factor for "< 15 min" will only result in an estimate of the exposure averaged over the full work shift.

2.3.3 Duration of activity and fugacity of the substance

The TRAv2 predicts dermal exposure expressed as the cumulative 8 hour skin loading (mg/cm^2/8hr). However for many substances, exposure durations of less than 8 hours will arise and these activities would normally be expected to be associated with significantly lower exposures than those expressed by an 8 hour value. Unlike inhalation exposure, the effect of duration of the work activity on the dermal exposure estimation is difficult to predict as it is related to the fate of the substance once it has been deposited onto the skin, with low / very low volatiles and 'dusty' solids remaining on the skin well beyond the cessation of the activity unless

intentionally removed by washing etc. However, it is reasonable to assume that for certain types of substance that are unlikely to reside on the skin due to their physical properties, task duration will affect the final skin loading (when expressed over 8 hours). There is no simple way to express the relationship between final concentration, duration and task / substance characteristics, but substances that are either more volatile or less dusty are less likely to reside on the skin for extended periods.

Therefore, it is proposed to apply the same TRA modifiers as for inhalation exposures (described in Appendix H of Technical Report No. 93 (ECETOC 2004) and shown in Table 5 below), but to limit their application to defined substance types. Exposure duration should be seen as distinct from any exposure control such as hand washing that may be applied during the course of a working day. The inherent conservatism of such a banded modifier is seen to be consistent with a screening approach.

Table 5: TRAv3 dermal exposure duration modifiers (which apply to all PROCs for high and moderate volatility liquids and non-dusty solid substances but do not apply to low / very low volatility liquids or moderate and high dusty solid)

Duration of activity	Exposure reduction (%)	Exposure modifying factor
> 4 hours	None (default)	1
1 - 4 hours	40	0.6
15 mins - 1 hour	80	0.2
< 15 mins	90	0.1

2.3.4 Concentration of the substance in a preparation

The TRAv2 does not allow for the concentration of substance in a mixture to be considered as a modifying factor for dermal exposure estimation, whereas this parameter clearly is an important exposure determinant. Version 3 will apply the same TRA modifiers as currently used in TRAv2 for inhalation exposures as shown in Table 6. The inherent conservatism of such a banded modifier is consistent with a screening approach

Table 6: Dermal exposure modifiers for substances in preparations

Percentage of substance in preparation	Exposure reduction (%)	Exposure modifying factor
>25%	None (default)	1
5-25%	40	0.6
1-5%	80	0.2
<1	90	0.1

2.3.5 Use of personal protection (gloves)

TRAv2 does not allow for the modification of dermal exposure estimates when dermal personal protection (gloves) is used, whereas this parameter is clearly a relevant exposure determinant. Version 3 allows for the use of dermal protection to be factored into exposures estimates using as a basis the modifier described in Appendix D-3 of Technical Report No. 107 (ECETOC, 2009). However, in contrast to the rationale applied to respiratory protection, the use of gloves is restricted and the choice of relevant PPE limited to two levels (80% and 90% effectiveness) for professional users; and three levels (80%, 90% and 95% effectiveness) for industrial users. The conservatism of such a modifier is then consistent with that also applied for inhalation exposures, whilst recognising that exposure reductions of >90% require control strategies that are only likely to be encountered in industrial settings. These features are summarised in Table 7 below.

Table 7: Exposure control efficiencies for different dermal protection strategies

Dermal Protection Characteristics	Indicated Efficiency %	Affected User Groups
a. Any glove / gauntlet without permeation data and without employee training	0	Applies to both industrial and professional users
b. Gloves with available permeation data indicating that the material of construction offers good protection for the substance	80	
c. Chemically resistant gloves (i.e. as #b above) with 'basic' employee training	90	
d. Chemically resistant gloves in combination with specific activity training (e.g. procedures for glove removal and disposal) for tasks where dermal exposure can be expected to occur	95	Industrial users only

The rationale applies to all substances and PROCs. It is not considered appropriate to include dermal protection having an assigned protection factor (APF) equivalent to >20 within the scope of a general Tier 1 model. It should also be noted that the exposed skin surface area varies according to task and so a judgement will also need to be applied in terms of how any linked RMMs are described i.e. the choice of gloves only relates to the hands, and gauntlets and other forms of RMM will be more appropriate where exposure to the wrists and/or forearms is also expected.

2.3.6 Other forms of exposure control

As indicated in section 2.1, although a number of suggested improvements and enhancements were put forward by users of TRAv2, most were discounted due to the fact that the scientific basis was either limited or that they were only applicable for a restricted range of conditions.

In respect to dermal exposures, a request was made to include 'hand washing' as a dermal exposure control. While the positive impact of hand washing for certain types of substance cannot be disputed (and particularly so for solids), ECETOC was unable to identify any robust basis for describing in simple terms the relationship between dermal exposure events; residual dermal exposure and hand washing (in terms of frequency, timing and intensity). As such, this parameter has not been included.

2.3.7 TRAv2 and TRAv3 comparison

Table 8 below summarises the changes introduced in version 3 with the functionality incorporated into version 2. It will be observed that, for dermal exposures, although version 3 now includes several new features, it also retains the basic structure of version 2.

Table 8: Comparison of features of TRAv2 vs TRAv3 (dermal exposure)

Applicability		**ECETOC-TRAv2**	**ECETOC-TRAv3**
Route		Dermal	Dermal
PROC Code		Yes	Yes
Task / Process		Yes	Yes
Covered physical state		solid liquid = volatile	solid liquid = volatile
Beyond Scope		Fibres, liquid aerosols or emissions from hot processes (e.g. fumes). Caution also needs to be exercised when applying to CMRs	Fibres, liquid aerosols or emissions from hot processes (e.g. fumes). Caution also needs to be exercised when applying to CMRs
Type of enterprises		Industrial and professional: common base estimates for each type	Industrial and professional. Base estimates vary for each type
Substance emission potential Volatility / Dustiness		Not included	Yes. Modifying factors (4 bands)
Amount of substance		Not included	Not included
Concentration of the substance		Not included	Yes. Modifying factors (4 bands)
Duration		Not included	Yes. Modifying factors (4 bands)
Frequency / Contact level		Not included	Not included
Farfield factors		Not included	Not included
Background factors		Not included	Not included
RMM		PROC-inherent OC	PROC-inherent OC
	Operational conditions (OC)	Local exhaust ventilation	Local exhaust ventilation effectiveness differs to v2 (default is 'no', but can be activated)
	PPE	No	Yes. Only addresses PPE with APFs of 5, 10 and 20 (latter for industrial uses only)

2.4 Ability for TRA to calculate exposures from mixtures

The TRA tool is not intended to calculate mixed exposures (whether derived from preparations or mixed exposure sources e.g. combustion products; emissions from articles). Rather it is intended to provide a conservative exposure estimate for single substances, including those substances which comprise preparations (and which are further discussed in section 2.1.8).

However, in limited cases, it may be possible to adapt this functionality to provide a conservative approximation of what such exposures might be. For example, when substances of similar volatility are blended together, then the TRA can be used to conservatively estimate the total exposures of the component substances (even though on a mass balance basis this may well exceed 100% of the mixture). However, such estimates are not possible when the mixture consists of substances with significantly different physico-chemical properties, where the exposures derive from the decomposition / degradation of the mixtures, or where exposure is 'modulated' in some way (such as when the substance or mixture has been incorporated into an article or matrix).

3. CONSUMERS

3.1 Enable creation of new product sub-categories for which all the required parameters could be set and justified

TRAv3 allows users to calculate exposure estimates and risk characterisation for product sub-categories if product use and consumer behaviour information are available. The sub-categories should be linked to the chemical product categories (PC) and article categories (AC) provided in ECHA guidance on the use descriptor system (ECHA, 2010a). A minimum set of product-specific and consumer use information is required before the tool generates exposure estimates. The minimum requirements are shown in Table 9.

Table 9: Minimum information requirements for building new subcategories

Minimum Input Parameter	Description
Product is a spray	For product subcategory linked to a PC. This parameter is used to select the release fraction to air.
Product is a solid	For product subcategory linked to a PC, and if not a spray. Parameter is used to calculate thickness layer in contact with the skin.
Route of exposure (dermal, oral, or inhalation)	If not selected, default is route of exposure is not relevant
Adult or child exposure	Selected in combination with the route of exposure. Used to select parameters (e.g., body weight) for exposure estimates.
Product ingredient fraction by weight	Substance concentration in product based on product-specific information
Body part exposed	Used to estimate surface area exposed
Surface area mouthed	Used to estimate contact area for oral exposures
Frequency of use	Based on product use information
Amount of product used per application	Based on product-specific information
Exposure time	Based on product use information and consumer habit

Users should substantiate input values with valid justification when calculating exposure estimates for product sub-categories not included in the TRA. This also makes communication of results more meaningful to downstream users. Appendix F includes a template, specific consumer exposure determinants (SCEDs), that can be used to collect information needed to calculate exposure estimates for new product subcategories.

3.2 Inhalation: Include an upper bound concentration (saturated vapour concentration)

TRAv2 provides conservative exposure estimates for non-aerosol products by assuming instantaneous release of 100% for substances with vapour pressure ≥10 Pa. This assumption can result in air concentrations that far exceed the upper bound saturated vapour

concentration for many scenarios in the tool (example below). The impact of this assumption on the estimated exposure, expressed in mg/kg/day, increases linearly with exposure duration.

Technical Report No. 107 (ECETOC, 2009) provides additional refinement options which have now been incorporated into TRAv3. The refinement options include comparison of the estimated inhalation exposure estimate to the substance's saturated vapour concentration.

In TRAv3, the calculation of saturated vapour concentration as the upper bound value of concentration of substance in air is applied to all of the inhalation scenarios for non-spray products. This is done as a two-step process:

a. Using the standard equation (Hawkins *et al*, 1991), saturated vapour concentration (SVC) of a substance 'i' in ppm can be calculated from its vapour pressure (VP):

$$SVC_i \text{ (ppm)} = (VP_i \text{ X } 10^6) / VP_{ambient}$$

VP units are Pascal

b. Using the standard equation [(ACGIH booklet 'Threshold Limit Values (TLVs™) for Chemical Substances and Physical Agents and Biological Exposure Indices (BEIs™)] the saturated vapour concentration in ppm can be converted to mg/m^3.

SVC (in mg/m^3) = (SVC in ppm) X (MW/24.45) [at standard temperature and pressure]

3.3 Inhalation: Include a 'standard' ventilation

Inhalation exposure estimates in TRAv2 do not account for basic ventilation. Even in homes with closed doors and windows and no active ventilation, a certain low level of air exchange occurs. For example, default values for air changes per hour (ACH) include 0.6 (Bremmer *et al*, 2006) and 0.45 ACH (US EPA, 2011). Higher ventilation rates of air change would be expected when active steps are taken to increase home ventilation.

Technical Report No. 107 (ECETOC, 2009) discusses refinement of exposure estimates by multiplying the inhalation exposure estimate by a dilution factor to account for basic ventilation indoor environments of residential dwelling. This refinement option is now included in TRAv3 to give users greater flexibility. The dilution fraction is calculated as follows:

$$\text{Dilution Fraction} = \frac{\text{Room Volume}}{(\text{Room volume} + (\text{ACH x exposure time x room volume}))}$$

A default value of 0.6 is used as the number of air changes per hour.

3.4 Dermal and oral transfer factors

In TRAv2, 100% of the substance in the thickness layer in contact with the skin was assumed to transfer from the product or article to the skin. Realistically, only a fraction of the substance is transferred to the skin and available for absorption via the skin or for ingestion when mouthing of the object. The amount transferred depends on various factors such as activity, contact surface, and age (US EPA, 2011). In TRAv3, users with relevant, specific information or knowledge on the pattern of transfer of a substance from a product or article matrix to skin or mouth can now enter transfer fraction values to refine dermal and oral exposure estimates. When no data is available, a conservative default value of 100% is assumed.

3.5 Calculation of combined total RCR values

Version 3 of the standalone TRA consumer tool calculates the combined total RCR (Risk Characterisation Ratio) values across different exposure routes in a different manner than version 2. In version 3, the combined total RCR value for each product or article category is calculated by adding up the RCR values from each individual route of exposure (oral, dermal, inhalation) pertaining to the product or article in question. This is the calculation method that is recommended by the REACH technical guidance (ECHA, 2010c). In the previous version of the consumer tool, the combined total RCR value was calculated by first adding up the predicted exposures from each of the relevant exposure routes of the product / article in question and then dividing that total exposure value over a proposed 'worst case' reference value (DNEL) for the substance under consideration. The main advantage of the new method of calculating the combined total RCR value is that it fully matches the REACH methodology and eliminates the need to define an overall reference value (hypothetical 'worst case' or lowest value among DNELs for the different exposure routes). Table 10 summarises the main differences between TRAv2 and TRAv3. In the tool, the RCR calculations are reported in the two results tabs ("Results by Sentinel Prod" and "Results by Prod Subcat").

Table 10: Summary of differences between the standalone Consumer TRAv3 and TRAv2

Consumer TRAv3	Consumer TRAv2
Capability to add / build specific product / article subcategories based on users-specific data	Fixed predefined product and article categories
Oral and dermal transfer factors values lower than 1 (100%) can be applied with relevant justification	Fixed default value of 1 (100%) for oral and dermal transfer factors
Ventilation rate taken into account for calculating inhalation exposure	No ventilation considered
Saturated vapour concentration is the maximum inhalation exposure value considered for non-aerosols	No upper limit for inhalation exposure estimations
Combined total RCR values calculated by summing up individual RCR values from each exposure route	Combined total RCR values calculated by dividing total exposure across all routes over a hypothetical "worst case" reference value

3.6 Additional Steps to Refine Consumer Exposure Estimates

The refinements implemented in this new version of the consumer TRA tool (TRAv3) reflect some of the potential enhancements detailed in Appendix F of ECETOC 2009. Opportunities for further improvement in future are described in Appendix G.

3.7 Comparison of results of TRAv3 with TRAv2 and ConsExpo (Appendixes H and I)

The new version of the consumer TRA tool (TRAv3) was compared to the consumer TRA (TRAv2), the ConsExpo model (v4.1), and (when available) measured data for six exposure scenarios: PC3 air care products - instant action, PC9 coatings, paints, thinners, paint removers – solvent rich (2 substances), PC13 fuels (automotive refuelling, garden equipment use), and PC35 washing and cleaning products – all purpose (liquid cleaner, trigger spray cleaner). Generally, for all the exposure scenarios tested, TRAv3 provided similar or lower exposure predictions than TRAv2, but higher exposure predictions (more conservative) than the ConsExpo model (see Appendix H). Detailed model inputs and outputs reports from TRAv2, TRAv3, and ConsExpo are given in Appendix I. along with a summary of the literature measured data.

4. ENVIRONMENT

The environmental exposure assessment in the ECETOC TRA has undergone rather limited modifications in going from v2 to v3. These changes are outlined below. In general, these changes do not affect the exposure prediction. In addition to these changes, this document will expand on Appendix I in order to provide more guidance on refined emission estimation (see 4.5).

4.1 Streamlined "ECETOC TRA Menu" structure

The ECETOC TRAv3 has been streamlined by combining the options for estimating the releases according to the A- and B- Tables and according to OECD emission scenario documents into one single option. This change affects the Tier 2 assessments and becomes apparent for the user in the 'Datasheets' of the ECETOC TRAM integrated tool exclusively. The standardised release estimations via ERCs (Tier 1 assessments) and the SpERCs (refined release estimates based on sets of defaults, which have been defined by sector organisations) remain unaltered.

In the new option, user-defined release fractions (dimensionless) can be used in combination with, for example site specific risk management measures and their efficiencies, and site-specific data on the wastewater stream or the receiving surface water to model for example specific sites. The A- and B-Tables of the old TGD (EC, 2006) or the OECD emission scenario documents can be a resource for deriving the release fractions. Please make sure to provide the rationale for the choice of the parameters used in the tier-2 release estimation in the Chemical Safety Report.

The second option provides for the possibility to enter release rates in [kg/day], which are based on measured data. This option is intended to characterise specific sites and requires that the release times per year (expressed as days per year), and the name of the monitoring site or other source of information be specified.

4.2 Enhanced guidance on SpERC provided in Cefic documents

As outlined above, SpERCs have been developed by sector organisations as instruments for refining the release estimate with standardised sets of defaults. The knowledge existing within the sector organisations has been used to develop SpERC as refined release estimates, which represent good practice in a sector. The responsibility for the content of the SpERCs is thus not with ECETOC but with the sector organisations. When Technical Report No. 107 (ECETOC, 2009) was published, there were no other publications on SpERC available, so a brief guidance on developing and documenting SpERCs was included as Appendix H.

