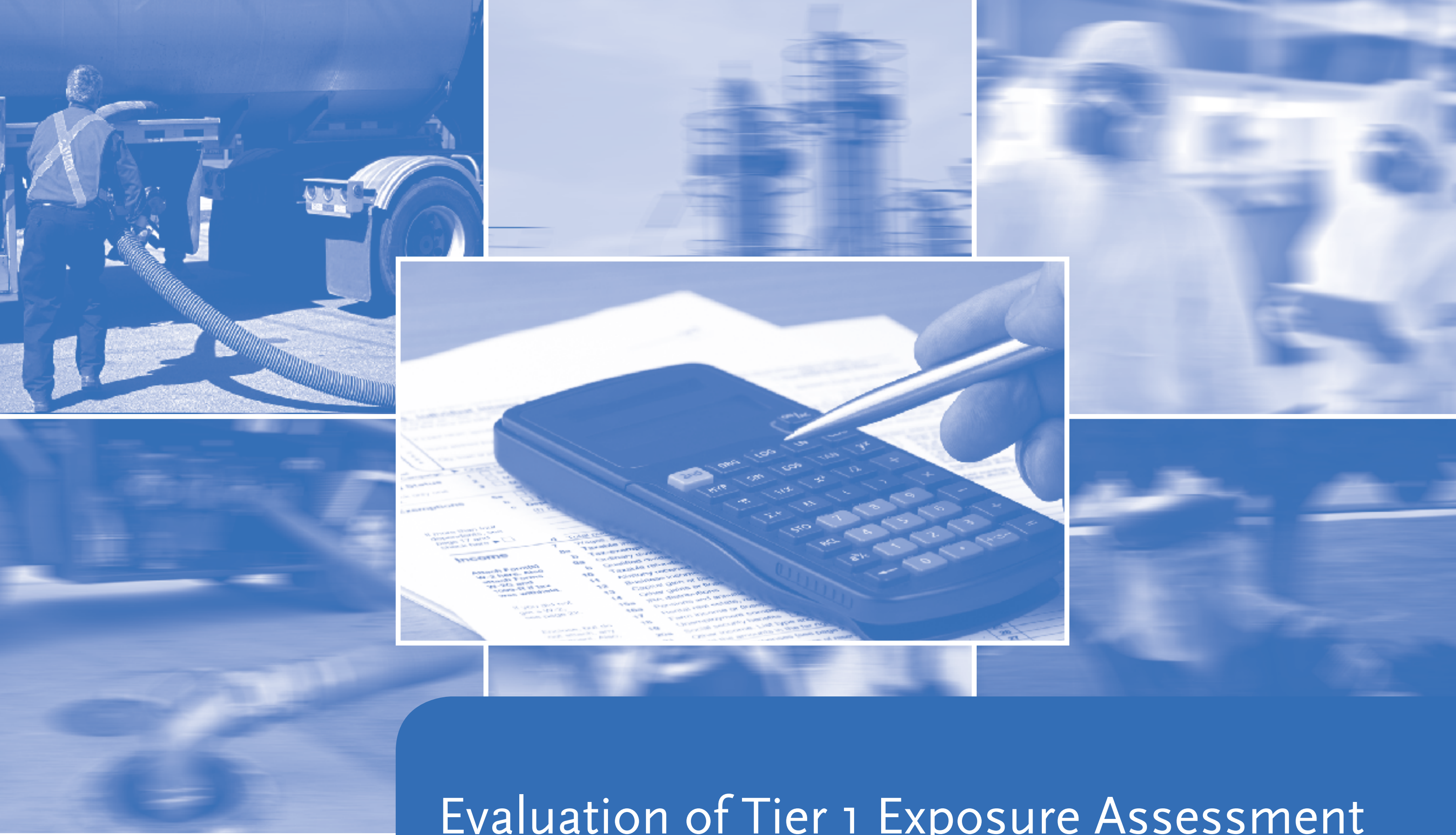

Evaluation of Tier 1 Exposure Assessment Models under REACH (eteam) Project

Final Overall Project Summary Report

J. Lamb, S. Hesse, B. G. Miller, L. MacCalman, K. Schroeder, J. Cherrie, M. van Tongeren

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The responsibility for the contents of this publication lies with the authors.

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Abstract

The Tier 1 exposure tools ECETOC TRA, MEASE, STOFFENMANAGER, EMKG-EXPO-TOOL and RISKOFDERM used for REACH are designed to be simple and easy to use by a range of assessors and to provide conservative estimate of exposure. The eteam Project aimed to carry out a comprehensive evaluation of the Tier 1 exposure tools. This report provides a summary of the main results of the evaluation together with the authors' assessment of the main implications. Recommendations are made for tool developers, users and regulators.
The project incorporated a range of qualitative and quantitative evaluation methods in the different work packages. These methods are detailed in the accompanying deliverable reports.

The tools differ in their underlying basis and in the number and definition of a limited range of input parameters. The tools were considered to be user-friendly and easy to access, download and use. However, extremely large variability was observed in outputs generated by a group of representative tool users (n=146) when assessing identical exposure situations. A small number of input parameters drove most of the variation; the task descriptor (PROC code or handling description), risk management measures and type of setting. This type of variability has been identified with all exposure assessment tools involving subjective assessment of parameters. An evaluation of tool uncertainty found that the type and level of uncertainty was heavily dependent on the individual situation being assessed, and should be considered in the context of the overall uncertainty of the exposure assessment process. The uncertainty arising from using Tier 1 tools is designed to be addressed by providing conservative estimates of exposure. Estimates of the tools were generally conservative, but did not always provide estimates that would be considered as a reasonable worst-case (as defined by the 90th percentile of exposure). Correlations between the measurement results and tool predictions were generally stronger for powders and non-volatile liquids than for the other exposure categories.

Comparison with measurement data suggested that the tools were generally conservative, but perhaps not always sufficiently so when compared with the reasonable worst case estimates as defined by the 90th percentiles of the exposure distribution. STOFFENMANAGER appeared to provide the most balanced performance with regard to the level of conservatism and predictive power for volatile liquids and powders. Furthermore, systems should be developed and applied to reduce the extreme levels of variability between users. Tool users must be more aware of the appropriate operation of the tools and their limitations. Improved quality assurance procedures including user certification and round-robin exercises, together with team-based assessments, the application of different models in tandem and corroboration of tool estimates with any available measurement data, should help improve the reliability of all of the tools.

Key words: exposure assessment; exposure modelling; REACH; inter-assessor variability; reliability; user-friendliness; uncertainty; conceptual basis; risk assess

Endbericht zur Evaluierung von Tier 1-Modellen (eteam-Projekt)

Kurzreferat

Die Tier 1-Expositionstools, wie ECETOC TRA, MEASE, STOFFENMANAGER, EMKG-EXPO-TOOL und RISKOFDERM, die unter REACH verwendet werden, sind mit dem Ziel entwickelt worden, den Anwendern unkompliziert und zuverlässig konservative Expositionsabschätzungen zu liefern. Das eteam-Projekt zielte darauf ab, die Tier 1-Tools umfassend zu evaluieren. Der Report gibt eine zusammengefasste Beurteilung der Autoren zu den wesentlichen Projektergebnissen sowie Empfehlungen für die Toolentwickler, Anwender und Regulatoren. Die Evaluierungsmethoden werden in den begleitenden Reports (Substudy Reports) ausführlich beschrieben.

Die Tools unterscheiden sich bezüglich der ihnen zu Grunde liegenden Datenbasis sowie in Anzahl und Definition der begrenzten Bandbreite ihrer Inputparametern. Sie sind allgemein als benutzerfreundlich und einfach auffindbar und anwendbar einzustufen. Allerdings wurde bei Modellberechnungen, durchgeführt von einer repräsentativen Gruppe von Toolanwendern (n=146) für identische Expositionssituationen eine sehr hohe Variabilität beobachtet. Eine kleine Gruppe an Inputparametern verursachte dabei einen Großteil der Variation: Die Beschreibung der Tätigkeit (PROC oder Beschreibung der Handhabung), Risikominimierungsmaßnahmen und der Arbeitsbereich („industrial“ (Industriebetrieb) vs. „professional“ (Handwerker)). Diese Variabilität wurde bei allen Tools identifiziert, die eine subjektive Zuordnung von Parametern verlangen.

Die Evaluierung der Toolunsicherheit kommt zum Ergebnis, dass Art und Ausprägung der Unsicherheit stark von der jeweilig betrachteten Situation abhängen. Daher ist die Gesamtunsicherheit des Expositionsbestimmungsprozesses im Kontext zu betrachten. Die Unsicherheiten von Tier 1-Tools müssen somit über ein entsprechend konservatives Design Berücksichtigung finden.

Ein Vergleich mit gemessenen Daten legt nahe, dass die Tools im Allgemeinen konservativ sind, allerdings nicht immer in ausreichendem Maße, wenn dies mit dem „reasonable worst case“, also dem 90. Perzentil der Expositionsverteilung, verglichen wird. Korrelationen zwischen Messergebnissen und Toolvorhersagen waren für Stäube und nicht-flüchtige Flüssigkeiten generell stärker als für andere Expositionskategorien. STOFFENMANAGER liefert die ausgewogenste Leistung im Hinblick auf das Schutzniveau und die Vorhersagekraft für flüchtige Flüssigkeiten und Stäube. Grundsätzlich sollten Lösungsansätze entwickelt werden, um die extremen Größenordnungen der Variabilität zwischen verschiedenen Anwendern zu reduzieren. Tool-Anwender müssen sich der angemessenen Bedienung der Tools und deren Beschränkungen mehr bewusst sein. Verbesserte Qualitätssicherungsmaßnahmen sollten helfen, die Verlässlichkeit aller Tools zu steigern. Dies schließt sowohl Anwenderzertifikate und Ringversuche als auch gruppenbasierte Berechnungen unter Anwendung verschiedener Modelle und anschließende Vergleiche mit zugänglichen Messdaten ein.

Schlagwörter: Expositionsabschätzung; Expositionsmodellierung; REACH; Variabilität zwischen Anwendern; Zuverlässigkeit; Anwenderfreundlichkeit; Unsicherheit; konzeptionelle Grundlagen; Risikoabschätzung

1 Introduction

Within the European Union, the Registration, Evaluation, Authorisation and restriction of Chemicals (REACH) Regulation (EU, 2007), requires the registration of chemicals by manufacturers and suppliers by a number of deadlines scheduled from 2008 until 2018. Following registration, substances will be authorised for use only in specified ways. As part of the registration process, the manufacturer or supplier is required to prepare a dossier of information on the substance, which includes a chemical safety report (CSR), containing an exposure assessment for the work activities for which the substance is used.

REACH guidance requires the sharing of toxicological and other data between companies, to improve the quality of hazard information available to the risk assessment process and reduce the need for unnecessary duplication of animal testing. The information within the dossier is used to provide guidance on safe working methods for intermediate and end users of the substances through the provision of detailed exposure scenarios and their dissemination via the supply chain. These describe the control measures needed to reduce exposure by a specified route to below the Derived No Effect Level (DNEL) or Derived Minimal Effect Level (DMEL) for the substance.

A number of computer-based tools have been developed to address the needs of industry, regulators and researchers in qualitatively and quantitatively assessing the exposure of workers to hazardous substances. These tools are used to predict exposures for a particular combination of workplace factors. The models vary in domain of application, level of detail and outputs, from simple screening tools, which are designed to easily and quickly differentiate those situations which may pose a risk to health from those which do not, to more advanced, higher level tools which give a more refined estimate of exposure.

Several screening (Tier 1) tools and higher level (Tier 2) tools that predict workers' inhalation and/or dermal exposures are mentioned in the REACH guidance, and are therefore used by registrants. Where the safety of a specific use of a substance is unclear at the first stage screening assessment, REACH guidance indicates that higher tier modelling and/ or measurements of exposure in the relevant situation should be carried out. The tools commonly used for Tier 1 assessments include the ECETOC Targeted Risk Assessment (TRA); -STOFFENMANAGER®; the EMKG-EXPO-TOOL; MEASE and RISKOFDERM. The Advanced REACH Tool (ART) has been developed and used to provide a more accurate prediction of exposure (Tier 2 assessments).

Tool predictions are used to identify, iterate and verify the risk management measures and operational conditions required to control exposure in workplaces, with information distributed to substance users via the supply chain. It is therefore important that the Tier 1 models are conservative in their estimation of exposure, i.e. generally overestimate exposure, while still being efficient screening tools. Although the Tier 1 tools claim to have a broad range of applicability, the performance of these tools has not been comprehensively evaluated. The German Federal Institute for Occupational Safety and Health (BAuA) therefore initiated and sponsored a comprehensive validation project Evaluation of the Tier 1 Exposure Assessment Models (“eteam”).