Subsequent to the release of the SpERCs and since the publication of Technical Report No. 107 (ECETOC, 2009), the SpERCs and the SpERC factsheets, which provide the underlying documentation, have been subject to review by the German Federal Environment Agency (UBA, 2011) and a multi-stakeholder workshop (Sättler *et al*, 2012). The workshop concluded that SpERCs are a valid instrument for estimating the substance releases to the environment. However, the SpERC factsheets were found to require improvement, particularly to better document the use conditions which correspond to the release fractions. Building on the feedback received from industry as well as from authorities, Appendix H (ECETOC, 2009) is being developed further into a Cefic guidance document on developing and documenting SpERCs. Its publication expected in 2012.

4.3 Changes in SpERCs in ECETOC TRAv3

As a result of the revision of the SpERCs and the SpERC factsheets the following changes are implemented in the ECETOC TRAv3.

1. Formulation of detergents – The AISE SpERCs AISE 2.1.d.v1, AISE 2.1.e.v1, and AISE 2.1.f.v1 define the release parameters for the formulation of compact granular detergents. These SpERCs have been removed from the ECETOC TRAv3 since AISE considers the AISE SpERCs for formulation of regular granular detergents (AISE 2.1.a.v1, AISE 2.1.b.v1, and AISE 2.1.c.v1) sufficient to cover the formulation of solid detergent and cleaning products. In addition, AISE changed the indicative worst case value for the substance use rate per site (M_{SpERC}) for the small scale formulation operations to 1000 kg/d. The respective changes have been including in the ECETOC TRAv3 for the 'AISE SpERCs AISE 2.1.c.v1, AISE 2.1.i.v1, and AISE 2.1.l.v1.

2. Formulation of adhesives. In the previous release, the SpERCs for formulation of adhesives are based on the assumption that strict emission control through containment is generally applied in adhesive formulation. This proved not to be the case. As a consequence, the release factors are increased and risk management measures are assumed for the use of solvents in the large scale manufacturing of solvent borne adhesives (FEICA SpERC 2.1b.v1).

3. The SpERC ESVOC (European solvent users platform) 1.1.v1 'Manufacture of the substance and subsequent recycling / recovery, including material transfers, storage, and maintenance' was corrected by setting the release fraction to air to 0.001 if VP exceeds 100 Pa and to 0.0001 if VP is below 100 Pa. For the SpERC ESVOC 4.3a.v1 the release fraction to air corrected to 0.98.

4.4 Risk management measures and related efficiency

In the ECETOC TRA RMMs for the environment are taken in to account in the Tier 2 approach and in the release estimation using the SpERCs. The degree by which RMMs for the environment reduce the release is specific per release pathway. For that reason, the ECETOC TRAv3 has been modified such that the RMMs and their efficiencies are detailed per release pathway. For example air scrubbing can be considered an obligatory RMM to reduce the releases to air by 90%. Where RMMs are specified, it is important to note that the release factors specified in the ECETOC TRAv3 always represent the effective release factors after accounting for the efficiency of the RMM. The so-called initial release factor which specifies the fraction of a substance released from an operation or a process is not considered a useful parameter for exposure assessment and therefore does not appear in the ECETOC TRAM.

However, as the Chemical Safety Report should be explicit in outlining the justification for the release factors used in the assessment the relationship between the initial release factor, the RMM and its efficiency and the effective release factor may need to be detailed in the CSR. The SpERC factsheets have been developed to provide the initial release factors.

4.5 Erroneous estimation of $PEC_{Local,Soil}$ for gases – A work around

In order to provide conservative estimates of PEC_{Local} for soil, the algorithms used in EUSES and in the TRA assume a steady deposition rate from air to soil and neglect that substances, particularly those with a high vapour pressure, may volatilise from soil to air. Typically, this leads to an over prediction of PEC_{Local} for soil. Usually, this is not relevant for the overall risk assessment results and can be disregarded.

However, caution should be applied when assessing gaseous substances. In that case, high concentrations in ambient air may be predicted by the model. According to the algorithms in EUSES and the TRA, these high concentrations in air lead to high deposition rates to soil and, due to neglecting the re-volatilisation from soil to air, to excessive values of PEC_{Local} for soil. The high estimates of PEC_{Local} for soil are thus artefacts of an inappropriate deposition model. A more appropriate estimation can be obtained by approximating PEC_{Local} for soil as the product of the PEC_{Local} in air multiplied by the partition coefficient soil-to-air. If no experimental data are available, this parameter can be estimated by dividing the partition coefficient soil-to-water by the Henry's Law constant. Values for these parameters can be retrieved from the EXCEL-File 'EUTGDSheet-TRAM.xls' in the tab 'Substance'. The partition coefficient soil-to water and the Henry's Law constant are specified in cell C29 and cell C42, respectively.

4.6 Alignment with scaling tools, i.e. introduce required removal (on-site) efficiencies etc.

Downstream users face the challenge of matching the set of operational conditions and risk management measures communicated to them in the Annex of the safety data sheet with the operational conditions and risk management measures which are in place in their operation. This matching procedure is also referred to as scaling. The concept of scaling is very recent and not yet well defined. However, the Generic Exposure Scaling Tool (GEST) and the so-called Simple ENvironmental Scaling tool (SENS) (both under development – expected to be published via CEFIC website) are two scaling tools, in which the rules of the ECETOC TRA are implemented. Both tools use the output of the ECETOC TRA as input. While they are not fully endorsed by ECETOC they are available as prototypes on the TRA website. NOTE: This feature is only available for assessments run via the datasheets (advanced mode) in TRAv3.

ECETOC is contributing to the discussion on scaling by offering an example of a seamless fit between the ECETOC TRAv3 output and two calculation tools. In addition, consistency is warranted through the use of the same set of rules in the registrants assessment and by Downstream Users checking whether their specific use is covered by the conditions specified by the supplier in the environmental part of the Exposure Scenario.

The respective input information for these two scaling tools can be made available by performing ECETOC TRAv3 batch mode assessments in the advanced mode. The information can be viewed in the datasheets in line 760ff. The information is organised such that it can be copy pasted into the GEST and SENS tools.

4.7 Tier 1 and refined emission

Both ECETOC TRAv2 and TRAv3, offer the possibility to refine the environmental exposure assessment as outlined in Section 4.3.7 of Technical Report No 107 (ECETOC, 2009). The basic refinement options are outlined in the Appendix I of Technical Report No. 107 (ECETOC, 2009). This section aims to provide more detailed guidance on emission estimation, in view of advances made in the TRA.

The emission estimation consists of two steps. In step one, the substance use over the whole life cycle is expressed by assigning amounts of a substance to the uses of the substances. The results are use rates (in tons per year) for all uses considered along the life-cycle. In the second step, the fractions of the substance which are released during these uses are defined per use. If measured data are available to define the emissions, it is not required to assume release fraction.

The result of the emission assessment is a set of values of release rates (expressed as kg/d) to air, soil and water for each life cycle step to both the local and the regional environment.

These release rates are the input to the environmental fate calculations according the REACH Guidance on Information Requirements and Chemical Safety Assessment R 16 (ECHA, 2010d).

Generally, there are three options for the emission estimation. The Environmental Release Categories (ERCs) are outlined in the REACH Guidance on Information Requirements and Chemical Safety Assessment R 16. They provide release fractions which are very broadly applicable and thus tend to overestimate releases. The specific ERCs, also referred to as SpERCs have been developed by industry sector organisations to provide refined yet standardised emission estimates. Further refinement of the emission assessment can be accomplished by customised estimations by the registrant or by using measured data.

The ECETOC TRAv3 employs the algorithms laid down in the REACH Guidance on Information Requirements and Chemical Safety Assessment R 16 to derive Predicted Environmental Concentrations (PEC) from the release rates, regardless of the option used in the emission estimation.

4.7.1 Step 1: Substance use rates over the life-cycle

For environmental assessments REACH requires that substance use rates are defined over the whole life-cycle. Starting point is the amount produced / imported by the registrant at the European scale (MT_{Total}), expressed as tonnes per year (t/a). The life cycle of a substance may include a variety of uses. This is exemplified in Figure 4. To assess environmental exposure under REACH, the substance amounts going into these individual uses (Q_{Use} in t/a) must be defined. Subsequently, regional and local scale tonnages, or estimates of these amounts, are required in order to perform the assessments.

Figure 4: Example illustration of relevant tonnages over the life-cycle of a hypothetical substance, required for registration

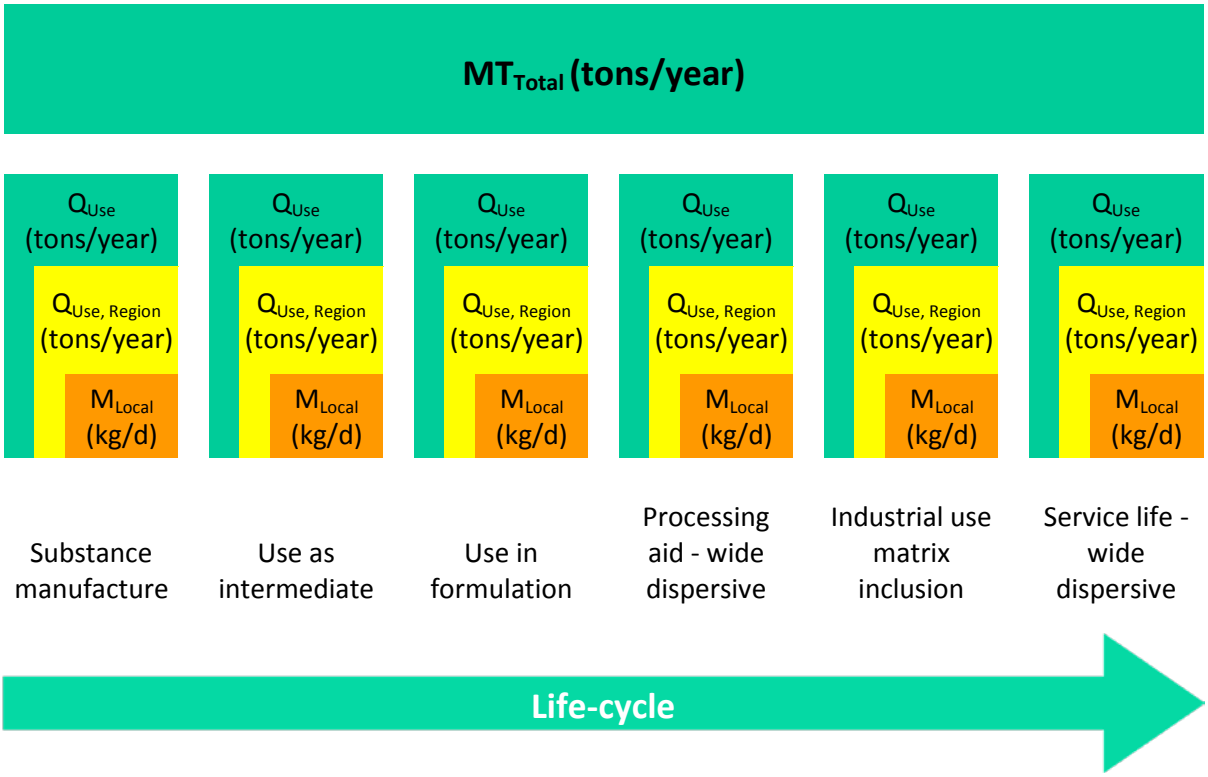


Table 11 gives an overview of the parameters used in the definition of the use rates and details the parameter values that the registrant has to define and document in the Chemical Safety Report. The three left-hand columns explain the parameters, their abbreviations and the units in which they are specified. The three columns on the right hand side outline the how the substance use rates are derived following the three emission estimation approaches.

Substance use rates – ERC approach

The 4th column (from left) outlines the default values according to the ECHA guidance. According to that approach, the substance use rates are defined in a top-down manner based on fixed values of F_{Region} and $F_{Mainsource}$. These parameters are used to break down the amount assigned to a use at EU-level to an amount used locally. According to the ECHA guidance F_{Region} can assume two values, 1 for large scale industrial uses and 0.1 for wide-dispersive uses. The ECETOC TRA allows to deviate from these defaults (in assessment via datasheets). Such deviations need to be justified in the CSR.

The ERC approach can be used via the interface and via the datasheets. $F_{Mainsource}$ typically assumes two values, 0.002 and 1. The value of 0.002 appears applicable for example for the industrial use of printing inks which occurs ubiquitously in Europe. In contrast the value of 1 is best applied if one industrial use is highly concentrated in one or few regions. With the two fractions – F_{Region} and $F_{Mainsource}$ – the amount used (e.g. M_{Local}) are defined and no further input is possible.

Substance use rates – SpERC

When the SpERC approach is used, assessments via the batch mode allow for more flexibility. When they are run via the interface, F_{Region} can assume two values, 0.1 and 1. As for ERC based assessments, user-defined values of F_{Region} can be employed when assessments are performed via the datasheets (batch mode).

The substance use rate M_{Local} for point source uses is derived by default according to the formulas used in the ERC approach. This default is overridden when an M_{SpERC} value is available. This is the case for a significant number of SpERCs. The derivation of M_{SpERC} is specific for the different processes assessed. The guidance on developing SpERCs provides an example of the derivation of M_{SpERC} (Cefic, 2010). The purpose of specifying M_{SpERC} is to provide the exposure assessor with a realistic worst case starting point of his assessments. The derivation of M_{SpERC} in the SpERC factsheets may be consulted in order to define more appropriate values of M_{Site}. Such user-defined values can be used to override both default estimates and the M_{SpERC}-values.

When a SpERC based assessment is selected, the user will be informed how the default tonnage is derived (equation based on ERC approach or specific M_{SpERC} defined. For point sources, the default value can be overridden and the assessment performed for the user defined M_{Local}.

Refining substance use rates when values of M_{SpERC} were used

If RCR <1, the assessor can conclude the assessment. If the assessment yields an RCR > 1, the assessor may communicate a value of M_{Safe} (M_{SpERC}/RCR) which is lower than M_{SpERC}. If the RCR »1, the assessor should consult the SpERC factsheet to check whether the assumptions made in the derivation of M_{SpERC} and those made in his own assessment can be reconciled. If he concludes so, he may decide that communicating a value of M_{Safe} which is significantly lower than M_{SpERC} is appropriate. This may for example be the case when the generic substance concentration assumed in the SpERC derivation is high, while the typically used concentration of the substance is low.

Substance use rates – Customised assessments

Alternatively, the assessor may have to conclude that the SpERC is inappropriate. In that case, another SpERC may have to be looked for, e.g. a SpERC which includes on-site emission reduction. If no alternative SpERCs are available, or if employing alternative SpERCs do not yield satisfactory results, further refinement can be achieved via a customised emission assessment. This option is accessible via the batch mode only.

Table 11: Overview of the parameters used in the REACH emission estimation and how they are used in Tier 1, SpERC-based, and higher tier assessments

Parameter	Abbreviation	Unit	ERC based emission assessment – ECHA Guidance	SpERC based emission assessment	Higher tier emission assessment
Mass of substance registered for a use in the EU	Q_{Use}	t / a	Defined by Registrant – use market intelligence	Defined by Registrant – use market intelligence	Defined by Registrant – use market intelligence
Fraction of Q_{Use} which is used in one region	F_{Region}	Unitless	Default values: 0.1 and 1.	Default values (0.1, 1) used in standard mode, free choice of value in advanced mode.	Default values: not defined
Mass of substance registered for a use which is used in a region	$Q_{Use,Region}$	t / a	$Q_{Use,Region} = Q_{Use} \times F_{Region}$	$Q_{Use,Region} = Q_{Use} \times F_{Region}$	Defined by Registrant – use market intelligence
For industrial uses: Fraction of amount used in a region ($Q_{Use,Region}$) which is used in one point source	$F_{Mainsource}$ Industrial use	Unitless	1	Not used in derivation of M_{Local}	Not used in derivation of M_{Local}
For wide dispersive uses: Fraction of amount used in a region ($Q_{Use,Region}$) which is use in the unit town	$F_{Mainsource}$ dispersive uses	Unitless	0.002	See SpERC factsheets*	Defined by Registrant
Number of days per year during which emissions occur	$T_{Emission}$	d / a	Default values:	Defined in SpERC factsheets	Defined by Registrant
For industrial uses - Mass of sub-stance used locally at a defined site	M_{Local}	Kg/d	$M_{Local} = Q_{Use, Region} \times 1000 \times F_{Mainsource} / T_{Emission}$	M_{SpERC} realistic worst case estimate of M_{Site}, can be overridden by Registrant	Defined by Registrant
For wide dispersive uses - Mass of substance used locally – dispersive	M_{Local}	Kg/d	$M_{Local,Dispersive} = Q_{Use,Region} \times 1000 \times F_{Mainsource} / T_{Emission}$		

4.7.2 Step 2: Defining release fractions

Once the substance use rates are defined along the life-cycle, the assessor has to define which fractions of the amounts used are released to the environment. This assessment specifies the

release fractions for water, air and soil as RF_{Air}, RF_{Water}, and RF_{Soil}. To that end, the ECETOC TRA provides three options.