Carried out by the Institute of Occupational Medicine (IOM Edinburgh) and the Fraunhofer Institute for Toxicology and Experimental Medicine (ITEM Hannover), the eteam project was intended to compare and contrast the different REACH Tier 1 exposure assessment models in terms of their conceptual and external validity, scope of application, functionality, reliability and user-friendliness. The following tools were evaluated in the eteam project:

- ECETOC TRAv2 and v3
- STOFFENMANAGER® v4.5 (referred to as “STOFFENMANAGER” henceforth)
- MEASE v1.02.01 (referred to as “MEASE” henceforth)
- EMKG-EXPO-TOOL
- RISKOFDERM Version 2.1 (referred to as “RISKOFDERM” henceforth)

An international Advisory Board provided objective scientific advice to the project and made available workplace exposure data for use in the external validation process.

Within the overall aim of a comprehensive evaluation process, a number of work packages were completed, each of which considered different theoretical and operational aspects of the tools. The range of work packages is shown below in Table 1.1, together with the relevant aims.

Focussing on the primary evaluation processes, as highlighted in bold in Table 1.1, this report provides a summary by work package of the evaluation methods and results, together with conclusions about overall performance of the tools and suggestions for areas of further development. Descriptions of these primary work packages and the ancillary activities in WPI.2, WPI.3 and WPI.4 are given in Chapter 2.

Table 1.1 Description of eteam Project work packages and aims

Work package	Title	Aim	
WPI.1	**Conceptual basis of models**	**To carry out a conceptual evaluation of the models**	
WPI.2	Evaluation of data sources	To evaluate potential sources of workplace exposure data for comparison with tool estimates	To collect a comprehensive and representative set of measurement data and contextual information for comparison with the tool estimates
WPI.3	Data gathering/ reporting protocol	To develop a protocol for gathering and reporting the workplace exposure data	
WPI.4	Data collection/ formation of exposure measurement database	To develop a comprehensive database of workplace exposure measurements with which to compare the tool estimates	
WPI.5	**Data evaluation/ comparison with tools**	**To compare tool estimates with the workplace measurement data**	
WPI.6	**Operational analysis**	**To determine the usability of the tools, i.e. their user-friendliness and between-user reliability**	
WPII.1	**Uncertainty of Tier 1 models**	**To review /describe any major uncertainties in the tools**	
WPII.2	**Comparison and suitability of tools**	**To compare the tools & identify the suitability domains**	
WPIII	Dissemination	To disseminate the project findings effectively	

2 Conceptual evaluation of the tools

2.1 Introduction

The underlying basis of the tools governs their applicability and validity both generally and in relation to the user's particular situation. The availability and transparency of information on the tool background, development and exposure estimation methods are therefore important in ensuring that it can be used in the most effective and appropriate manner.

The aim of this work package was to evaluate the conceptual background of Tier 1 occupational exposure assessment tools. This mainly refers to the ECETOC TRA, MEASE, EMKG-EXPO-TOOL, STOFFENMANAGER and RISKOFDERM, which have been evaluated in this project. For the conceptual evaluation the EASE tool was also included, as this is the basis of several more recent exposure assessment tools (e.g. MEASE, ECETOC TRA). However, EASE will not be further discussed in this summary report. In this report, the various software implementation packages will be referred to as the exposure assessment "tools" whilst the underlying mathematical bases and corresponding determinants of the prediction methods referred to as the "models".

A general evaluation of the underlying concepts of the tools was carried out. The origin, development, design and functionality of the tools were described in detail. The tool algorithms and estimation processes were also evaluated, including appraisal of the relevant underlying datasets and fundamental principles of operation.

An applicability matrix was developed, which included a summary of the tools' scope and could thus be used to identify appropriate tool(s) for assessing different exposure situations. A use-map was also developed, which facilitates the between- tool conversion of different use categorisation systems (e.g. Dermal Exposure Operation (DEO) units, Process codes (PROCs).

The outcomes of this work package can therefore be of assistance to users when comparing the scope and use of different tools and served as a basis for other parts of the project where detailed knowledge of the model algorithms was required.

2.2 Method

There are several publications describing concepts that can be used as a basis for exposure models (Cherrie et al, 1996; Tielemans et al, 2008; Schneider et al, 1999). However, the Tier 1 tools included in this project are intended to be easy to use with a limited amount of information available on the substance and its uses. Thus, they should not be designed in a complex way and as a consequence, cannot fulfil all requirements set by the publications mentioned above.

Rather than regarding the published concepts as a gold standard, a more generalised approach was therefore used to evaluate the tools' background. The conceptual basis of the tools were evaluated in relation to the underlying empirical evidence, the model algorithm, scope and the supporting documentation for the tool, i.e. the transparency with which information about the tools is available.

The results of this work package are described fully in the corresponding report (eteam Project Deliverable Report D5: WPI-1 Conceptual evaluation). The main findings are summarised in the following sections, including amongst others a summary of the scope (applicability matrix) and a comparison of the implemented parameters.

2.3 Tools

2.3.1 ECETOC TRA (v2 and v3)

Two versions of the ECETOC TRA have been evaluated in the project: version 2 (2009) and version 3 (2012). In both cases the tool is based on a set of Excel sheets and can be used for estimating occupational dermal and inhalation exposure.

For both versions of ECETOC TRA, user guidance documents are available on the ECETOC homepage together with reports describing the tool background, algorithm and scope (ECETOC, 2009; ECETOC 2014). Moreover, a large amount of information concerning defaults and the algorithm is stored in the Excel sheets, either directly in the user interface or in the underlying sheets.

The ECETOC TRA output is based on an initial estimate defined by core exposure determinants, such as volatility/ dustiness and the type of use (PROC, type of setting), which can then be refined by operational conditions, such as duration or concentration and risk mitigation measures (mainly ventilation) and personal protective equipment (respiratory equipment, gloves):

Tool estimate = Modifier(s) x Initial estimate **Equation 2.1**

In general, version 3 of the tool offers more parameters to define a situation, e.g. version 3 includes a parameter on the use of gloves and more options for the ventilation conditions are available compared with version 2.

2.3.2 MEASE – "The metals' EASE" (v. 1.02.01)

MEASE is an Excel-based tool contained in a single worksheet in which all necessary information can be entered and the results are presented. Background information and user guidance can be found in the glossary within the tool itself and the HERAG Fact Sheet 01 (HERAG, 2007), which contains detailed information about the underlying measured data supporting the dermal model. Additional information can be found in Fransman et al. (2008), detailing data about the efficiency of risk mitigation measures which has been incorporated into MEASE (ECEL database).

The MEASE algorithm is a combination of refined versions of ECETOC TRAv2 (for the inhalation part) and EASE (for the dermal part).

Concerning the inhalation part, the ECETOC algorithm has been refined mainly for the metal-related processes using measured data from the metal industry. Options for the physical form of the substance have been implemented ("massive objects", "aqueous solutions", "gaseous"). Additional risk mitigation measures based on the data collected by Fransman et al. have been also implemented.

The dermal tool part is based on the set of logic criteria that were used in the EASE algorithm. EASE exposure outputs have however been replaced by values derived from measured dermal exposures and several enhancements implemented, for example gloves and refined skin areas.

2.3.3 EMKG-EXPO-TOOL

The EMKG-EXPO-TOOL is also implemented in Excel. It can only be used for inhalation exposure and is part of the EMKG ("Einfaches Maßnahmenkonzept Gefahrstoffe" = "Easy to use workplace concept control scheme for hazardous substances"). Background information can be found in BAuA publications about the EMKG (Kahl et al., 2008; Kahl et al., 2011), but also in publications related to COSHH (Control of Substances Hazardous to Health) Essentials, which is the control banding tool developed in the UK by the Health and Safety Executive and on which the EMKG and the corresponding exposure tool are based. There is also a help function within the tool offering guidance for users.

The exposure estimate of this tool is defined by two principles: the exposure potential of a substance (based on the amount of substance used and its volatility/ dustiness) and the control approach. To appropriately use this tool, the user must refer to external control guidance sheets, which can be obtained from the COSHH Essentials homepage and partly (in a German version) the BAuA homepage. The control guidance sheets contain detailed information concerning the use description and implemented risk management measures that have to be followed in order to ensure an appropriate estimation of exposure.
Overall these influences are combined into a set of logic criteria, which is almost identical to the COSHH Essentials algorithm. However, for the application on surfaces, for example painting, a refinement of the algorithm has been implemented.

2.3.4 STOFFENMANAGER

STOFFENMANAGER is a web-based tool that can only be used online. The tool consists of several modules: a control banding section (dermal and inhalation, no quantitative results), a general quantitative section and a REACH-oriented quantitative section (both only inhalation). This evaluation mainly refers to the REACH part of version 4.5, which was the most recent implementation of the tool when the eteam project started. An updated version (version 5) has since been made available, which offers some additional options and refinements including in the REACH part, the exposure estimation starting with input of the PROC codes. The quantitative and REACH-oriented tool sections of STOFFENMANAGER are based on the same algorithms and background and should therefore result in identical estimates.

Background information about the tool can be found in several publications (Schinkel et al., 2010; Tielemans et al., 2008; Marquart et al., 2008); however, no history of the most recent tool updates is publicly available. User guidance is also available via a help function within the tool.

STOFFENMANAGER is based on the model concept described by Tielemans et al. (2008), which defines a concentration score (C_t) based on various parameters:

$$C_t = [(\varepsilon_i \cdot h \cdot \eta_{lc} \cdot d_{gv,NF}) + (\varepsilon_i \cdot h \cdot \eta_{llc} \cdot d_{gv,FF}) + (\varepsilon_i \cdot a)] \cdot \eta_{PPE} \quad \textbf{Equation 2.2}$$

ε_i : intrinsic emission score of substance i
h: handling (or task) score
η_{lc}: multiplier for the effect of local control measures
$d_{gv,NF}$: multiplier for the effect of general ventilation in relation to the room size on the exposure due to near-field sources
$d_{gv,FF}$: multiplier for the effect of general ventilation in relation to the room size on the exposure due to far-field sources
a: multiplier for the relative influence of background sources.
η_{PPE}: modifier for the reduction of exposure due to control measure at the worker

This score is then fitted to a set of measured exposure values via mixed effect regression modelling to result in the final exposure algorithms:

$$\text{Ln}(Y_{ij}) = X_{ij} = ß_0 + ß_1 \cdot \text{Ln}(C_T) + \delta_i + \varepsilon_{ij} \quad \textbf{Equation 2.3}$$

Y_{ij}: exposure level for i^{th} company and the j^{th} worker (measurement)
X_{ij}: log-transformed exposure level
$ß_0$: intercept
$ß_1$: represents the fixed effect of the log of STOFFENMANAGER scores, slope of the regression line
δ_i: random effect of the i^{th} company, variance σ^2_{bc}
ε_{ij}: random effect for the j^{th} worker in the i^{th} company, variance σ^2_{wc}

2.3.5 RISKOFDERM

RISKOFDERM is an Excel-based tool for estimation of dermal exposure to hands and the body. Background information about the tool and its use is available in the user guidance and the underlying publication by Warren et al. (2006). There is also a help function within the tool which indicates when parameters outside of the underlying model boundaries are entered.

The exposure algorithm is based on a set of measured exposure data to which linear mixed effects modelling has been applied:

$$Y_{i,j} = \alpha_0 + \alpha_1 X_1 + \alpha_2 I_{2,ij} + ... + \beta_i + \Sigma_{ij} \quad \textbf{Equation 2.4}$$

- $Y_{i,j}$: j^{th} log-transformed measurement on the i^{th} worker
- α_0: mean log-transformed potential dermal exposure for the corresponding DEO unit. $\alpha_{i,0}$: includes a default setting for each implemented determinant.

- α_n: n^{th} fixed effect (n = 1,2, ...; defines the determinants of an exposure setting, e.g. quality of ventilation)
- $I_{1,ij}$: becomes 1, if the first fixed effect was present for the j^{th} measurement on the i^{th} worker and 0 otherwise.
- X_1: logarithm of the application rate
- $ß_i$: random effect for the i^{th} worker; describes the scattering of exposure values caused by the fact that different individuals were measured.
- Σ_{ij} : random error associated with the j^{th} measurement on the i^{th} individual; describes the scattering of exposure values caused by the fact that different measurements on one single individual were performed.

2.4 Comparison and discussion

2.4.1 General comparison and scope

The tools evaluated in this report are very different concerning their handling, design, purpose, scope and implemented determinants. Some tools have been designed specifically for screening purposes under REACH, e.g. the ECETOC TRA and MEASE. Other tools, for example STOFFENMANAGER and the EMKG-EXPO-TOOL, were designed originally to estimate workplace exposures, and have been subsequently adapted for REACH purposes. A basic overview of the different scopes and implemented influences is given in Table 2.1 and Table 2.2.