Standardised release fractions – ERCs

In the REACH Guidance on IR&CSA ERCs are introduced as generic, broadly applicable emission scenarios. They define the fractions of a substance emitted during a process / application, and provide default assumptions for the local environmental properties. In combination with an amount used per ERC, a generic emission estimate can be derived. As Tier 1 scenarios, they are simple and provide conservative emission estimates. This is clearly acknowledged in the REACH Guidance on Information Requirements and Chemical Safety Assessment R 16 (ECHA, 2010d) which states "ERC should be used as a starting point for emission estimation" and which explicitly encourages the use of more refined or specific information for emissions.

Standardised release fractions – SpERCs

One of the refining options for the release fractions are the specific ERCs or SpERCs. ECETOC has provided a framework for specifying the emission estimations based on the ERCs (see Appendix J in Technical Report No. 107, ECETOC, 2009). According to this framework, the emission estimation parameters for each of the ERCs can be made specific for emissions as they occur in different sectors. SpERCs are developed by sector organisations. This ensures that SpERCs are standardised and can feed into a standardised communication. The responsibility for the SpERCs resides with the sector organisations. Hence, the parameter values of the SpERCs in the TRA tool have been proposed by the sector organisations and ECETOC does not assume responsibility for their correctness. It is the SpERC originators' obligation to provide documentation on the SpERCs along with the justification of the assumed release fractions. Guidance on the development and documentation of the SpERCs such that the required quality and transparency are warranted will shortly be available from Cefic (Cefic, in preparation).

Customised release assessments

When SpERCs are not available or when SpERC-based assessments do not allow for concluding that a use of a substance is safe, further refinement of the emission assessment may be necessary. This can be achieved by improving the release fractions, for instance by measuring them, or by measuring the release rates. The information underlying these refinements should be documented and justified in the Chemical Safety Report. A subset of this information may need to be

included in the Annex of the Safety Data Sheet such that the downstream user is able to check whether the use at his specific site is covered by the Exposure Scenario generated by the supplier.

4.7.3 Emission estimation – The release rates

When the substance use rates (M) and the release factors (RF) for the different pathways (air, (waste)water, and soil) are defined then the release rates are calculated for the regional level and the local level. The algorithms applied in ECETOC TRA are displayed in Table 12. The release rates are the outcome of the emission assessment. They form the link to the estimation of the environmental concentrations. In the ECETOC TRA they are handed over from the emission assessment module to the multimedia fate calculation module, which calculates the values of PEC.

Table 12: Algorithms used in ECETOC TRA for deriving the release rates

Use Rates		Release Factors	Amounts Emitted	
Regional	**Local**		**Regional**	**Local**
$Q_{Use,Region}$	M_{Local}	RF_{Air}	$E_{Regional,Air} = Q_{Use,Region} \times RF_{Air}$	$E_{Local,Air} = M_{Local} \times RF_{Air}$
		RF_{Water}	$E_{Regional,Water} = Q_{Use,Region} \times RF_{Water}$	$E_{Local,Water} = M_{Local} \times RF_{Water}$
		RF_{Soil}	$E_{Regional,Soil} = Q_{Use,Region} \times RF_{Soil}$	$E_{Local,Soil} = M_{Local} \times RF_{Soil}$

4.7.4 Communicating the results of environmental assessments

Distinguishing wide dispersive from point source uses

The purpose of downstream communication of the results of REACH environmental assessments is to enable the downstream user to check whether from an environmental perspective a use is covered by the environment part of an Exposure Scenario. In this regard wide dispersive uses have to be distinguished from industrial uses (Table 13). This distinction has first been elaborated in the SpERC Guidance (Cefic, 2010). Wide dispersive uses are those uses by consumers and professionals. These uses result in more or less evenly distributed substance emissions over time and in the geographical region under assessment. In addition, there are typically no technical measures by which consumers and professionals can control emissions. However, instructions such as “Do not pour down the drain” serve to control emissions and can be communicated to customers and professionals. For the rest, it is sufficient to inform downstream users that wide dispersive uses are included in an assessment and have been assessed to be safe.

Table 13: Mapping industrial, professional and consumer uses to point source and wide dispersive uses

User group	Emission permit and/or access to general technical emission control	Obligation to follow SDS re-commendation	Relevant environmental release classes	Input for exposure scenario checking
Industrial	Yes	Yes	Point source use: ERC1 to 7, 12	Explicit information (see below)
Professional*	No**	Yes	Wide dispersive use: ERC 8 to 11	Statement: wide dispersive use is covered
Consumer*	No	No		None

* Professional and consumer uses are in charge of release control by following instructions for equipment cleaning and disposal.

** Specific measures may be encountered in some professional uses.

In contrast, the emission assessments for industrial uses define the emissions for unit point sources for certain applications and processes with regard to the emissions of substances to the environment. This encompasses that assumptions are made on the typical size of an operation, the typical way a process / application is operated and the risk management measures which are typically applied. This information is communicated down the supply chain such that the operators of point sources are able to check whether their specific use is covered by the environmental part of the exposure scenario provided by their suppliers.

As outlined above, the environmental exposure assessment in ECETOC TRA uses the algorithms laid down in the REACH Guidance on Information Requirements and Chemical Safety Assessment R 16 (ECHA, 2010d) to derive PECs regardless of the option used in the emission estimation. Hence, the emission estimation is the feature which can be used to distinguish between different types of exposure assessments in the supply chain communication of the environmental part of the Exposure Scenarios.

Standardised emission assessment – ERCs

In cases where the environmental part of the Exposure Scenario is developed on the basis of an ERC emission assessment, the downstream user may be provided with the PECs and the resulting values of RCR for all compartments. In addition, the information on the amount used locally (M_{Local}) may need to be provided. Alternatively, the maximum values which may be used locally (M_{Safe}) and the identity of the compartment with the highest value of RCR can be provided.

The downstream user may take eventual differences in the dilution, and the amount used into account when checking whether his specific conditions are covered. ERCs are defined to represent worst case emission situations with a broad range of applicability. For that reason, operational conditions are not specified for ERCs. A check of operational conditions is only

possible if the registrant specifies the operational conditions in the annex of the safety data sheet he provides.

Standardised emission assessment – SpERCs

In cases where the environmental part of the Exposure Scenario is developed on the basis of an SpERC emission assessment, the downstream user is provided with additional information on operational conditions and, if applicable, risk management measures. A short description of the operational conditions and the risk management measures is provided in the annex of the SDS. A detailed description is available via the SpERC Factsheets. The registrant may alert downstream users to these documents in order to make them aware of the detailed description of the operational conditions assumed in the SpERC-based emission assessment.

Typically, a downstream user operates one or a few 'uses' at one site. For these he has to identify which SpERCs are applicable for uses. Once the relevant SpERCs are identified, the downstream user should compare the specific operational conditions and risk management measures assumed in these SpERCs with the situation at his site. Where in-depth information is being sought, the SpERC factsheets should be consulted. If not, the information in the annex of the safety data sheet may be sufficient.

Customised assessments

There is no standardisation for customised assessment,. Consequently, the downstream user may have to be informed about the information mentioned above. In addition, the supplier has to specify release factors, detailed information on operational conditions and risk management measures. The downstream user should consider all this information when evaluating whether or not his specific operation is covered by the supplier's customised assessment.

4.8 Exposure prediction in TRAv3 and TRAv2

While the environment tools of ECETOC TRAv2 and TRAv3 generally produce equivalent results, there are two exceptions which need to be noted. In section 4.3 a number of modified SpERCs are identified. Their use in TRAv3 may result in exposure predictions which deviate from TRAv2. Such deviations may also occur when the value of amount of a substance used locally (M_{Local}) exceeds that of the amount of a substance which used is registered for a use (Q_{Use}). Such a parameter setting is possible in the TRAv3 as a result of the increased flexibility in the emission assessment.

5. FUTURE DIRECTIONS

5.1 TRAv3 and the ECHA CHESAR Tool

The ECETOC TRA provides the basis for the worker and consumer exposure estimates used within the European Chemicals Agency's (ECHA) CHESAR (Chemical Safety Assessment and reporting tool). In 2010, ECHA announced its intention to significantly upgrade CHESAR. ECETOC has therefore worked with ECHA to ensure that not only will there be full alignment between the TRAv3 and CHESAR v2, but that the TRAv3 also incorporates many of ECHA's observations concerning human exposure estimation resulting from the Phase 1 REACH registrations.

Version 2 of CHESAR [http://CHESAR.echa.europa.eu/] is planned for release in summer 2012. It will include added functionality to enable industry CSA/ES activities such as supply chain use mapping and Specific Environmental Release Categories (SpERCs) to be more readily accessed and applied. The SpERC concept was first proposed by ECETOC, (see Technical Report No. 107 (ECETOC, 2009) Appendix H) in order to provide a basis for more realistic environmental exposure estimates. In a similar vein, this report proposes the Specific Consumer Exposure Determinant (SCED) as a verifiable basis for more realistic consumer exposure estimates (see Appendix F). It can also be expected that CHESAR v2 will allow the incorporation of the SCEDs that conform to the format set out in Appendix F in order to further enhance the utility of CHESAR.

5.2 Sustaining the TRA tools: Future ECETOC intentions

Over the period 2002-2012, ECETOC has developed 3 versions of the TRA. ECETOC, 2004, describes the technical basis for version 1 and ECETOC, 2009, deals with version 2. Versions 1 and 2 differed in a number of important areas, notably in the need to ensure that the features and attributes of version 1 could be seen to align with the expectations of REACH. The revisions necessary to achieve such an objective resulted in version 2 being significantly different to version 1. Version 3 of the TRA is a refinement of version 2 i.e. although it offers improved functionality and accuracy, its underlying structure remains similar to version 2.

Version 3 incorporates the considerable experiences of TRA users arising from the 2009/10 REACH Phase 1 registration period. It is not to be expected that these experiences will materially differ during subsequent REACH registration phases. As such, no further upgrades to the TRA are envisaged in the foreseeable future. However, as ECETOC retains oversight of the science underpinning the TRA, future developments affecting the TRA (such as any changes to the REACH Regulation or supporting Technical Guidance) will be monitored and responded to accordingly.

ABBREVIATIONS

AC	Article category
ACH	Air changes per hour
ACGIH	American Conference of Industrial Hygienists
AISE	Association Internationale de la Savonnerie, de la Détergence et des Produits d'Entretien (International Association for Soaps, Detergents and Maintenance Products)
APF	Assigned protection factor
ART model	Advanced REACH tool model
BEI	Biological exposure index
CEFIC	The European Chemical Industry Council
CHESAR	Chemical safety assessment and reporting tool
CMR	Carcinogenic, mutagenic and reprotoxic
COSHH	Control of substances hazardous to health
CSA	Chemical safety assessment
CSR	Chemical safety report
DNEL	Derived No Effect Level
EASE	Estimation and assessment of substance exposure model
ECHA	European Chemicals Agency
EGRET	ESIG GES Risk and Exposure Tool
ERC	Environmental Release Categories
ES Tool	Exposure Scenario Tool
ESIG	European Solvents Industry Group
ESVOC	European solvent users platform
EUSES	European unified system for the evaluation of substances
FEICA	Fédération Européenne des Industries de Colles et Adhésifs (Association of European Adhesive and Sealant Industry)
GEST	Generic Exposure Scaling Tool
GV	General ventilation
H&P	Habits and practices

IRCSA	Information requirements and chemicals safety assessment
LEV	Local exhaust ventilation
MEASE	Metals Estimation and Assessment of Substance Exposure
MW	Molecular weight
OC	Operational conditions
OECD	Organisation for Economic Co-operation and Development
PC	Product categories
PEC	Predicted environmental concentrations
PPE	Personal protective equipment
PROC	Process category
RCR	Risk characterisation ratio
REACH	Registration, Evaluation, Authorisation and restriction of CHemicals
RF	Release factor
RMM	Risk management measure
RPE	Respiratory protective equipment
SCED	Specific Consumer Exposure Determinants
SDS	Safety data sheet
SENS	Simple ENvironmental Scaling tool (under development)
SpERCs	Specific Environmental Release Classes
SVC	Saturated vapour concentration
TGD	Technical Guidance Document
TLVs	Threshold limit values
TRA	Targeted risk assessment
TRAM	Targeted risk assessment modular model
UVCB substance	Substance of Unknown or Variable composition, Complex reaction products or Biological materials
VP	Vapour pressure

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APPENDIX A: RATIONALE FOR TRAv3 WORKER INHALATION PREDICTIONS

Table A-1: Rationale Behind TRAv3 Worker Exposure Predictions

PROC	Exposure scenario	LEV	Fugacity	Industrial exposure prediction	Professional exposure prediction	LEV effectiveness industrial (%)	LEV effectiveness professional (%)
1	**Use in closed process, no likelihood of exposure**	yes	High			n/a	n/a
	(solids)	no		0.01	0.1		
	mg/m^3	yes	Moderate			n/a	n/a
		no		0.01	0.01		
		yes	Low			n/a	n/a
		no		0.01	0.01		
	(volatiles)	yes	High			n/a	n/a
	ppm	no		0.01	0.1		
		yes	Moderate			n/a	n/a
		no		0.01	0.01		
		yes	Low			n/a	n/a
		no		0.01	0.01		
		yes	Very Low			n/a	n/a
		no		0.01	0.01		
2	**Use in closed, continuous process with occasional controlled exposure**	yes	High			90	80
	(solids)	no		1	5		
	mg/m^3	yes	Moderate			90	80
		no		0.5	1		
		yes	Low			90	80
		no		0.01	0.01		
	(volatiles)	yes	High			90	80
	ppm	no		**25**	50		
		yes	Moderate			90	80
		no		**5**	20		
		yes	Low			90	80
		no		1	5		
		yes	Very Low			90	80
		no		0.1	0.1		
3	**Use in closed batch process (synthesis or formulation)**	yes	High			90	80
	(solids)	no		1	5		
	mg/m^3	yes	Moderate			90	80
		no		1	1		
		yes	Low			90	80
		no		0.1	0.1		

	(volatiles)	yes	High			90	80
	ppm	no		**50**	100		
		yes	Moderate			90	80
		no		**10**	25		
		yes	Low			90	80
		no		3	3		
		yes	Very Low			90	80
		no		0.1	0.1		
4	**Use in batch and other process (synthesis) where opportunity for exposure arises**	yes	High			90	80
	(solids)	no		25	50		
	mg/m^3	yes	Moderate			90	80
		no		5	5		
		yes	Low			90	80
		no		0.5	1		
	(volatiles)	yes	High			90	80
	ppm	no		100	250		
		yes	Moderate			90	80
		no		20	50		
		yes	Low			90	80
		no		5	10		
		yes	Very Low			90	80
		no		0.1	0.1		
5	**Mixing or blending in batch processes (multistage and/or significant contact)**	yes	High			90	80
	(solids)	no		25	50		
	mg/m^3	yes	Moderate			90	80
		no		5	5		
		yes	Low			90	80
		no		0.5	1		
	(volatiles)	yes	High			90	80
	ppm	no		250	500		
		yes	Moderate			90	80
		no		50	100		
		yes	Low			90	80
		no		5	10		
		yes	Very Low			90	80
		no		0.1	0.1		
6	**Calendering operations**	yes	High			90	80
	(solids)	no		25	50		
	mg/m^3	yes	Moderate			90	80
		no		5	5		
		yes	Low			90	80
		no		0.1	1		