Inhalation exposure to liquid aerosols is only covered by STOFFENMANAGER and MEASE and exposure to fumes can only be estimated with MEASE. Furthermore, fibres are mostly excluded from the models' scope, while gaseous substances only covered by MEASE.

Not every process can be described and estimated with all tools, but there is a considerable overlap of situations which are applicable for all tools. All tools can be used for the following PROCs:

- PROC3 (use in closed batch process)
- PROC4 (use in batch or other process, where opportunity for exposure arises)
- PROC5 (mixing process, batch process, multistage or significant contact)
- PROC7/11 (spray process, industrial or professional)
- PROC8a/8b/9 (transfer operations)
- PROC 10 (roller application).
- PROC13 (treatment of articles by dipping and pouring)
- PROC14 (production of articles by tabletting, compression etc.)
- PROC15 (laboratory reagents).

In the external validation exercise, these common PROCs were used as the basis for collecting workplace measurement data, to maximise the usefulness of the dataset across the tools.

Table 2.1 Applicability matrix (inhalation models)

Applicability	EMKG-EXPO-TOOL	STOFFENMANAGER	ECETOC TRAv2	ECETOC TRAv3	MEASE
PROC codes	not included	not included; however, a suggested relation between PROCs and Handling Classes is presented	yes	yes	yes
Covered physical state	solid liquid	solid liquid	solid liquid = volatile	solid liquid = volatile	solid liquid gaseous
Beyond Scope	dusts by abrasive techniques, open spray, gases, pesticides, fumes (soldering, welding, acid fumes), wood dusts, CMR substances	fibres, gases or hot working techniques (welding, soldering, acid fumes); abrasion and impact of solid objects not recommended	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	organic substances & some restrictions concerning special combinations of PROC/physical properties
Type of enterprises	small and medium sized companies	industrial & professional	industrial & professional	industrial & professional	industrial & professional
Basis of use description	task based (control guidance sheets)	task based	process based	process based	process based

* GOHP: Good occupational hygiene practice

Table 2.2 Applicability matrix (dermal models)

Applicability	ECETOC TRAv2	ECETOC TRAv3	MEASE	RISKOFDERM
PROC Code	yes	yes	yes	not included
Covered physical state	solid liquid = volatile	solid liquid = volatile	solid liquid gaseous	solids liquids
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	organic substances	sometimes restrictions due to original data set ("only on manual tasks for powders") fumes not covered
Type of enterprises	industrial & professional	industrial & professional	industrial & professional	industrial & professional
Basis of use description	process based	process based	process based	task based

2.4.2 User Guidance

The level of detail included in the user help functions varies between the evaluated tools. In MEASE guidance is given via its glossary, in ECETOC TRA via comments and information in the underlying Excel sheets, in the EMKG-EXPO-TOOL, STOFFENMANAGER and RISKOFDERM via help texts appearing during tool usage (e.g. pop-up windows).

RISKOFDERM is the only tool that additionally, and instantaneously, advises users as to whether their input values are inside the specified boundaries of the model and if the resulting exposure outcome is beyond what is considered to be a reasonable maximum exposure. Specific user manuals and/or reports are only available for RISKOFDERM and ECETOC TRA. The EMKG-EXPO-TOOL, MEASE and STOFFENMANAGER refer the user to sets of underlying publications.

2.4.3 Transparency / Tool background

The tools included in this project offer very different amounts of information about their development and the underlying model algorithms. The EMKG-EXPO-TOOL offers some information which is mostly available via COSHH Essentials-specific literature. Differences between COSHH Essentials and the EMKG-EXPO-TOOL were not publicly available until reported by this project. A lot of information is available about the algorithm and development of the ECETOC TRA via project reports and the tool itself. Information about MEASE is available via underlying publications but not via specific documentation or report files. Detailed publications containing information about the underlying model algorithms and their derivation are also available for RISKOFDERM and STOFFENMANAGER.

Real exposure data have been used to a varying extent during the development of all of the tools, but these measurements differ in many features (quality, methodology, age, country, exposure situation). Thus, a sufficient amount of information about the underlying datasets is an important part of a transparent tool concept. However, the exposure situation descriptions assigned to the available measurements differ widely in quality and level of detail, as measurements are usually not performed with the intention of tool development. Tool-development specific measurements have however been performed and used, together with data collected for other purposes, in the validation and calibration of STOFFENMANAGER.

While STOFFENMANAGER and RISKOFDERM are based on a mathematical fitting procedure applied to a well-documented set of measured data, MEASE can only partly be retraced to certain datasets that are documented in a less detailed and transparent way. There are no specific datasets published for the EMKG-EXPO-TOOL and the ECETOC TRA.

2.4.4 Algorithm and exposure determinants

All implemented tool parameters are categorised into one of four basic groups (intrinsic substance properties, process description/ operational conditions, risk management measures at the source, personal protective equipment) and listed in Table 2.3.

In general, the level of detail per tool varies greatly, with the highest level of detail obtained with MEASE and STOFFENMANAGER. However, this also depends on the situation and the route of exposure that is to be assessed. As an example, RISKOFDERM may offer more options for a certain process than the dermal parts of MEASE and ECETOC TRA.

Although a parameter is represented in every tool, its influence, categorisation or definition within the tool may still differ from tool to tool, as outlined below.

2.4.4.1 Intrinsic substance properties

All of the tools include an option to define the fugacity of a substance or product. Most commonly used are the vapour pressure for a liquid (all tools) and the dustiness for solids (all tools except RISKOFDERM), however, there are also other approaches, e.g. using the vapour pressure of a solid to describe its presence in a liquid mixture (STOFFENMANAGER). In addition, RISKOFDERM partly offers a definition of a product’s viscosity (for DEO unit 3: Dispersion with hand-held tools).

The molecular weight is needed for unit conversions of the inhalation estimates of ECETOC TRA and MEASE from ppm to mg m^{-3}. The ECETOC TRA, MEASE and STOFFENMANAGER allow the substance concentration in a mixture to be entered.

The physical form needs to be defined in all tools, but the number of options depends on the tools’ scopes, e.g. while MEASE and EASE include gaseous products, all other tools only refer to solid or liquid substances and/ or products.

Solutions of solids in liquids are only addressed explicitly in STOFFENMANAGER (all solutions) and in MEASE (aqueous solutions of inorganics), but with different approaches concerning the fugacity. The parameter ‘very low dustiness’ is reintroduced in case of MEASE and the vapour pressure of the solid substance is used in case of STOFFENMANAGER.

2.4.4.2 Process description and operational conditions

Almost all tools implement user categorisation of the substance use and handling. The EMKG-EXPO-TOOL does not include categorisation within the tool itself, however refers the user to external Control Guidance Sheets (CGSs) for this purpose. The CGSs comprise a number of discrete operations.

The PROC code-based use descriptor system which is recommended by ECHA is implemented in ECETOC TRA and MEASE. For STOFFENMANAGER v.5 (REACH part) a list of recommendations for a conversion of the different categorisation approaches is implemented.

In general, task-based approaches and process-based use categorisations exist. Whereas a task generally only represents one defined activity (e.g. sampling of a reactor), a process may include several sub-activities (e.g. mixing in a closed batch process, including sampling activities). While in the case of STOFFENMANAGER, RISKOFDERM and the EMKG-EXPO-TOOL task-based approaches are used, the ECETOC TRA and MEASE use process (PROC code) based descriptions.

In addition to the general use description, a definition of the type of setting (professional vs. industrial, i.e. skilled trade vs. industrial companies) is offered by the ECETOC TRA and MEASE tools. Duration or frequency modifiers are also common parameters (ECETOC TRA, STOFFENMANAGER, MEASE).

Further options concerning the operational conditions, such as the level of automation or the process location (indoors/ outdoors), process temperature or the amount of substance are also offered by some models.

Exposure determinants related to far-field factors (i.e. external to the worker's breathing zone) and background exposure, i.e. exposure induced by other sources in the same room, or by a lack of cleaning respectively, are only directly implemented in STOFFENMANAGER.

2.4.4.3 Risk management measures (RMMs)

Some simple RMMs are implemented in several of the tools included in this project, e.g. the option "LEV" (Local Exhaust Ventilation) is implemented in all tools with varying levels of detail and the option "general ventilation" can be used in all tools except ECETOC TRAv2. More specific control measures at the process level, e.g. wetting of powders to prevent the release of dust, are addressed in MEASE and STOFFENMANAGER.

Best practice occupational hygiene and health and safety principles recommend a hierarchy of effective controls: elimination; substitution; technical/ engineering controls; organisational controls and finally personal protective equipment. It is therefore desirable to use exposure assessment tools which allow refinement of controls in accordance with this principle, i.e. in practice reducing release from the source should be favoured over using personal protective equipment.

There are also some risk management measures which overlap with general operational conditions, for example the room size input in STOFFENMANAGER, (where large rooms are assumed to result in lower exposures via additional dilution) , and the distance between emission source and worker (STOFFENMANAGER and RISKOFDERM) which also reduces the exposure. These factors can thus be specified for safe use and incorporated into the overall risk control approach.

2.4.4.4 Personal protective equipment

The personal protective equipment options within the tools are restricted to the use of gloves for controlling dermal exposure or respiratory protective equipment (RPE) for reduction of inhalation exposure. RPE is included in all of the tools except the EMKG-EXPO-TOOL, with gloves only implemented in version 3 of ECETOC TRA and MEASE.

Table 2.3 Overview of determinants and separation into the four main areas of an exposure situation

		Inhalation					Dermal			
		ECETOC TRA v2	**ECETOC TRA v3**	**MEASE**	**EMKG-EXPO-TOOL**	**STOFFEN-MANAGER**	**ECETOC TRA v2**	**ECETOC TRA v3**	**MEASE**	**RISKOF-DERM**
Intrinsic substance properties	*physical state*	✓	✓	✓	✓	✓	✓	✓	✓	✓
	dust description (fibrous or not)	-	-	-	-	-	-	-	-	-
	volatility / solids (dustiness based)	✓	✓	✓	✓	✓	-	-	-	✓
	volatility / solids (vapour pressure based)	-	-	-	-	✓	-	-	-	-
	volatility / liquids	✓	✓	✓	✓	✓	-	-	-	✓
	molecular weight[1)]	✓	✓	✓	-	-	-	-	-	-
	concentration of component in product / preparation	✓	✓	✓	-	✓	-	✓	✓	-
	viscosity	-	-	-	-	-	-	-	-	✓
Process description / operational conditions	*generic process categorisation*	✓	✓	✓	-	✓	✓	✓	✓	✓
	descriptor system	✓	✓	✓	-	-	✓	✓	✓	-
	process temperature	Mix	✓ | Mix	Mix	-	-	-	-	-	-
	automation rate	-	-	-	-	-	-	-	-	✓
	duration of task	✓	✓	✓	✓	✓[(1)]	-	✓	✓	✓
	frequency of task / contact frequency	-	-	-	-	-	-	-	✓	✓
	direction of work (e.g. downwards)	-	-	-	-	-	-	-	-	✓

		Inhalation					Dermal			
		ECETOC TRA v2	**ECETOC TRA v3**	**MEASE**	**EMKG-EXPO-TOOL**	**STOFFEN-MANAGER**	**ECETOC TRA v2**	**ECETOC TRA v3**	**MEASE**	**RISKOF-DERM**
	type of contact (light, extensive)	Not relevant					-	-	-	✓
	professional / industrial	✓ Mix	✓ Mix	- Mix	-	-	-	✓ Mix	-	-
	amount of substance	-	-	-	✓	Mix	-	-	-	-
	background exposure (e.g. other workers in the same room)	-	-	-	-	✓	-	-	-	-
	passive exposure	-	-	-	-	✓	-	-	-	-
	application outdoors	✓	✓	-	-	✓	-	-	-	-
Risk management Measures	*LEV*	✓	✓	✓	✓	✓	✓	✓	-	✓
	general ventilation	-	✓	✓	✓	✓	-	-	-	✓
	suppression techniques (e.g. wetting the source)	-	-	✓	-	✓	-	-	-	-
	segregation (cabin, other room)	-	-	-	-	✓	-	-	-	✓
	containment	Mix	Mix	Mix	✓	✓	Mix	Mix	Mix	-
	direct / not direct handling	Not relevant					-	-	✓	-
	distance to worker	-	-	-	-	✓	-	-	-	✓
	room size	-	-	-	-	✓	-	-	-	-
PPE	respiratory protection / gloves	✓	✓	✓	-	✓	-	✓	✓	-

KEY: ✓ determinant implemented; "-": determinant not implemented; Mix: "mixed determinants"- included in process description. Determinants in italics fall under the Tier 1 definition as described in ECHA, 2010b [1)]used for conversion of units only[(1)] tool allows task duration input for calculation of 8 hr time weighted average exposure

2.4.5 Application under REACH

All tools evaluated in this project have been recommended for exposure assessments under REACH in the official ECHA guidance document R14. However, their applicability varies for certain REACH specific features such as different hazard values (short-term/ long-term DNELs/ DMELs) or the necessity to produce a CSR.