	(volatiles)	yes	High			90	80
	ppm	no		250	500		
		yes	Moderate			90	80
		no		50	100		
		yes	Low			90	80
		no		5	10		
		yes	Very Low			90	80
		no		0.1	0.1		
7	**Industrial spraying**	yes	High			95	n/a
	(solids)	no		100	n/a		
	mg/m^3	yes	Moderate			95	n/a
		no		20	n/a		
		yes	Low			95	n/a
		no		1	n/a		
	(volatiles)	yes	High			95	n/a
	ppm	no		500	n/a		
		yes	Moderate			95	n/a
		no		250	n/a		
		yes	Low			95	n/a
		no		100	n/a		
		yes	Very Low			95	n/a
		no		100	n/a		
8a	**Transfer of chemicals from/to vessels/large containers at non dedicated facilities**	yes	High			90	80
	(solids)	no		50	50		
	mg/m^3	yes	Moderate			90	80
		no		5	**10**		
		yes	Low			90	80
		no		0.5	0.5		
	(volatiles)	yes	High			90	80
	ppm	no		250	500		
		yes	Moderate			90	80
		no		50	100		
		yes	Low			90	80
		no		10	25		
		yes	Very Low			90	80
		no		0.1	0.1		
8b	**Transfer of chemicals from/to vessels/large containers at dedicated facilities**	yes	High			95	80
	(solids)	no		25	50		
	mg/m^3	yes	Moderate			95	80
		no		**1**	5		
		yes	Low			95	80
		no		0.1	0.5		

	(volatiles)	yes	High			95	90
	ppm	no		150	250		
		yes	Moderate			95	90
		no		**25**	50		
		yes	Low			95	90
		no		5	10		
		yes	Very Low			95	90
		no		0.1	0.1		
9	**Transfer of chemicals into small containers (dedicated filling line)**	yes	High			90	80
	(solids)	no		20	20		
	mg/m^3	yes	Moderate			90	80
		no		5	5		
		yes	Low			90	80
		no		0.1	0.5		
	(volatiles)	yes	High			90	80
	ppm	no		200	250		
		yes	Moderate			90	80
		no		50	100		
		yes	Low			90	80
		no		5	10		
		yes	Very Low			90	80
		no		0.1	0.1		
10	**Roller application or brushing**	yes	High			90	80
	(solids)	no		10	10		
	mg/m^3	yes	Moderate			90	80
		no		5	5		
		yes	Low			90	80
		no		0.5	0.5		
	(volatiles)	yes	High			90	80
	ppm	no		250	500		
		yes	Moderate			90	80
		no		50	100		
		yes	Low			90	80
		no		10	25		
		yes	Very Low			TRA provides estimate of 0.1ppm when LEV applied	
		no		10	25		
11	**Non-industrial spraying**	yes	High			n/a	80
	(solids)	no		n/a	200		
	mg/m^3	yes	Moderate			n/a	80
		no		n/a	20		
		yes	Low			n/a	80
		no		n/a	1		

	(volatiles)	yes	High			n/a	80
	ppm	no		n/a	1000		
		yes	Moderate			n/a	80
		no		n/a	500		
		yes	Low			n/a	80
		no		n/a	100		
		yes	Very Low			n/a	80
		no		n/a	100		
12	**Use as a blowing agent**	yes	High			n/a	n/a
	(solids)	no		n/a	n/a		
	mg/m^3	yes	Moderate			n/a	n/a
		no		n/a	n/a		
		yes	Low			n/a	n/a
		no		n/a	n/a		
	(volatiles)	yes	High			90	80
	ppm	no		100	500		
		yes	Moderate			90	80
		no		20	100		
		yes	Low			90	80
		no		2	10		
		yes	Very Low			90	80
		no		2	10		
13	**Treatment of articles by dipping and pouring**	yes	High			90	80
	(solids)	no		5	5		
	mg/m^3	yes	Moderate			90	80
		no		1	5		
		yes	Low			90	80
		no		0.1	0.5		
	(volatiles)	yes	High			90	80
	ppm	no		250	250		
		yes	Moderate			90	80
		no		50	100		
		yes	Low			90	80
		no		10	10		
		yes	Very Low			90	80
		no		0.1	0.1		
14	**Production of preparations or articles by tabletting, compression, extrusion, pelletisation**	yes	High			90	80
	(solids)	no		10	50		
	mg/m^3	yes	Moderate			90	80
		no		1	5		
		yes	Low			90	80
		no		0.1	1		

	(volatiles)	yes	High			90	80
	ppm	no		250	500		
		yes	Moderate			90	80
		no		50	100		
		yes	Low			90	80
		no		5	10		
		yes	Very Low			90	80
		no		0.1	0.1		
15	**Use of laboratory reagents in small scale laboratories**	yes	High			90	80
	(solids)	no		5	5		
	mg/m^3	yes	Moderate			90	80
		no		0.5	0.5		
		yes	Low			90	80
		no		0.1	0.1		
	(volatiles)	yes	High			90	80
	ppm	no		50	50		
		yes	Moderate			90	80
		no		10	10		
		yes	Low			90	80
		no		5	5		
		yes	Very Low			90	80
		no		0.1	0.1		
16	**Using material as fuel sources (limited exposure to unburned product to be expected)**	yes	High			90	80
	(solids)	no		10	50		
	mg/m^3	yes	Moderate			90	80
		no		5	20		
		yes	Low			90	80
		no		0.1	5		
	(volatiles)	yes	High			90	80
	ppm	no		25	50		
		yes	Moderate			90	80
		no		5	10		
		yes	Low			90	80
		no		1	1		
		yes	Very Low			90	80
		no		0.1	0.1		
17	**Lubrication at high energy conditions and in partly open process**	yes	High			90	80
	(solids)	no		50	200		
	mg/m^3	yes	Moderate			90	80
		no		20	50		
		yes	Low			90	80
		no		1	10		

	(volatiles)	yes	High			90	80
	ppm	no		100	500		
		yes	Moderate			90	80
		no		50	200		
		yes	Low			90	80
		no		20	50		
		yes	Very Low			90	80
		no		20	50		
18	**Greasing at high energy conditions**	yes	High			90	80
	(solids)	no		50	200		
	mg/m^3	yes	Moderate			90	80
		no		20	50		
		yes	Low			90	80
		no		1	5		
	(volatiles)	yes	High			90	80
	ppm	no		100	500		
		yes	Moderate			90	80
		no		50	200		
		yes	Low			90	80
		no		20	50		
		yes	Very Low			90	80
		no		20	50		
19	**Hand-mixing with intimate contact (only PPE available)**	yes	High			90	80
	(solids)	no		25	50		
	mg/m^3	yes	Moderate			90	80
		no		5	5		
		yes	Low			90	80
		no		0.5	0.5		
	(volatiles)	yes	High			90	80
	ppm	no		250	500		
		yes	Moderate			90	80
		no		50	100		
		yes	Low			90	80
		no		10	25		
		yes	Very Low			TRA provides estimate of 0.1ppm when LEV applied	
		no		10	25		
20	**Heat and pressure transfer fluids (closed systems) in dispersive use**	yes	High			n/a	80
	(solids)	no		n/a	5		
	mg/m^3	yes	Moderate			n/a	80
		no		n/a	1		
		yes	Low			n/a	80
		no		n/a	0.01		

	(volatiles)	yes	High			n/a	80
	ppm	no		n/a	50		
		yes	Moderate			n/a	80
		no		n/a	20		
		yes	Low			n/a	80
		no		n/a	5		
		yes	Very Low			n/a	80
		no		n/a	0.1		
21	**Low energy manipulation of substances bound in materials and/or articles**	yes	High			90	80
	(solids)	no		10	20		
	mg/m^3	yes	Moderate			90	80
		no		3	5		
		yes	Low			90	80
		no		1	3		
	(volatiles)	yes	High			n/a	n/a
	ppm	no		n/a	n/a		
		yes	Moderate			n/a	n/a
		no		n/a	n/a		
		yes	Low			n/a	n/a
		no		n/a	n/a		
		yes	Very Low			n/a	n/a
		no		n/a	n/a		
22	**Potentially closed operations with minerals at elevated temperature**	yes	High			90	n/a
	(solids)	no		10	n/a		
	mg/m^3	yes	Moderate			90	n/a
		no		3	n/a		
		yes	Low			90	n/a
		no		1	n/a		
	(volatiles)	yes	High			n/a	n/a
	ppm	no		n/a	n/a		
		yes	Moderate			n/a	n/a
		no		n/a	n/a		
		yes	Low			n/a	n/a
		no		n/a	n/a		
		yes	Very Low			n/a	n/a
		no		n/a	n/a		
23	**Open processing and transfer of minerals at elevated temperature**	yes	High			90	80
	(solids)	no		10	20		
	mg/m^3	yes	Moderate			90	80
		no		3	5		
		yes	Low			90	80
		no		1	3		

	(volatiles)	yes	High			n/a	n/a
	ppm	no		n/a	n/a		
		yes	Moderate			n/a	n/a
		no		n/a	n/a		
		yes	Low			n/a	n/a
		no		n/a	n/a		
		yes	Very Low			n/a	n/a
		no		n/a	n/a		
24	**High (mechanical) energy work-up of substances bound in materials and/or articles**	yes	High			80	75
	(solids)	no		10	20		
	mg/m^3	yes	Moderate			80	75
		no		3	5		
		yes	Low			80	75
		no		1	3		
	(volatiles)	yes	High			n/a	n/a
	ppm	no		n/a	n/a		
		yes	Moderate			n/a	n/a
		no		n/a	n/a		
		yes	Low			n/a	n/a
		no		n/a	n/a		
		yes	Very Low			n/a	n/a
		no		n/a	n/a		
25	**Hot work operations with metals**	yes	High			90	80
	(solids)	no		5	10		
	mg/m^3	yes	Moderate			90	80
		no		5	10		
		yes	Low			90	80
		no		5	10		
	(volatiles)	yes	High			n/a	n/a
	ppm	no		n/a	n/a		
		yes	Moderate			n/a	n/a
		no		n/a	n/a		
		yes	Low			n/a	n/a
		no		n/a	n/a		
		yes	Very Low			n/a	n/a
		no		n/a	n/a		

APPENDIX B: RATIONALE FOR TRAv3 INDUSTRIAL WORKER DERMAL EXPOSURE ESTIMATES

blue upward revision compared to TRAv2 i.e. trends towards a higher exposure estimate

red downward revision compared to TRAv2 i.e. trends towards a lower exposure estimate

		LEV present?	Assigned inhalation LEV efficiency (%)	Initial predicted v3 dermal exposure (ug/cm^2/day)	Exposed skin surface (cm^2)	Predicted dermal exposure (mg/kg/day)
PROC	**Wide Dispersive Uses**					
1	**Use in closed process, no likelihood of exposure**	Yes	0	10		0.03
		No	0	**10**	240	0.03
2	**Use in closed, continuous process with occasional controlled exposure**	Yes	90	20		0.14
		No	0	200	480	1.37
3	**Use in closed batch process (synthesis or formulation)**	Yes	90	**20**		0.07
		No	0	**200**	240	0.69
4	**Use in batch and other process (synthesis) where opportunity for exposure arises**	Yes	90	100		0.69
		No	0	1000	480	6.86
5	**Mixing or blending in batch processes (multistage and/or significant contact)**	Yes	90	**200**		1.37
		No	0	2000	480	13.71
6	**Calendering operations**	Yes	90	**200**		2.74
		No	0	2000	960	27.43
7	**Industrial spraying**	Yes	95	100		2.14
		No	0	2000	1500	42.86
8a	**Transfer of chemicals from/to vessels / large containers at non dedicated facilities**	Yes	90	**100**		1.37
		No	0	1000	960	13.71
8b	**Transfer of chemicals from/to vessels / large containers at dedicated facilities**	Yes	95	**50**		0.69
		No	0	1000	**960**	13.71
9	**Transfer of chemicals into small containers (dedicated filling line)**	Yes	90	100		0.69
		No	0	1000	480	6.86
10	**Roller application or brushing**	Yes	**0**	**2000**		27.43
		No	0	2000	960	27.43

11	**Non industrial spraying**	Yes	n/a			
		No	n/a			
12	**Use of blowing agents for foam production**	Yes	**90**	10		0.03
		No	0	100	240	0.34
13	**Treatment of articles by dipping and pouring**	Yes	90	**200**		1.37
		No	0	2000	480	13.71
14	**Production of preparations or articles by tabletting, compression, extrusion, pelletisation**	Yes	90	50		0.34
		No	0	500	480	3.43
15	**Use of laboratory reagents in small scale laboratories**	Yes	90	10		0.03
		No	0	100	240	0.34
16	**Using material as fuel sources, limited exposure to unburned product to be expected**	Yes	90	10		0.03
		No	0	100	240	0.34
17	**Lubrication at high energy conditions and in partly open process**	Yes	**90**	**200**		2.74
		No	0	2000	960	27.43
18	**Greasing at high energy conditions**	Yes	**90**	**100**		1.37
		No	0	1000	960	13.71
19	**Hand-mixing with intimate contact (only PPE available)**	Yes	**0**	**5000**		141.43
		No	0	5000	1980	141.43
20	**Heat and pressure transfer fluids (closed systems) in dispersive use**	Yes	n/a			
		No	n/a			
21	**Low energy manipulation of substances bound in materials and/or articles**	Yes	90	10		0.28
		No	0	100	1980	2.83
22	**Potentially closed operations with minerals at elevated temperature**	Yes	90	**10**		0.28
		No	0	100	1980	2.83
23	**Open processing and transfer of minerals at elevated temperature**	Yes	90	5		0.14
		No	0	50	1980	1.41
24	**High (mechanical) energy work-up of substances bound in materials and/or articles**	Yes	80	**20**		0.57
		No	0	100	1980	2.83
25	**Hot work operations with metals**	Yes	90	**1**		0.03
		No	0	10	1980	0.28

APPENDIX C: RATIONALE FOR TRAv3 WORKER PROFESSIONAL DERMAL EXPOSURE ESTIMATES

blue upward revision compared to TRAv2 i.e. trends towards a higher exposure estimate

red downward revision compared to TRAv2 i.e. trends towards a lower exposure estimate

		LEV present?	Assigned inhalation LEV efficiency (%)	Initial predicted v3 dermal exposure (ug/cm^2/day)	Exposed skin surface (cm^2)	Predicted dermal exposure (mg/kg/day)
PROC	**Wide Dispersive Uses**					
1	**Use in closed process, no likelihood of exposure**	Yes	0	10		0.03
		No	0	**10**	240	0.03
2	**Use in closed, continuous process with occasional controlled exposure**	Yes	80	**40**		0.27
		No	0	200	480	1.37
3	**Use in closed batch process (synthesis or formulation)**	Yes	80	**40**		0.14
		No	0	**200**	240	0.69
4	**Use in batch and other process (synthesis) where opportunity for exposure arises**	Yes	80	**200**		1.37
		No	0	1000	480	6.86
5	**Mixing or blending in batch processes (multistage and/or significant contact)**	Yes	80	**400**		2.74
		No	0	2000	480	13.71
6	**Calendering operations**	Yes	80	**400**		5.49
		No	0	2000	960	27.43
7	**Industrial spraying**	Yes	n/a			
		No	n/a			
8a	**Transfer of chemicals from/to vessels/ large containers at non dedicated facilities**	Yes	80	**200**		2.74
		No	0	1000	960	13.71
8b	**Transfer of chemicals from/to vessels/ large containers at dedicated facilities**	Yes	80	**200**		2.74
		No	0	1000	**960**	13.71
9	**Transfer of chemicals into small containers (dedicated filling line)**	Yes	80	**200**		1.37
		No	0	1000	480	6.86
10	**Roller application or brushing**	Yes	**0**	**2000**		27.43
		No	0	2000	960	27.43

11	**Non industrial spraying**	Yes	80	**1000**		21.43
		No	0	5000	1500	107.14
12	**Use of blowing agents for foam production**	Yes	80	**20**		0.07
		No	0	100	240	0.34
13	**Treatment of articles by dipping and pouring**	Yes	80	**400**		2.74
		No	0	2000	480	13.71
14	**Production of preparations or articles by tabletting, compression, extrusion, pelletisation**	Yes	80	**100**		0.69
		No	0	500	480	3.43
15	**Use of laboratory reagents in small scale laboratories**	Yes	80	**20**		0.07
		No	0	100	240	0.34
16	**Using material as fuel sources, limited exposure to unburned product to be expected**	Yes	80	**20**		0.07
		No	0	100	240	0.34
17	**Lubrication at high energy conditions and in partly open process**	Yes	90	**200**		2.74
		No	0	2000	960	27.43
18	**Greasing at high energy conditions**	Yes	90	**100**		1.37
		No	0	1000	960	13.71
19	**Hand-mixing with intimate contact (only PPE available**	Yes	**0**	**5000**		141.43
		No	0	5000	1980	141.43
20	**Heat and pressure transfer fluids (closed systems) in dispersive use**	Yes	80	**50**		0.34
		No	0	250	480	1.71
21	**Low energy manipulation of substances bound in materials and/or articles**	Yes	80	**20**		0.57
		No	0	100	1980	2.83
22	**Potentially closed operations with minerals at elevated temperature**	Yes	n/a			
		No	n/a			
23	**Open processing and transfer of minerals at elevated temperature**	Yes	80	**10**		0.28
		No	0	50	1980	1.41
24	**High (mechanical) energy work-up of substances bound in materials and/or articles**	Yes	75	**25**		0.71
		No	0	100	1980	2.83
25	**Hot work operations with metals**	Yes	80	**2**		0.06
		No	0	10	1980	0.28

APPENDIX D: LEVEL OF CONTAINMENT ASSUMED FOR EACH PROC

The basis for the worker Process Categories (PROCs) is described in Appendix R12-3 of Chapter R12 of the REACH Technical Guidance. Many of these PROCs have a close similarity to the terms originally used in the TRAv1 to describe circumstances of worker exposure (ECETOC, 2004, Appendix G) although the later PROCs originate from other sources. The TRAv2 used these TGD descriptions to help ensure that the associated exposure estimates duly reflect any inherent operational condition or risk management measure that might be reasonably considered to be associated with that PROC (see Appendix C, ECETOC 2009). Version 3 continues with this approach. It has become clear, however, that despite the documentation in ECETOC 2004 and ECETOC 2009, some TRA users are unaware of the assumptions that ECETOC has applied in the development of the exposure estimates. Table D-1 summarises these.