2.4.5.1 Risk characterisation

Depending on the specific hazard characterisation (chronic vs. acute effects) of a substance, risk assessments may be necessary for both long-term and short-term exposure under REACH.

Long-term exposure corresponds to full shift average concentrations and can be predicted by all of the tools discussed in this project. RISKOFDERM, MEASE, ECETOC TRAv2 and v3 and the EMKG-EXPO-TOOL include a parameter reflecting duration of exposure, so that the full-shift estimate takes account of non-exposed periods during a shift. STOFFENMANAGER also allows the actual task duration to be entered where the user selects the daily average concentration route within the tool, thus allowing conversion of the task-based estimate to an 8 hour time weighted average exposure.

In contrast to this, short-term exposure refers to peak exposure values with durations of 15 minutes of less. Procedures to extrapolate short term values from long term exposure are suggested in ECHA document Chapter R14, (ECHA, 2012), however predictions are only directly provided by one of the models within this project, ECETOC TRAv3.

2.4.5.2 Presentation of results

The tools do not provide standardised outputs. Only the ECETOC TRA allows direct calculation of a risk characterisation ratio (RCR), i.e. the ratio of the estimated exposure to the DNEL, DMEL or other limit value. Where the RCR is >1, suitable RMMs can then be selected within the tool to reduce exposure and derive a safe scenario.

STOFFENMANAGER also offers the option to enter a limit value for the assessed substance but does not provide the corresponding risk characterisation ratio.

At the time the tools were evaluated, none produced report files that offered a full description of an exposure scenario as required for the REACH CSR. However there are additional tools and templates using the same model algorithm that are able to fill this gap, for example the CEFIC GES/ ES template and Chesar, as described below.

The CEFIC GES/ES template (release 2010) is available as an Excel spreadsheet and can be used for developing generic exposure scenarios for occupational exposure, translating available sector-specific Generic Exposure Scenarios (GES) into substance-specific exposure scenarios and transferring data into certain IT systems. It can be used together with ECETOC TRAv2.

Chesar (Chemical Safety Assessment and Reporting tool) (ECHA, 2014) can be used in combination with the widely used IUCLID (International Uniform Chemical Information Database) software which is able to store and exchange various information related to chemicals. The first version of Chesar was released in 2010 by the European Chemicals Agency (ECHA) and is used to carry out chemical safety assessments (CSAs) and prepare CSRs and exposure scenarios (ES) for communication in the supply chain.

The tool algorithm of ECETOC TRAv3 is already implemented in Chesar; furthermore, the most recent version of STOFFENMANAGER (v.5 REACH part) allows for the export of Chesar compatible xml-files.

Although the MEASE tool algorithm is not included in Chesar, the corresponding tool input parameters will become available as options within the tool and form a template that is able to simulate the MEASE inherent scenario design. Moreover it will be possible to create xml-files with MEASE which can be directly imported into Chesar and facilitate the conversion process (Vetter and Battersby, 2012; personal communication).

A similar conversion process is planned for the EMKG-EXPO-TOOL: it is intended that the Chesar user will be able to upload an xml-file containing the assessment related information and the results of the exposure assessment carried out with the EMKG-EXPO-TOOL. There are considerations to implement the EMKG-EXPO-TOOL as a plug-in into Chesar in a second step in future. For this purpose, it will be necessary to recode the tool in Chesar (Walendzik, 2012; personal communication).

2.5 Conclusion and Recommendations

As all evaluated tools can be classified screening tools (at Tier 1 or Tier 1.5 level), it cannot be expected that all details of an exposure situation are incorporated in a realistic way. However, there are some important differences in the applicability domains between the tools. Therefore, prior to the use of any tool, the user should be aware of the underlying concepts, strengths and limitations of the various tools.

3 Evaluation of data sources, DATA GATHERING PROTOCOL and development of the database

3.1 Introduction

This chapter summarises work packages I.2 (Evaluation of data sources), I.3 (Data gathering/ reporting protocol) and I.4 (Data collection/ formation of exposure measurement database). These three intrinsically linked and overlapping work packages covered the iterative process of identifying, selecting, collecting, collating and cleaning workplace exposure data from a range of providers, through to the completion of the final database used for storing the exposure situation descriptions, measurement data, tool inputs and tool-generated estimates. The methods used are therefore summarised and described collectively below.

3.2 Evaluation of data sources

All potential data providers for the project were asked to supply an initial summary of their expected submissions. From these summaries, a detailed evaluation of the potential total dataset was presented to the Advisory Board. During this evaluation, it was apparent that some of the potential data sources were much larger than others, and that a consolidation process would be required to ensure balance in terms of numbers of data points, as well as adequate coverage of tool parameters and workplace situations. Similarly, some rationalisation of identified data was required in terms of applicability within the scope of the tools and/or the overall project aim relating to the use of the tools for Tier 1 assessments under REACH. During the data collection phase, it became evident that it would not be possible to collect sufficient dermal data of sufficient variety, quantity and homogeneity of sampling method to allow a comprehensive validation of the exposure predictions from dermal assessment tools to be carried out. Further information on the data evaluation and selection process is available in eteam Project report Deliverable D16 Final report on external validation exercise (Lamb et al., 2014).

General aspects of the data rationalisation/ consolidation process are described below.

3.2.1 General Criteria for Data Selection

An initial data selection process was carried out with consideration given to the following factors.

3.2.1.1 Common PROC codes/ Handling categories

During the conceptual evaluation phase of the project (WP I-1), a number of PROC codes (PROCs 3, 4, 5, 7, 8a, 8b, 9, 10, 11, 13, 14 and 15) and equivalent STOFFENMANAGER handling categories were identified as being within the scope of all of the tools. It was noted that identification of those exposure situations, which were described by these codes, would maximise the usefulness of the data and potentially allow comparison of estimates across the range of tools.

However, it was also recognised that there were specific applications of some tools which required evaluation outside of this list of common PROCs. For example, MEASE can provide estimates of exposure to fumes from hot metal processes, and dust from handling inorganic substances and the mechanical treatment of metals (PROCs 22, 23, 24, 25, 26, 27a, 27b). Suitable data from several providers were therefore included accordingly.