Table D-1: Level of containment assumed for each PROC

PROC	Process categories	Examples and explanations (from TGD ChR12)	"Level of control" assumed by TRA
PROC1	Use in closed process, no likelihood of exposure	Use of the substances in high integrity contained system where little potential exists for exposures, e.g. any sampling via closed loop systems.	Closed system. Minimal release or contact expected during routine operation.
PROC2	Use in closed, continuous process with occasional controlled exposure	Continuous process but where the design philosophy is not specifically aimed at minimising emissions. It is not high integrity and occasional expose will arise e.g. through maintenance, sampling and equipment breakages.	Closed continuous process with occasional controlled exposure.
PROC3	Use in closed batch process (synthesis or formulation)	Batch manufacture of a chemical or formulation where the predominant handling is in a contained manner, e.g. through enclosed transfers, but where some opportunity for contact with chemicals occurs, e.g. through sampling.	Closed batch process with occasional controlled exposure.
PROC4	Use in batch and other process (synthesis) where opportunity for exposure arises	Use in batch manufacture of a chemical where significant opportunity for exposure arises, e.g. during charging, sampling or discharge of material, and when the nature of the design is likely to result in exposure.	Partially closed batch process with occasional controlled exposure.
PROC5	Mixing or blending in batch processes for formulation of preparations* and articles (multistage and/or significant contact)	Manufacture or formulation of chemical products or articles using technologies related to mixing and blending of solid or liquid materials, and where the process is in stages and provides the opportunity for significant contact at any stage.	Predominantly open mixing and blending of chemicals / preparations. Potential for occasional significant exposure. Level of control is lower than PROC4 due to staged character of the process.
PROC6	Calendering operations	Processing of product matrix Calendering at elevated temperature an large exposed surface.	Open processing of a polymer or similar matrix at temperatures above ambient. Potential for significant exposure.

PROC	Process categories	Examples and explanations (from TGD ChR12)	"Level of control" assumed by TRA
PROC7	Industrial spraying	Air dispersive techniques Spraying for surface coating, adhesives, polishes/cleaners, air care products, sandblasting; Substances can be inhaled as aerosols. The energy of the aero-sol particles may require advanced exposure controls; in case of coating, overspray may lead to waste water and waste.	Industrial spraying (and similar techniques) applications by manual or automated methods. Potential for significant exposures depending on the level of containment and ventilation control of the spraying activity itself.
PROC8a	Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at non-dedicated facilities	Sampling, loading, filling, transfer, dumping, bagging in non- dedicated facilities. Exposure related to dust, vapour, aerosols or spillage, and cleaning of equipment to be expected.	Open transfers of the substance. No expectation for dedicated engineering controls aimed at managing exposures. Potential for significant release.
PROC8b	Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities	Sampling, loading, filling, transfer, dumping, bagging in dedicated facilities. Exposure related to dust, vapour, aerosols or spillage, and cleaning of equipment to be expected.	Partially closed transfers of the substance. Provision of dedicated engineering controls results in potential for only occasional controlled exposure.
PROC9	Transfer of substance or preparation into small containers (dedicated filling line, including weighing)	Filling lines specifically designed to both capture vapour and aerosol emissions and minimise spillage.	Material transfers into small containers. Potential for occasional controlled exposure.
PROC10	Roller application or brushing	Low energy spreading of e.g. coatings. Including cleaning of surfaces. Substance can be inhaled as vapours, skin contact can occur through droplets, splashes, working with wipes and handling of treated surfaces.	Open manual pouring, brushing and rolling of coatings onto surface of article. Potential for significant exposures.
PROC11	Non industrial spraying	Air dispersive techniques Spraying for surface coating, adhesives, polishes/cleaners, air care products, sandblasting. Substances can be inhaled as aerosols. The energy of the aero-sol particles may require advanced exposure controls.	(In general open) spraying (and similar techniques) applications by professional groups using manual or automated methods. Potential for significant exposures.
PROC12	Use of blowing agents in manufacture of foam		Blowing of foams. Typically in predominantly enclosed systems. Potential for occasional controlled exposure.
PROC13	Treatment of articles by dipping and pouring	Immersion operations. Treatment of articles by dipping, pouring, immersing, soaking, washing out or washing in substances; including cold formation or resin type matrix. Includes handling of treated objects (e.g. after dying, plating). Substance is applied to a surface by low energy techniques such as dipping the article into a bath or pouring a preparation onto a surface.	Wet immersion operations with no specific exposure controls. Potential for occasional uncontrolled exposures.

PROC	Process categories	Examples and explanations (from TGD ChR12)	"Level of control" assumed by TRA
PROC14	Production of preparations* or articles by tabletting, compression, extrusion, pelletisation	Processing of preparations and/or substances (liquid and solid) into preparations or articles. Substances in the chemical matrix may be exposed to elevated mechanical and/or thermal energy conditions. Exposure is predominantly related to volatiles and/or generated fumes, dust may be formed as well.	Mechanical forming of solid preparations and articles. No specific exposure controls. Potential for incidental exposures.
PROC15	Use as laboratory reagent	Use of substances at small scale laboratory (< 1 l or 1 kg pre-sent at workplace). Larger laboratories and R+D installations should be treated as industrial processes.	Open manual handling of substances in laboratory. Potential for incidental exposures.
PROC16	Using material as fuel sources, limited exposure to unburned product to be expected	Covers the use of material as fuel sources (including additives) where limited exposure to the product in its unburned form is expected. Does not cover exposure as a consequence of spill-age or combustion.	Use of fuel in contained equipment. No substance transfers. Minimal release or contact expected during routine operation.
PROC17	Lubrication at high energy conditions and in partly open process	Lubrication at high energy conditions (temperature, friction) between moving parts and substance; significant part of process is open to workers. The metal working fluid may form aerosols or fumes due to rapidly moving metal parts.	Open or semi-closed lubrication of moving machinery and equipment. Potential for significant exposures to vapours and aerosols.
PROC18	Greasing at high energy conditions	Use as lubricant where significant energy or temperature is applied between the substance and the moving parts.	Greasing between moving parts in open or semi-closed systems. Potential for significant exposures.
PROC19	Hand-mixing with intimate contact and only PPE available	Addresses occupations where intimate and intentional contact with substances occurs without any specific exposure controls other than PPE.	Open manual mixing of chemicals. Potential for significant exposures, especially via dermal contact.
PROC20	Heat and pressure transfer fluids in dispersive, professional use but closed systems	Motor and engine oils, brake fluids Also in these applications, the lubricant may be exposed to high energy conditions and chemical reactions may take place during use. Exhausted fluids need to be disposed of as waste. Repair and maintenance may lead to skin contact.	Use of functional fluids in contained / dedicated equipment. No substance transfers. Potential for incidental exposures.
PROC21	Low energy manipulation of substances bound in materials and/or articles	Manual cutting, cold rolling or assembly / disassembly of material / article (including metals in massive form), possibly resulting in the release of fibres, metal fumes or dust.	Open forming, assembly and disassembly of material or articles (manual or automated). Potential for incidental exposures.
PROC22	Potentially closed processing operations with minerals/metals at elevated temperature Industrial setting	Activities at smelters, furnaces, refineries, coke ovens. Exposure related to dust and fumes to be expected. Emission from direct cooling may be relevant.	Partially closed processes and activities with metals / minerals at elevated temperature. Potential for incidental exposures.

PROC	Process categories	Examples and explanations (from TGD ChR12)	"Level of control" assumed by TRA
PROC23	Open processing and transfer operations with minerals / metals at elevated temperature	Sand and die casting, tapping and casting melted solids, drossing of melted solids, hot dip galvanising, raking of melted solids in paving. Exposure related to dust and fumes to be expected.	Open processing and transfer of hot and/or molten minerals. Potential for significant exposures to fumes and other aerosols.
PROC24	High (mechanical) energy work-up of substances bound in materials and/or articles	Substantial thermal or kinetic energy applied to substance (including metals in massive form) by hot rolling / forming, grinding, mechanical cutting, drilling or sanding. Exposure is pre-dominantly expected to be to dust. Dust or aerosol emission as result of direct cooling may be expected.	Open mechanical forming of material or articles including surface treatment. Potential for significant exposures to dusts.
PROC25	Other hot work operations with metals	Welding, soldering, gouging, brazing, flame cutting. Exposure is predominantly expected to fumes and gases.	Open assembly or disassembly of metal material or articles by melting metals. Potential for exposures to aerosols.
PROC26	Handling of solid inorganic substances at ambient temperature	Transfer and handling of ores, concentrates, raw metal oxides and scrap; packaging, un-packaging, mixing / blending and weighing of metal powders or other minerals.	*Not covered by the TRA*
PROC27a	Production of metal powders (hot processes)	Production of metal powders by hot metallurgical processes (atomisation, dry dispersion).	*Not covered by the TRA*
PROC27b	Production of metal powders (wet processes)	Production of metal powders by wet metallurgical processes (electrolysis, wet dispersion).	*Not covered by the TRA*

APPENDIX E: ESTIMATING WORKER EXPOSURES TO PROCESS FUMES

In general, the ECETOC TRA predictions do not account for the likelihood that under certain conditions, exposure will be predominantly to fumes (rather than vapours or liquid aerosols). The exception to this is for PROCs 22 to 27b which account for the fact that many processes involving metals are undertaken at temperatures above the melting point of the metal. However, as explained in Appendix B (ECETOC, 2009), the exposure estimates applied in these circumstances are based upon exposure measurements that only relate to the metals sector (note that this only applies to the PROCs 22 to 25; the ECETOC TRA does not provide predictions for PROC26, 27a and 27b).

Exposures to fumes will also occur when other types of substances which are solid at ambient temperature are handled at temperatures above their melting point, for example to facilitate their transport or mixing. Emissions from these substances at elevated temperature can be viewed as vapour, but which will condense to particles upon contact with air at (near-) ambient temperatures. In such circumstances, and in the absence of representative measured data for the use/substance, ECETOC is aware that users have applied the TRA to deliver a pragmatic and conservative approach to the prediction of fume exposures.

ECETOC is aware that, as part of the 2010 Registration process, some groups/Consortia have applied TRAv2 predictions to derive general inhalation estimates of 'fume' exposure, in circumstances (other than PROCs 22-27b) where the substance is handled above its melting point. The approaches used for such estimates vary, but can be summarised as:

1. The dustiness estimates (in mg/m^3) are applied as 'fume surrogates' for each PROC. In some cases, these are as the 'moderate' dustiness estimate (based on the fume having these characteristics). But in other cases (for example when limited actual measurements enable some form of bootstrapping for a representative range of PROCs), then the low dustiness estimates have been applied.

2. The low volatility estimate (in ppm) is used as a base exposure estimate (as molten solids are rarely handled at temperatures significantly above their melting point), which is then converted to mg/m^3 using the molecular weight of the substance. In some cases, the volatility band based on the substance's vapour pressure has been applied to provide conservative exposure estimates. The exposure assessment was then refined, if required, by an assessment of the operating conditions, physical form, and physical chemical properties of the substance.

3. Either #1 or #2 above are only applied to those PROCs where uncontained/uncontrolled exposures to the substance might reasonably be expected to occur at elevated

temperatures (and which is likely to vary, depending upon the physical and chemical properties of the substance)

None of these approaches have been formally implemented within the TRAv3 because they are based more on pragmatism than empirical data. But ECETOC has reviewed both #1 and #2 above and determined that there is a very low likelihood of any ‘false negative’ predictions. Indeed, both approaches are likely to deliver the opposite i.e. to provide very conservative (cautionary) estimates of fume exposure (with #2 generally being the most conservative).

ECETOC is unaware of any approaches that have attempted to predict dermal exposure to "fumes", other than for the metal PROCs. Presumably these exposures are generally low, based on the fact that fume exposures occur when workers are in the proximity of activities undertaken at elevated temperatures (which constitute a hazard in themselves due to burns etc.), and therefore direct skin contact is highly unlikely.

APPENDIX F: TEMPLATE OF THE SPECIFIC CONSUMER EXPOSURE DETERMINANTS (SCEDs) WITH A HOLISTIC EXAMPLE: A FUEL USE SCENARIO

Specific Consumer Exposure Determinants (SCEDs) are similar to Specific Environmental Release Categories (SpERCS). The SCEDs template can be used to adapt the conditions of use at a generic level with more refined or specific use conditions in consumer exposure scenarios. In application, it could be very useful to refine more general scenarios in the TRA consumer with exposure determinants more specific to uses or use sectors. The SCEDs template provides a transparent, consistent format to specify these more specific determinants and their basis, and facilitate the communications in the supply chain as well. The following is the consumer SCEDs, completed with an automobile refuelling scenario as an example.

Table F-1: Example of SCED for automobile refuelling scenario

Exposure Descriptor or Determinant	Value	Justification
Use description	**Consumer re-fuelling of cars and similar vehicles**	
Product/Article Use Category	PC13	
PC/AC Subcategory	None	Automobile refuelling
Product Characteristics / Properties	Insert narrative that enables the relationship between the determinants and the Product Characteristics / Properties to be ascertained e.g. volatile liquid having a VP of 1K Pa	
Product Ingredient Fraction (by weight)	100%	
Frequency of Use (events/day, and for an infrequently used product also provide days/year)	0.14	Once/week
Relevant Route(s) of Exposure	Dermal / inhalation	Oral exposure not considered relevant for this use
Dermal Specific Parameters		
Skin Contact Area (cm^2)	210	Palm of one hand, only one hand holds fuel nozzle
Skin Transfer Factor	0.05	Assumed value of no greater than 5% of material transferred from contaminated pump handle / item to skin. Long standing contamination eliminated through evaporation. Contact invariably is indirect with contaminated surfaces rather than virgin product.
Inhalation Specific Parameters		
Amount of product used per application (g)	37500	Based on 50 litres and density of 750 g/l
Exposure Time (hr)	0.05	3 minutes, 97th% value from Vainiotalo *et al*, 1999
Is product used outdoors only?	Outdoor use	
Room Volume (m^3)	100	100m^3 used as default volume (consistent with Stoffenmanager)
Ventilation specified or likely due to properties (i.e. odour, etc.) – if so what type – (open window, fan)	0.6	Outdoor air exchange rate considered to equivalent to value cited by RIVM for garages (0.6x)
Inhalation factor (fraction of total amount handles lost to air)	0.2%	Evaporative losses during refuelling expected to be <<1% based on mass balances
Oral Specific Parameters		
Volume Ingested (cm^3)	n/a	
Oral Transfer Factor	n/a	
Sector / organisation with responsibility for the sheet		

APPENDIX G: ADDITIONAL STEPS TO REFINE CONSUMER EXPOSURE ESTIMATES

Inhalation: Average the event exposure concentration(s) over the day for comparing with long-term DNEL where sufficient evidence is available for the number of events per day

The TRA tool currently assumes product use occurs daily. In reality, however, many products are used infrequently. Often infrequent use is associated with greater amounts of product per use (for example, coatings- paints), where frequent use is associated with smaller amounts. ECHA has provided some guidance on this, indicating that daily use values should first be provided, but then the assessment may be refined based upon use frequency (ECHA chapter R15, 2010c).

It is to be noted that for products used infrequently, use frequency should not be used to average out exposure over a longer time period. In the first instance, exposure should be calculated for the actual duration of an event (event exposure) and then expressed as that concentration per day. If the derived risk characterisation ratio (RCR) is lower than 1, the conclusion of the assessment is that there is no relevant risk even from the acute exposure. If the derived RCR is above 1, the assessment may be refined by using available data on event exposure, frequency, duration of exposure and other information to refine the exposure estimate. Only in situations where a substance is classified for its acute systemic toxicity, the derivation of an acute DNEL and the assessment of peak exposure would be required.

Examples of tools that incorporate the capability to refine exposure estimates based upon use frequency include the ESIG GES Risk and Exposure Tool (EGRET) and the ConsExpo model.

Inhalation / dermal: Take into account "containment" for transfer of mixtures (e.g. filling de-icing fluid from a container into another container)

For some products, a fraction of the total use amount (<1) can be spilled or evaporated during the transferring process (e.g. filling or refueling). This fraction represents the percentage of the total use amount available for inhalation or for dermal contact. It can be applied as a simple multiplier to the total use amount to further refine its dermal or inhalation exposure estimate. The EGRET tool provides an example (Appendix C in EGRET user manual) on how to implement this capability in an exposure assessment.

Introduction of additional manual transfer factors

Users can choose to make simple modifications, such as addition of manual transfer factors, to make more realistic exposure estimates. Consumer exposure equations which include the use of

transfer factors are described in SDA (2005) and HERA (2005). Equations are similar to those in the TRA, but with the addition of a factor to represent percentage retained on skin or transferred to skin, depending upon product type. Values for transfer factors are provided for several specific chemicals in the SDA document.

Take into account the fact that the product is diluted before use (dermal)

When a substance involves a dilution prior to or during use, e.g. dilution of washing solution by rinsing, the user can apply a dilution factor to further refine its dermal exposure estimate. A dilution factor (<1) is a ratio of aliquot volume of a product used to its final volume (aliquot + diluent). For example, one ml of a product was mixed with 99ml of water before its use, the dilution factor will be equal to 0.01 (or 1/100).

When appropriate, a dilution factor has been applied in both HERA and EGRET for dermal exposure assessment. ConsExpo also takes dilution factor into account in its dermal estimate for cleaning products. For example, ConsExpo used a dilution factor (80 times) in its dermal estimate for a cleaning scenario with all-purpose liquid cleaner (Prud'homme de Lodder L *et al*., 2006).

Developing an exposure scenario as a whole

When developing an exposure scenario, the user needs to develop it in an integrated fashion.

In several scenarios, using the most conservative assumptions (small room size and high use volume) result in combinations of use descriptors that are inappropriate as they are mismatched. For example, for the lubricant scenario, while the amount of product used (5000 g) may be representative of lubrication of a larger motor, such a scenario would take place in a garage or outdoors. Similarly, lawn care products are designed for outdoor use, and so large amounts should be matched with a scenario that reflects outdoor use, or use amounts should be adjusted lower for indoor use. The TRA tool does not allow for such changes per se, but because the supporting default assumptions are clearly stated (see Appendix E, ECETOC 2009), then it is possible for users to identify where such mismatch might be considered to occur and to account accordingly (assuming suitable supporting justification can be provided).

This concept was applied within EGRET when developing new scenarios.

APPENDIX H: COMPARISON OF RESULTS FROM TRAv3, TRAv2, AND CONSEXPO v4.1

Summary of Consumer TRA (v3) Tool Comparison Results

The new version of the consumer TRA tool (TRAv3) was compared to the consumer TRA (TRAv2), the ConsExpo model (v4.1), and measured data (where available) for six exposure scenarios: PC3 air care products – instant action, PC9 coatings, paints, thinners, paint removers – solvent rich (2 substances), PC13 fuels (automotive refueling), PC13 fuels (garden equipment use), and PC35 washing and cleaning products – all purpose (liquid cleaner), PC35 washing and cleaning products – all purpose (trigger spray cleaner).

Approach:

1. TRAv3 and TRAv2 were run using a hypothetical solvent: MW = 200g/mole, VP = 2000Pa, $\log K_{ow}$ = 2 for all the testing scenarios except for PC13 fuels. Fuel scenarios were tested using a substance closer to a hypothetical fuel (MW = 105 g/mole, VP = 90000 Pa, $\log K_{ow}$ of 4). These MW and VP values were chosen so that exposure estimates based upon the tool would fall below the saturated vapour concentration of the hypothetical substance.

2. Next, ConsExpo was run in three different settings for the two hypothetical substances:
    a. In ConsExpo default settings (default mode and values)
    b. In lower tier (LT) mode with TRAv3 defaults as input values (instantaneous release for inhalation, instant application for dermal)
    c. In higher tier (HT) mode with TRAv3 defaults as input values (evaporation release for inhalation, constant application for dermal)

3. Measured exposure values from publications were available for four exposure scenarios: solvent rich wall painting, automotive refueling, garden equipment use, and trigger spray cleaning (see Appendix I).
    a. ConsExpo was run in a higher tier mode with the published inputs for these scenarios, except for the 2 fuel use scenarios. For the two fuel scenarios, ConsExpo was run with TRA defaults instead, as scenario descriptive parameters were not available in the publications.
    b. Similarly, TRAv3 was run with its defaults for the fuel scenarios, and published input values for the other scenarios.

Detailed model inputs and outputs reports from TRAv2, TRAv3, ConsExpo, and a summary of the literature measured data are shown in the Appendix I. ConsExpo scenarios considered most representative of the evaluated scenarios were used: pest control product with electrical evaporators used to simulate air freshener – instant action (PC3) representative of a plug-in dispenser; painting with solvent rich paints by using brush and roller used for painting scenarios (PC9); cleaning and washing with all-purpose cleaners (liquid cleaner and spray cleaner) for cleaning scenarios (PC35). There was no matched scenario in ConsExpo to simulate the TRA fuel scenarios. Thus, ConsExpo was run in evaporation mode for inhalation and constant release mode for dermal, as most representative of these scenarios, with input parameters based upon TRA defaults.

Generally, for the exposure scenarios tested (see Table H-1), TRAv3 provided similar or lower exposure predictions than the TRAv2, but higher exposure predictions (more conservative) than the ConsExpo model under default settings. When ConsExpo was run with TRA defaults, its exposure predictions were similar or lower than those from TRA tool. This reflected the inherent conservativeness of the TRA tool. With publication values as model inputs, the results obtained from the ConsExpo model were closer to the measured inhalation concentrations than the exposure estimates from TRAv2 and v3. Compared to TRAv2, TRAv3 delivers an improved realism in the consumer exposure estimates for the scenarios tested.

Table H-1: Summary Results of TRAv2, TRAv3, ConsExpo and Data Comparison

Exposure scenarios	Inhalation Event Concentration (mg/m^3)				Dermal External Event Concentration (mg/kg/day)		
	TRA v2	TRA v3	ConsExpo 4.1	Measured	TRA v2	TRA v3	ConsExpo 4.1
PC3 aircare, instant action – instant action							
generic solvent[1]	1000	870	Defaults in spray mode: 0.5; TRA v3 defaults in LT: 232; TRA v3 defaults in HT: 218	–	No dermal route in the scenario		
PC9 painting – solvent rich							
generic solvent	32500	14000	Defaults in HT: 8680; TRA v3 defaults in LT: 18000; TRA v3 defaults in HT: 11100	–	35.7	35.7	Defaults in HT: 27.2; TRA v3 defaults in LT: 35.8; TRA v3 defaults in HT: 30
substance a[2]	32500	10900	Publication values in HT: 338	Range: 16-403, Time weighted average value: 43.5	35.7	35.7	Publication defaults in HT: 0.36
substance b[2]	32500	14000	Publication values in HT: 80.5	Range: 0.17-22.1, Time weighted average value: 2.8	35.7	35.7	Publication defaults in HT: 0.034
PC13 fuel use							
generic solvent – automotive refuel[3]	125000	36800	TRA v3 defaults in HT: 506	Typical value: 113, Worst case value: 531	71.5	71.5	TRA v3 defaults in HT: 1.5
Generic solvent – garden equipment use[4]	125000	36800	TRA v3 defaults in HT: 86.9	Typical value: 22, Worst case value: 69	No dermal route in the scenario		
PC35 washing and cleaning products							
generic solvent – liquid cleaner	6250	5220	Defaults in HT: 1.6; TRA v3 defaults in LT: 7.1; TRA v3 defaults in HT: 2.4	–	71.5	71.5	Defaults in LT: 0.18; TRA v3 defaults in LT: 0.13; TRA v3 defaults in HT: 0.0063
generic solvent – trigger spray cleaner	350	103	Defaults in HT: 76.7; TRA v3 defaults in LT: 133; TRA v3 defaults in HT: 128	–	28.6	28.6	Defaults in LT: 0.49; TRA v3 defaults in LT: 1.17; TRA v3 defaults in HT: 0.4
substance c – trigger spray cleaner [5]	350	103	Publication values in HT: 2.3	1.41	28.6	28.6	Publication defaults in HT: 0.78

[1] To simulate plug in air freshener, used ConsExpo pest control product, electrical evaporators and weight fraction of 0.5

[2] Data for 2 substances in paint given in ARCADIS, 1998

[3] No matching default scenario in ConsExpo. The automotive refueling scenario was based upon literature values (Hakkola and Saarinen, 2000; Vainiotalo *et al*, 1999)

[4] No matching default scenario in ConsExpo. The garden equipment use scenario was based upon literature values (Nilsson *et al*, 1987)

[5] Data for trigger spray cleaning product use was based on the literature (Singer *et al*, 2006)

APPENDIX I: COMPARISON OF RESULTS FROM TRAv3, TRAv2, AND CONSEXPO v4.1: DETAILED MODEL INPUT AND OUTPUT

Appendix I-1. TRA runs

Table I-1-1: TRA version 2 defaults

		Default Route of Relevance							Dermal Exposure			Oral Exposure				Inhalation		Derm/Oral	All	
		ADULT			CHILD															
Descriptor	Product Subcategory	Dermal	Oral	Inhalation	Dermal	Oral	Inhalation	Product Ingredient (g/g)	Body Part Considered	Adult Contact Area (cm^2)	Child Contact Area (cm^2)	Volume Prod Swallowed (cm^3)	Body Part Considered	Adult Contact Area (cm^2)	Child Contact Area (cm^2)	Amount of prod for formula (g/event)	Exposure Time (hr)	Thickness Layer (cm)	Density (g/cm^3)	FreQ of Use (events/day)
PC3:Air care products	Aircare, instant action (aerosol sprays)	n	n	y	n	n	n	0.5								10	0.25			4
	Aircare, continuous action (solid & liquid)	y	n	y	n	n	n	0.1	1: fingertips	35.7						50	8	0.001	1	1
PC9a: Coatings, paints, thinners, removers	Waterborne latex wall paint	y	n	y	n	n	n	0.5	2: inside hands / one hand / palm of hands	428.8						3750	2.2	0.01	1	1
	Solvent rich, high solid, water borne paint	y	n	y	n	n	n	0.5	2: inside hands / one hand / palm of hands	428.8						1300	2.2	0.01	1	1
	Aerosol spray can	n	n	y	n	n	n	0.5								300	0.33			1
	Removers (paint-, glue-, wall paper-, sealant-remover)	y	n	y	n	n	n	0.9	3: hands	857.5						2000	4	0.01	1	1
PC13:Fuels	Liquids	y	n	y	n	n	n	0.5	3: hands	857.5						5000	4	0.01	1	1
PC35:Washing and cleaning products (including solvent based products)	Laundry and dish washing products	y	n	y	n	n	n	0.6	3: hands	857.5						50	1	0.01	1	1
	Cleaners, liquids (all purpose cleaners, sanitary products, floor cleaners, glass cleaners, carpet cleaners, metal cleaners)	y	n	y	n	n	n	0.5	3: hands	857.5						250	0.33	0.01	1	1
	Cleaners, trigger sprays (all purpose cleaners, sanitary products, glass cleaners)	y	n	y	n	n	n	0.2	3: hands	857.5						35	4	0.01	1	1

Table I-1-2: Sub-population specific default parameters

Sub-Population Specific Default Parameters

Default Surface Areas (Dermal Exposure)					
	Child	Adult	Child	Adult	
	Skin Contact Area		% of body surface		Comment
Whole body	4800	17500			
1: fingertips	10.6	35.7	0.2	0.20	5 finger tips
2: inside hands / one hand / palm of hands	127.2	428.8	2.7	2.5	inside hands = one hand
3: hands	254.4	857.5	5.3	4.9	
4: hands and forearms	556.8	2082.5	11.6	11.9	
5: upper part of the body	2400	8750	50	50	half body surface
6: lower part of the body	2400	8750	50	50	half body surface
7: whole body except feet, hands and head	3393.6	14315	70.7	81.8	
8: whole body	4800	17500	100	100	
Default Surface Areas (Oral Exposure)					
	Child	Adult			
1: some fingertips	10.6	35.7			same as dermal
2: fingers one hand	63.6	214.4	1.3	1.2	
3: inside one hand, all fingers	127.2	428.8	2.7	2.5	
4: area product mouthed	10	NA			
Other default parameters					
	Child	Adult			
Body Weight (kg)	10	60			
Inhalation Rate (m^3/hr)	not used	1.37			
Room volume (m^3)	not used	20			
Weight fraction (sprays only)	not used	1			

Table I-1-3: TRA version 2 – Predicted exposure concentrations (two hypothetical substances)

Descriptor	Product Subcategory	Dermal Exposure Estimate (mg/kg/day)	Oral Exposure Estimate (mg/kg/day)	Inhalation Exposure Estimate (mg/kg/day)	Inhalation Exposure Estimate (mg/m^3)
PC3:Air care products	Aircare, instant action (aerosol sprays)			**5.71E+00**	**1.00E+03**
	Aircare, continuous action (solid & liquid)				
PC9a: Coatings, paints, thinners, removers	Waterborne latex wall paint				
	Solvent rich, high solid, water borne paint	**3.57E+01**		**1.63E+03**	**3.25E+04**
	Aerosol spray can				
	Removers (paint-, glue-, wall paper-, sealant-remover)				
PC13:Fuels	Liquids	**7.15E+01**		**1.14E+04**	**1.25E+05**
PC35:Washing and cleaning products (including solvent based products)	Laundry and dish washing products				
	Cleaners, liquids (all purpose cleaners, sanitary products, floor cleaners, glass cleaners, carpet cleaners, metal cleaners)	**7.15E+01**		**4.76E+01**	**6.25E+03**
	Cleaners, trigger sprays (all purpose cleaners, sanitary products, glass cleaners)	**2.86E+01**		**3.20E+01**	**3.50E+02**

Table I-1-4: TRA version 3 defaults

		Default Route of Relevance ADULT			CHILD				Dermal Exposure			Oral Exposure				Inhalation			Derm/Oral	All	Derm/Oral
Descriptor	**Product Subcategory**	**Dermal**	**Oral**	**Inhalation**	**Dermal**	**Oral**	**Inhalation**	**Product Ingredient (g/g)**	**Body Part Considered**	**Adult Contact Area (cm^2)**	**Child Contact Area (cm^2)**	**Volume Prod Swallowed (cm^3)**	**Body Part Considered**	**Adult Contact Area (cm^2)**	**Child Contact Area (cm^2)**	**Amount of prod for formula (g/event)**	**Exposure Time (hr)**	**FreQ of Use (events/day)**	**Thickness Layer (cm)**	**Density (g/cm^3)**	**FreQ of Use (events/day)**
PC3:Air care products	**Aircare, instant action (aerosol sprays)**	n	n	y	n	n	n	0.5								10	0.25	4			
	Aircare, continuous action (solid & liquid)	y	n	y	n	n	n	0.1	1: fingertips	35.7						50	8	1	0.001	1	1
PC9a: Coatings, paints, thinners, removers	**Waterborne latex wall paint**	y	n	y	n	n	n	0.5	2: inside hands / one hand / palm of hands	428.8						3750	2.2	1	0.01	1	1
	Solvent rich, high solid, water borne paint	y	n	y	n	n	n	0.5	2: inside hands / one hand / palm of hands	428.8						1300	2.2	1	0.01	1	1
	Aerosol spray can	n	n	y	n	n	n	0.5								300	0.33	1			1
	Removers (paint-, glue-, wall paper-, sealant-remover)	y	n	y	n	n	n	0.9	3: hands	857.5						2000	4	1	0.01	1	1
PC13:Fuels	**Liquids**	y	n	y	n	n	n	0.5	3: hands	857.5						5000	4	1	0.01	1	1
PC35:Washing and cleaning products (including solvent based products)	**Laundry and dish washing products**	y	n	y	n	n	n	0.6	3: hands	857.5						50	1	1	0.01	1	1
	Cleaners, liquids (all purpose cleaners, sanitary products, floor cleaners, glass cleaners, carpet cleaners, metal cleaners)	y	n	y	n	n	n	0.5	3: hands	857.5						250	0.33	1	0.01	1	1
	Cleaners, trigger sprays (all purpose cleaners, sanitary products, glass cleaners)	y	n	y	n	n	n	0.2	3: hands	857.5						35	4	1	0.01	1	1

Table I-1-5: Sub-population specific default parameters

Sub-Population Specific Default Parameters

Default Surface Areas (Dermal Exposure)					
	Child	Adult	Child	Adult	
	Skin Contact Area		% of body surface		Comment
Whole body	4800	17500			
1: fingertips	10.6	35.7	0.2	0.20	5 finger tips
2: inside hands / one hand / palm of hands	127.2	428.8	2.7	2.5	inside hands = one hand
3: hands	254.4	857.5	5.3	4.9	
4: hands and forearms	556.8	2082.5	11.6	11.9	
5: upper part of the body	2400	8750	50	50	half body surface
6: lower part of the body	2400	8750	50	50	half body surface
7: whole body except feet, hands and head	3393.6	14315	70.7	81.8	
8: whole body	4800	17500	100	100	
Default Surface Areas (Oral Exposure)					
	Child	Adult			
1: some fingertips	10.6	35.7			same as dermal
2: fingers one hand	63.6	214.4	1.3	1.2	
3: inside one hand, all fingers	127.2	428.8	2.7	2.5	
4: area product mouthed	10	NA			
Other default parameters					
	Child	Adult			
Body Weight (kg)	10	60			
Inhalation Rate (m^3/hr)	not used	1.37			
Room volume (m^3)	not used	20			
Weight fraction (aerosols and sprays only)	not used	1			
Room ventilation (air changes per hour)		0.6			

Table I-1-6: TRA version 3 – Predicted exposure concentrations (two hypothetical substances)

Summary of Results for Consumer Product Exposure (By Product Subcategory)

Descriptor	Product Subcategory	Dermal Exposure Estimate (mg/kg/day)	Oral Exposure Estimate (mg/kg/day)	Inhalation Exposure Estimate (mg/kg/day)	Inhalation Exposure Estimate (mg/m^3)	Worst-case Exposure Scenario
PC3:Air care products	Aircare, instant action (aerosol sprays)			**4.97E+00**	**8.70E+02**	**Adult**
	Aircare, continuous action (solid & liquid)					
PC9a: Coatings, paints, thinners, removers	Waterborne latex wall paint					
	Solvent rich, high solid, water borne paint	**3.57E+01**		**7.04E+02**	**1.40E+04**	**Adult**
	Aerosol spray can					
	Removers (paint-, glue-, wall paper-, sealant-remover)					
PC13:Fuels	Liquids	**7.15E+01**		**3.36E+03**	**3.68E+04**	**Adult**
PC35:Washing and cleaning products (including solvent based products)	Laundry and dish washing products					
	Cleaners, liquids (all purpose cleaners, sanitary products, floor cleaners, glass cleaners, carpet cleaners, metal cleaners)	**7.15E+01**		**3.93E+01**	**5.22E+03**	**Adult**
	Cleaners, trigger sprays (all purpose cleaners, sanitary products, glass cleaners)	**2.86E+01**		**9.41E+00**	**1.03E+02**	**Adult**

Table I-1-7: TRA version 3 – Predicted exposure concentrations – inhalation (substance a for PC9 painting)

		Parameter:	Product Ingredient (g/g)	Amount Product Used per Application (g/event)	FreQuency of Use (events / day)	Fraction Released to Air[1] (g/g)	Dilution Fraction (unitless)	Exposure Time (hr)	Inhalation Rate (m^3/hr)	Conversion Factor	Room Volume (m^3)	Body Weight (kg)	Exposure (mg/m3)	Basis for inhalation exposure
		Algorithm:	(PI	A	FQ	F	DF	ET	IR	1000)	/ (V	BW)		SVC=saturated vapour concentration
PC9:Coatings and paints, fillers, putties, thinners	Waterborne latex wall paint													
	Solvent rich, high solid, water borne paint		0.5	1300	1	1	0.43	2.2	1.37	1000	20	60	1.09E+04	SVC
	Aerosol spray can													

Table I-1-8: TRA version 3 – Predicted exposure concentrations – inhalation (substance b for PC9 painting)

		Parameter:	Product Ingredient (g/g)	Amount Product Used per Application (g/event)	FreQuency of Use (events / day)	Fraction Released to Air[1] (g/g)	Dilution Fraction (unitless)	Exposure Time (hr)	Inhalation Rate (m^3/hr)	Conversion Factor	Room Volume (m^3)	Body Weight (kg)	Exposure (mg/m3)	Basis for inhalation exposure
		Algorithm:	(PI	A	FQ	F	DF	ET	IR	1000)	/ (V	BW)		SVC=saturated vapour concentration
PC9:Coatings and paints, fillers, putties, thinners	Waterborne latex wall paint													
	Solvent rich, high solid, water borne paint		0.5	1300	1	1	0.43	2.2	1.37	1000	20	60	1.40E+04	
	Aerosol spray can													

Appendix I-2. ConsExpo runs

Table I-2-1: PC3 air care products, pest control product with electric evaporators (generic solvent) – ConsExpo defaults, exposure to spray for inhalation

ConsExpo 4.1 report

Compound

Compound name	generic solvent	
CAS number		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	150	1/year
body weight	65	kilogram

Inhalation model: Exposure to spray

weight fraction compound	0.5	fraction
exposure duration	480	minute
room volume	16	m^3
ventilation rate	1	1/hr
mass generation rate	2.2E-5	g/sec
spray duration	480	minute
airborne fraction	1	fraction
weight fraction non-volatile	1	fraction
density non-volatile	1.5	g/cm^3
room height	2.5	metre
inhalation cut-off diameter	15	micrometre
Spraying away from exposed person		

Uptake model: Fraction

Output

Inhalation (point estimates)

inhalation mean event concentration :	0.507	mg/m^3
inhalation mean concentration on day of exposure:	0.169	mg/m^3
inhalation air concentration year average :	0.0694	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Oral non-respirable: point estimates

oral external dose :	0	mg/kg
oral acute (internal) dose :	-	mg/kg
oral chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	0	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note: weight fraction was based on TRAv3 default.

Table I-2-2: PC3 air care products, pest control product with electric evaporators (generic solvent) – TRAv3 defaults, instantaneous mode for inhalation

ConsExpo 4.1 report

Compound

Compound name :	generic solvent	
CAS number :		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	1460	1/year
body weight	60	kilogram

Inhalation model: Exposure to vapour : instantaneous release

weight fraction compound	0.5	fraction
exposure duration	0.25	hour
room volume	20	m^3
ventilation rate	0.6	1/hr
applied amount	10	gram

Uptake model: Fraction

Output

Inhalation (point estimates)

inhalation mean event concentration :	232	mg/m^3
inhalation mean concentration on day of exposure:	9.67	mg/m^3
inhalation air concentration year average :	9.67	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	0	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Table I-2-3: PC3 air care products, pest control product with electric evaporators (generic solvent) – TRAv3 defaults, evaporation mode for inhalation

ConsExpo 4.1 report

Compound

Compound name:	generic solvent	
CAS number:		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	1460	1/year
body weight	60	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.5	fraction
exposure duration	0.25	hour
room volume	20	m^3
ventilation rate	0.6	1/hr
applied amount	10	gram
release area	800	cm^2
application duration	0.25	hour
mass transfer rate	2.66E3	m/min

Uptake model: Fraction

Output

Inhalation (point estimates)

inhalation mean event concentration :	218	mg/m^3
inhalation mean concentration on day of exposure:	9.06	mg/m^3
inhalation air concentration year average :	9.06	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	0	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note: application time = exposure duration; release area = $20m^3/2.5m=800cm^2$

Table I-2-4: PC9 painting, solvent rich (generic solvent) – ConsExpo defaults, evaporation mode for inhalation, constant application for dermal

ConsExpo 4.1 report

Product

Compound

Compound name:	generic solvent	
CAS number:		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	1	1/year
body weight	65	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.5	fraction
exposure duration	132	minute
room volume	20	m^3
ventilation rate	0.6	1/hr
applied amount	1E3	gram
release area	1E5	cm^2
application duration	120	minute
mol weight matrix	300	g/mol
mass transfer rate	2.66E3	m/min

Uptake model: Fraction

Dermal model: Direct dermal contact with product : constant rate

weight fraction compound	0.5	fraction
exposed area	429	cm^2
contact rate	30	mg/min
release duration	7.2E3	second

Uptake model:

Output

Inhalation (point estimates)

inhalation mean event concentration :	8.68E3	mg/m^3
inhalation mean concentration on day of exposure:	796	mg/m^3
inhalation air concentration year average :	2.18	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Dermal : point estimates

dermal load :	4.2	mg/cm^2
dermal external dose :	27.7	mg/kg
dermal acute (internal) dose :	-	mg/kg
dermal chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	27.7	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note, both weight fraction and exposed area were based on TRAv3 defaults

Table I-2-5: PC9 painting, solvent rich (generic solvent) – TRAv3 defaults, instantaneous mode for inhalation, instant application for dermal

ConsExpo 4.1 report

Compound

Compound name:	generic solvent	
CAS number:		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	1	1/day
body weight	60	kilogram

Inhalation model: Exposure to vapour : instantaneous release

weight fraction compound	0.5	fraction
exposure duration	2.2	hour
room volume	20	m^3
ventilation rate	0.6	1/hr
applied amount	1.3E3	gram

Uptake model: Fraction

uptake fraction	1	fraction
inhalation rate	34.7	m3/day

Dermal model: Direct dermal contact with product : instant application

weight fraction compound	0.5	fraction
exposed area	429	cm^2
applied amount	4.3	gram

Uptake model: fraction

uptake fraction	1	fraction

Output

Inhalation (point estimates)

inhalation mean event concentration :	1.8E4	mg/m^3
inhalation mean concentration on day of exposure:	1.65E3	mg/m^3
inhalation air concentration year average :	1.65E3	mg/m^3/day
inhalation acute (internal) dose :	957	mg/kg
inhalation chronic (internal) dose :	957	mg/kg/day

Dermal : point estimates

dermal load :	5.01	mg/cm^2
dermal external dose :	35.8	mg/kg
dermal acute (internal) dose :	35.8	mg/kg
dermal chronic (internal) dose :	35.8	mg/kg/day

Integrated (point estimates)

total external dose:	992	mg/kg
total acute dose (internal):	992	mg/kg
total chronic dose (internal):	992	mg/kg/day

Table I-2-6: PC9 painting, solvent rich (generic solvent) – TRAv3 defaults, evaporation mode for inhalation, constant application for dermal

ConsExpo 4.1 report

Compound

Compound name:	generic solvent	
CAS number:		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	1	1/year
body weight	60	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.5	fraction
exposure duration	2.2	hour
room volume	20	m^3
ventilation rate	0.6	1/hr
applied amount	1.3E3	gram
release area	1E5	cm^2
application duration	120	minute
mol weight matrix	300	g/mol
mass transfer rate	2.66E3	m/min

Uptake model: Fraction

Dermal model: Direct dermal contact with product : constant rate

weight fraction compound	0.5	fraction
exposed area	429	cm^2
contact rate	30	mg/min
release duration	7.2E3	second

Uptake model:

Output

Inhalation (point estimates)

inhalation mean event concentration :	1.11E4	mg/m^3
inhalation mean concentration on day of exposure:	1.02E3	mg/m^3
inhalation air concentration year average :	2.79	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Dermal : point estimates

dermal load :	4.2	mg/cm^2
dermal external dose :	30	mg/kg
dermal acute (internal) dose :	-	mg/kg
dermal chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	30	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note, ConsExpo defaults were used for release area, dermal contact rate, and application time.

Table I-2-7: PC9 painting, solvent rich (substance a) – publication defaults, evaporation mode for inhalation, constant application for dermal

ConsExpo 4.1 report

Compound

Compound name:	substance a	
CAS number:		
molecular weight	142	g/mol
vapour pressure	191	Pascal
KOW	5.01	10Log

General Exposure Data

exposure frequency	1	1/year
body weight	60	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.0214	fraction
exposure duration	33.7	minute
room volume	30.3	m^3
ventilation rate	0.48	1/hr
applied amount	4.93E3	gram
release area	29.5	m^2
application duration	33.7	minute
mol weight matrix	300	g/mol
mass transfer rate	3.16E3	m/min

Uptake model: Fraction

uptake fraction	1	fraction
inhalation rate	32.9	m^3/day

Dermal model: Direct dermal contact with product : constant rate

weight fraction compound	0.0214	fraction
exposed area	429	cm^2
contact rate	30	mg/min
release duration	33.7	minute

Uptake model: fraction

uptake fraction	1	fraction

Output

Inhalation (point estimates)

inhalation mean event concentration :	338	mg/m^3
inhalation mean concentration on day of exposure:	7.9	mg/m^3
inhalation air concentration year average :	0.0216	mg/m^3/day
inhalation acute (internal) dose :	4.34	mg/kg
inhalation chronic (internal) dose :	0.0119	mg/kg/day

Dermal : point estimates

dermal load :	0.0504	mg/cm^2
dermal external dose :	0.361	mg/kg
dermal acute (internal) dose :	0.361	mg/kg
dermal chronic (internal) dose :	0.000987	mg/kg/day

Integrated (point estimates)

total external dose:	4.7	mg/kg
total acute dose (internal):	4.7	mg/kg
total chronic dose (internal):	0.0129	mg/kg/day

Note, ConsExpo default was used for dermal contact rate. application duration = exposure duration, release duration = exposure duration

Table I-2-8: PC9 painting, solvent rich (substance b) – publication defaults, evaporation mode for inhalation, constant application for dermal

ConsExpo 4.1 report

Compound

Compound name :	substance b	
CAS number :		
molecular weight	106	g/mol
vapour pressure	881	Pascal
KOW	3.12	10Log

General Exposure Data

exposure frequency	1	1/year
body weight	60	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.00202	fraction
exposure duration	33.7	minute
room volume	30.3	m^3
ventilation rate	0.48	1/hr
applied amount	4.93E3	gram
release area	29.5	m^2
application duration	33.7	minute
mol weight matrix	300	g/mol
mass transfer rate	3.66E3	m/min

Uptake model: Fraction

uptake fraction	1	fraction
inhalation rate	32.9	m^3/day

Dermal model: Direct dermal contact with product : constant rate

weight fraction compound	0.00202	fraction
exposed area	429	cm^2
contact rate	30	mg/min
release duration	33.7	minute

Uptake model: fraction

uptake fraction	1	fraction

Output

Inhalation (point estimates)

inhalation mean event concentration :	80.5	mg/m^3
inhalation mean concentration on day of exposure:	1.88	mg/m^3
inhalation air concentration year average :	0.00516	mg/m^3/day
inhalation acute (internal) dose :	1.03	mg/kg
inhalation chronic (internal) dose :	0.00283	mg/kg/day

Dermal : point estimates

dermal load :	0.00476	mg/cm^2
dermal external dose :	0.034	mg/kg
dermal acute (internal) dose :	0.034	mg/kg
dermal chronic (internal) dose :	9.32E-5	mg/kg/day

Integrated (point estimates)

total external dose:	1.07	mg/kg
total acute dose (internal):	1.07	mg/kg
total chronic dose (internal):	0.00292	mg/kg/day

Note, ConsExpo default was used for dermal contact rate. application duration = exposure duration, release duration = exposure duration

Table I-2-9: PC13 fuels – TRAv3 defaults, evaporation mode for inhalation, instant mode for dermal

ConsExpo 4.1 report

Compound

Compound name :	automotive refuel	
CAS number :		
molecular weight	105	g/mol
vapour pressure	9E4	Pascal
KOW	4	10Log

General Exposure Data

exposure frequency	1	1/week
body weight	60	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	1	fraction
exposure duration	3	minute
room volume	100	m^3
ventilation rate	0.6	1/hr
applied amount	75	gram
release area	40	cm^2
application duration	3	minute
mass transfer rate	3.67E3	m/min

Uptake model: Fraction

uptake fraction	1	fraction
inhalation rate	32.9	m^3/day

Dermal model: Direct dermal contact with product : constant rate

weight fraction compound	1	fraction
exposed area	210	cm^2
contact rate	30	mg/min
release duration	3	minute

Uptake model: fraction

uptake fraction	1	fraction

Output

Inhalation (point estimates)

inhalation mean event concentration :	506	mg/m^3
inhalation mean concentration on day of exposure:	1.05	mg/m^3
inhalation air concentration year average :	0.151	mg/m^3/day
inhalation acute (internal) dose :	0.578	mg/kg
inhalation chronic (internal) dose :	0.0826	mg/kg/day

Dermal : point estimates

dermal load :	0.429	mg/cm^2
dermal external dose :	1.5	mg/kg
dermal acute (internal) dose :	1.5	mg/kg
dermal chronic (internal) dose :	0.214	mg/kg/day

Integrated (point estimates)

total external dose:	2.08	mg/kg
total acute dose (internal):	2.08	mg/kg
total chronic dose (internal):	0.297	mg/kg/day

Note, release area = π*(D/2)2= π*(7/2)2=40cm^2, 7cm is a conservative estimated diameter of an automotive gas tank nozzle (¾" based upon [http://www.opwglobal.com/Product.aspx?pid=1]). Application duration = exposure duration, release duration = exposure duration. ConsExpo default contact rate for painting-solvent rich scenario was used.

Table I-2-10: PC13 fuels – TRAv3 defaults, evaporation mode for inhalation, constant mode for dermal

ConsExpo 4.1 report

Compound

Compound name :	garden equipment use	
CAS number :		
molecular weight	105	g/mol
vapour pressure	9E4	Pascal
KOW	4	10Log

General Exposure Data

exposure frequency	0.5	1/week
body weight	60	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	1	fraction
exposure duration	2	hour
room volume	100	m^3
ventilation rate	0.6	1/hr
applied amount	15	gram
release area	40	cm^2
application duration	2	hour
mass transfer rate	3.67E3	m/min

Uptake model: Fraction

uptake fraction	1	fraction
inhalation rate	32.9	m^3/day

Output

Inhalation (point estimates)

inhalation mean event concentration :	86.9	mg/m^3
inhalation mean concentration on day of exposure:	7.25	mg/m^3
inhalation air concentration year average :	0.518	mg/m^3/day
inhalation acute (internal) dose :	3.97	mg/kg
inhalation chronic (internal) dose :	0.284	mg/kg/day

Integrated (point estimates)

total external dose:	3.97	mg/kg
total acute dose (internal):	3.97	mg/kg
total chronic dose (internal):	0.284	mg/kg/day

Table I-2-11: PC35 washing and cleaning products, all-purpose liquid cleaner (generic solvent) – ConsExpo defaults, evaporation mode for inhalation, instant application for dermal

ConsExpo 4.1 report

Compound

Compound name :	generic solvent	
CAS number :		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	104	1/year
body weight	65	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.000625	fraction
exposure duration	240	minute
room volume	58	m^3
ventilation rate	0.5	1/hr
applied amount	400	gram
release area	1E5	cm^2
application duration	20	minute
mol weight matrix	18	g/mol
mass transfer rate	2.66E3	m/min

Uptake model: Fraction

inhalation rate	24.1	litre/min

Dermal model: Direct dermal contact with product : instant application

weight fraction compound	0.000625	fraction
exposed area	1.9E3	cm^2
applied amount	19	gram

Uptake model:

Output

Inhalation (point estimates)

inhalation mean event concentration :	1.57	mg/m^3
inhalation mean concentration on day of exposure:	0.262	mg/m^3
inhalation air concentration year average :	0.0746	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Dermal : point estimates

dermal load :	0.00625	mg/cm^2
dermal external dose :	0.183	mg/kg
dermal acute (internal) dose :	-	mg/kg
dermal chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	0.323	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note, weight fraction = TRAv3 product ingredient (0.5) divided by a dilution factor of 80 based upon RIVM cleaning products fact sheet.

Table I-2-12: PC35 washing and cleaning products, all-purpose liquid cleaner (generic solvent) – TRAv3 defaults, instantaneous mode for inhalation, instant application for dermal

ConsExpo 4.1 report

Compound

Compound name :	generic solvent	
CAS number :		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	1	1/year
body weight	60	kilogram

Inhalation model: Exposure to vapour : instantaneous release

weight fraction compound	0.000625	fraction
exposure duration	0.33	hour
room volume	20	m^3
ventilation rate	0.6	1/hr
applied amount	250	gram

Dermal model: Direct dermal contact with product : instant application

weight fraction compound	0.000625	fraction
exposed area	858	cm^2
applied amount	12.5	gram

Uptake model:

Output

Inhalation (point estimates)

inhalation mean event concentration :	7.09	mg/m3
inhalation mean concentration on day of exposure:	0.0975	mg/m3
inhalation air concentration year average :	0.000267	mg/m3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Dermal : point estimates

dermal load :	0.00911	mg/cm^2
dermal external dose :	0.13	mg/kg
dermal acute (internal) dose :	-	mg/kg
dermal chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	0.187	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note, weight fraction = TRAv3 product ingredient (0.5) divided by a dilution factor of 80 based upon RIVM cleaning products fact sheet. Applied amount on skin = 5% of product amount used.

Table I-2-13: PC35 washing and cleaning products, all-purpose liquid cleaner (generic solvent) – TRAv3 defaults, evaporation mode for inhalation, constant application for dermal

ConsExpo 4.1 report

Compound

Compound name :	generic solvent	
CAS number :		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	1	1/year
body weight	60	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.000625	fraction
exposure duration	0.33	hour
room volume	20	m^3
ventilation rate	0.6	1/hr
applied amount	250	gram
release area	1E5	cm^2
application duration	20	minute
mol weight matrix	18	g/mol
mass transfer rate	2.66E3	m/min

Uptake model: Fraction

Dermal model: Direct dermal contact with product : constant rate

weight fraction compound	0.000625	fraction
exposed area	858	cm^2
contact rate	30	mg/min
release duration	1.2E3	second

Uptake model:

Output

Inhalation (point estimates)

inhalation mean event concentration :	2.4	mg/m^3
inhalation mean concentration on day of exposure:	0.033	mg/m^3
inhalation air concentration year average :	9.04E-5	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Dermal : point estimates

dermal load :	0.000437	mg/cm^2
dermal external dose :	0.00625	mg/kg
dermal acute (internal) dose :	-	mg/kg
dermal chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	0.00625	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note, weight fraction = TRAv3 product ingredient (0.5) divided by a dilution factor of 80 based upon RIVM cleaning products fact sheet. ConsExpo default contact rate for painting-solvent rich scenario was used.

Table I-2-14: PC35 washing and cleaning products, all-purpose trigger spray cleaner (generic solvent) – ConsExpo defaults, evaporation mode for inhalation, instant application for dermal

ConsExpo 4.1 report

Compound

Compound name :	generic solvent	
CAS number :		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	365	1/year
body weight	65	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.2	fraction
exposure duration	60	minute
room volume	15	m^3
ventilation rate	2.5	1/hr
applied amount	16.2	gram
release area	1.71E4	cm^2
application duration	10	minute
mol weight matrix	22	g/mol
mass transfer rate	2.66E3	m/min

Dermal model: Direct dermal contact with product : instant application

weight fraction compound	0.2	fraction
exposed area	215	cm^2
applied amount	0.16	gram

Uptake model:

Output

Inhalation (point estimates)

inhalation mean event concentration :	76.7	mg/m^3
inhalation mean concentration on day of exposure:	3.2	mg/m^3
inhalation air concentration year average :	3.19	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Dermal : point estimates

dermal load :	0.149	mg/cm^2
dermal external dose :	0.492	mg/kg
dermal acute (internal) dose :	-	mg/kg
dermal chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	2.2	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note, weight fraction = TRAv3 product ingredient (0.5)

Table I-2-15: PC35 washing and cleaning products, all-purpose trigger spray cleaner (generic solvent) – TRAv3 defaults, instantaneous mode for inhalation, instant application for dermal

ConsExpo 4.1 report

Compound

Compound name :	generic solvent	
CAS number :		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	1	1/year
body weight	60	kilogram

Inhalation model: Exposure to vapour : instantaneous release

weight fraction compound	0.2	fraction
exposure duration	4	hour
room volume	20	m^3
ventilation rate	0.6	1/hr
applied amount	35	gram

Uptake model: Fraction

inhalation rate	24.1	litre/min

Dermal model: Direct dermal contact with product : instant application

weight fraction compound	0.2	fraction
exposed area	858	cm^2
applied amount	0.35	gram

Uptake model:

Output

Inhalation (point estimates)

inhalation mean event concentration :	133	mg/m^3
inhalation mean concentration on day of exposure:	22.1	mg/m^3
inhalation air concentration year average :	0.0605	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Dermal : point estimates

dermal load :	0.0816	mg/cm^2
dermal external dose :	1.17	mg/kg
dermal acute (internal) dose :	-	mg/kg
dermal chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	13.9	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note, applied amount on skin = 1% of product amount used.

Table I-2-16: PC35 washing and cleaning products, all-purpose trigger spray cleaner (generic solvent) – TRAv3 defaults, evaporation mode for inhalation, constant application for dermal

ConsExpo 4.1 report

Compound

Compound name :	generic solvent	
CAS number :		
molecular weight	200	g/mol
vapour pressure	2E3	Pascal
KOW	2	10Log

General Exposure Data

exposure frequency	1	1/year
body weight	60	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.2	fraction
exposure duration	4	hour
room volume	20	m^3
ventilation rate	0.6	1/hr
applied amount	35	gram
release area	1E5	cm^2
application duration	20	minute
mol weight matrix	18	g/mol
mass transfer rate	2.66E3	m/min

Uptake model: Fraction

Dermal model: Direct dermal contact with product : constant rate

weight fraction compound	0.2	fraction
exposed area	858	cm^2
contact rate	6	mg/min
release duration	20	minute

Uptake model:

Output

Inhalation (point estimates)

inhalation mean event concentration :	128	mg/m^3
inhalation mean concentration on day of exposure:	21.3	mg/m^3
inhalation air concentration year average :	0.0584	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Dermal : point estimates

dermal load :	0.028	mg/cm^2
dermal external dose :	0.4	mg/kg
dermal acute (internal) dose :	-	mg/kg
dermal chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	0.4	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Note, contact rate of 6mg/min was used (assume 1/5 of contact rate used in ConsExpo for all purpose cleaner liquid).

Table I-2-17: PC35 washing and cleaning products, all-purpose trigger spray cleaner (substance c) – publication values, evaporation mode for inhalation, constant application for dermal

ConsExpo 4.1 report

Compound

Compound name :	substance c	
CAS number :		
molecular weight	118	g/mol
vapour pressure	117	Pascal
KOW	0.83	10Log

General Exposure Data

exposure frequency	1	1/day
body weight	60	kilogram

Inhalation model: Exposure to vapour : evaporation

weight fraction compound	0.026	fraction
exposure duration	60	minute
room volume	50	m^3
ventilation rate	0.52	1/hr
applied amount	6.3	gram
release area	0.56	m^2
application duration	2	minute
mol weight matrix	22	g/mol
mass transfer rate	3.47E3	m/min

Dermal model: Direct dermal contact with product : constant rate

weight fraction compound	0.026	fraction
exposed area	215	cm^2
contact rate	30	mg/min
release duration	1	hour

Uptake model: fraction

Output

Inhalation (point estimates)

inhalation mean event concentration :	2.29	mg/m^3
inhalation mean concentration on day of exposure:	0.0953	mg/m^3
inhalation air concentration year average :	0.0953	mg/m^3/day
inhalation acute (internal) dose :	-	mg/kg
inhalation chronic (internal) dose :	-	mg/kg/day

Dermal : point estimates

dermal load :	0.218	mg/cm^2
dermal external dose :	0.78	mg/kg
dermal acute (internal) dose :	-	mg/kg
dermal chronic (internal) dose :	-	mg/kg/day

Integrated (point estimates)

total external dose:	0.78	mg/kg
total acute dose (internal):	-	mg/kg
total chronic dose (internal):	-	mg/kg/day

Appendix I-3. References for the measured data

PC9 – painting scenarios for 2 substances

The painting scenarios included are based on an EPA test house painting study (ARCADIS, 1998): painting gypsum walls of a bedroom with solvent rich paint. Two of the chemical components in the paint (substance a and b) were used for this test. The measured concentration of substance a ranged from 16 to 403 mg/m^3 over 24 hrs, with an event concentration of 43.5 mg/m^3. The measured concentration of substance b ranged from 0.17 to 22.1 mg/m^3, with an event concentration of 2.8 mg/m^3. The study parameters are given in Table I-3-1 . With these study parameters as inputs, the predictions from the ConsExpo are 338 mg/m^3 for substance a and 80.5 mg/m^3 for substance b, more conservative than the measured concentrations.

Table I-3-1 Parameter values used to estimate PC9 exposures

Parameters from the Study	Substance a	Substance b
Molecular weight (g/mol)	142	106
Vapour pressure (Pa)	191	881
LogK_{ow}	5.01	3.12
Weight fraction	0.0214	0.00202
Exposure duration (mins)	33.7	
Room volume (m^3)	30.3	
Ventilation rate (1/hr)	0.48	
Applied amount (g)	4930	
Release area (m^2)	29.5	
Predictions based on ConsExpo (mg/m^3)	**338**	**80.5**
Measured data (mg/m^3)	**43.5 (16-403)**	**2.8 (0.17-22.1)**

PC13 – two fuel use scenarios

Two fuel use scenarios were used in this test: automotive refueling and garden equipment use. For the automotive refueling scenario, a typical airborne concentration was 113 mg/m^3 and a reasonable worst case value was as a typical value and 531 mg/m^3 based upon Hakkola and Saarinen (2000). For a 70-kg person with an exposed skin area of 420 cm^2 and dermal uptake rate of 0.03 mg/day, predicted dermal intake using the SkinPerm model was 0.0004 mg/kg/day. For garden equipment use scenario, a typical airborne concentration measurement was 22 mg/m^3

and a worst case value was 69 mg/m^3 based upon Nilsson *et al* (1987). No dermal contact from the use of garden equipment was expected.

The study measurements and model predictions for all the scenarios are given in Table I-3-2. With these study parameters as inputs, the predictions from ConsExpo (87-506 mg/m^3 for inhalation, 1.5mg/kg/day for dermal) were more conservative than their corresponding typical measured inhalation values (22-113 mg/m^3) and SkinPerm predicted dermal uptake (0.0004 mg/kg/day).

Table I-3-2: Measured data and model predictions for PC13

Concentrations	Automotive refuel	Garden equipment use
Inhalation predictions based on ConsExpo (mg/m^3)	506	86.9
Measured data – inhalation (mg/m^3)	113 (median value), 531 (worst case value)	22, 69 (worst case value)
Dermal predictions based on ConsExpo (mg/kg/day)	1.5	–
Dermal predictions based on SkinPerm – dermal (mg/kg/day)	0.0004	–

PC35 – washing and cleaning products with trigger spray

A simulated cleaning experiment with a trigger spray cleaner was conducted by Singer *et al*, (2006). One of the product constituents (substance c) was used in this test. First, 6ml of the product was sprayed onto a 0.56-m^2 section of a laminate table top. The wetted surface was wiped clean with paper towels 1min after the application. The spray and clean procedure lasted for 2 mins. The study parameters are given in Table I-3-3. No dermal exposure measurement was provided in the study. The inhalation prediction from the ConsExpo provides a conservative estimate.

Table I-3-3: Summary of study parameters from Singer et al. (2006)

Parameters from the Studies	Substance c
Molecular weight (g/mol)	118
Vapour pressure (Pa)	117
LogK_{ow}	0.83
Weight fraction	0.026
Application duration (mins)	2
Room volume (m^3)	50
Ventilation rate (1/hr)	0.52
Applied amount (g)	6.3
Release area (cm^2)	5200
Inhalation predictions based on ConsExpo (mg/m^3)	**2.3**
Measured data – inhalation (mg/m^3)	**1.41**

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