3.2.1.2 Physical form of substances

For the grouping purposes, we refer to measurements of the respirable fraction as “respirable dust”, and for simplicity included this fraction within the overall category of “powder”. It was also noted during the conceptual evaluation process and in subsequent discussions with the tool developers, that no measurements of the respirable fraction (according to EN 481) had been used in the development of the various tools. Measurements of this type were therefore considered to be out of scope for the project and were excluded from the validation dataset. It is recognised that the STOFFENMANAGER database has since been revised to include respirable dust measurements; however, these were not included at the time of the original data collection exercise. Gases were also excluded from the database as these are outside the scope of all tools except MEASE. Furthermore, acid mist-related situations were excluded as the applicability of each of the tools to this physical form was not explicitly stated.

Where more than one suitable physical form was present in the situation, for example a solid and a vapour (but not originating from the same substance), the exposure situation description was duplicated to allow evaluation of tool performance for both forms to be undertaken. A unique identifier was assigned to each of the duplicate situations.

3.2.1.3 Samples with multiple analytes

Where a suite of analyses had been carried out for the same sample (e.g. measurements of several organic solvents taken using the same sorbent tube/diffusive sampler), the following selection process was performed:

- Where no information on percentage concentration for the material was available, a single analyte was chosen randomly from the given set of measurements, excluding those for whom the result was less than the limit of detection. This method ensured that substances which were not present in the material, but which were routinely included in an analysis, were not included erroneously.
- Where a percentage concentration of the substance in the product was available, a random selection was made from the whole set of available measurements (or from those substances with this information), including those which were below the limit of detection. Situations where some or all of the results were below the limit of detection were included in the evaluation.

The limits of detection supplied by the data providers were used in the analyses if the analyte was not detectable in a given sample.

3.2.1.4 Sample type

To ensure that the workplace exposure measurements used for the external validation reflected the conditions of exposure modelled by the tools, only personal samples collected on workers were selected from the various datasets. The data selected included both long-term (8-hour/ shift long) time weighted average samples and task-based measurements.

3.2.1.5 Purpose of sampling

A large part of the original data submissions originated from datasets collected by government or other authorities for various purposes including inspection visits, routine surveys and industry-specific monitoring campaigns, with the remainder being sourced from research/ consultancy. However, as the majority of these data were not gathered for enforcement reasons, there was no assumed bias towards the higher end of exposure distributions.

3.2.1.6 REACH-relevance

The eteam Project was concerned primarily with the use of the tools for Tier 1 exposure assessments under the REACH regulation. Data collection was therefore focussed on substances relevant to this legislation, i.e. those which have been registered or will require registration. Measurements of generic inhalable dust, which could not easily be related to a single agent, were generally excluded, as were process generated exposures, such as stone and wood dust, rubber fume or welding fume which did not include a specific metal.

3.2.2 Summary of data by provider

A descriptive summary of the data supplied by each provider and subsequently used in the external validation exercise is given in Table 3.1. Additional detail regarding the numbers and types of situations used for the external validation exercise are given in eteam Project Deliverable D15: Final report on external validation exercise.

Table 3.1 Summary of data by provider

Provider	Data format	Exposure type	Detail contextual information	eteam data collection template used?	Language translation required	Measurement data type	Reason for sampling exercise	Data access arrangements	Overall quality
A	Coded database entries + textual activity description	Inhalation	high	Amended version of template used	For activity descriptions only: coded entries in English	Individual data points	Routine exposure measurements/ specific chemical hazard sampling campaigns	Descriptive information provided with relevant measurement results	Good
B	Textual description	Inhalation	high	Yes: information split into separate situations where required by IOM	No	Individual data points + limited number of Type 1 aggregated data	Surveys of workplace exposures/ specific chemical hazard sampling campaigns	Descriptive information provided with relevant individual or summarised measurement results	Individual data: Good
C	Detailed coded database entries plus clear legend + limited textual description	Inhalation	high	No	For activity descriptions: coded entries mainly supplied in English	Type 2 aggregated data	Routine exposure measurements/ specific chemical hazard sampling campaigns/ research	Descriptive information provided without measurement results. Data provider supplied statistical summaries for grouped data	Type 2aggregate d data: Medium/ good
D	Textual description	Inhalation	high	Yes	No	Individual data points	Exposure model validation sampling programme	Descriptive information provided with relevant measurement results	Good

Table 3.1 (continued)

Provider	Data format	Exposure type	Detail contextual information	eteam data collection template used?	Language translation required	Measurement data type	Reason for sampling exercise	Data access arrangements	Overall quality
E	Textual description	Inhalation + dermal	high	Yes	No	Individual data points	Regulatory risk assessment/ dermal model validation sampling programme	Descriptive information provided with relevant measurement results	Good
F	Textual description	Dermal	high	Yes	No	Individual data points	Dermal exposure research sampling programme	Descriptive information provided with relevant measurement results	Good
G	Textual description	Inhalation and dermal	High	No: information extracted from MS Word documents by IOM	No	Individual data points	Regulatory investigations into workplace exposures/ specific chemical hazard sampling campaigns	Descriptive information provided with relevant measurement results	Good
H	Textual descriptions of generic exposure scenarios	Inhalation	high	No: information extracted from Word document by IOM	No	Type 1 aggregated data	Industry/ sector specific sampling programme	Descriptive information supplied with relevant measurement results	Good

Table 3.1 (continued)

Provider	Data format	Exposure type	Detail contextual information	eteam data collection template used?	Language translation required	Measurement data type	Reason for sampling exercise	Data access arrangements	Overall quality
J	Textual descriptions in database	Dermal	high	No: information extracted from database by IOM	No	Individual data points	Dermal model development- routine/ regulatory and research sampling programmes	Descriptive information supplied with relevant measurement results	Good
K	Coded database entries	Inhalation	med	No: information extracted from database by IOM	Yes	Individual data points	Routine exposure measurements/ specific chemical hazard sampling campaigns/ tool validation exercise	Descriptive information supplied with relevant measurement results	Good
M	Textual descriptions in database	Inhalation	high	Yes	No	Individual data points	Inhalation model development- routine/ regulatory and research sampling programmes	Descriptive information supplied with relevant measurement results	Medium/ good

3.3 Data gathering protocol

Providers were asked to submit their data on a Microsoft Excel based data collection template. This had been developed by the project team to allow the required inhalation and dermal tool input parameters to be collected in the form of either written descriptions and/ or coded parameters. Comprehensive guides were also developed and distributed to assist data owners during the collation and submission process.

During the final submission process, data provider formatting and resourcing issues resulted in only a small number of data being supplied on the agreed collection templates, with the majority supplied as Microsoft Excel, Access or Word documents.

3.4 Database development

The selected data were extracted from the relevant submissions from each of the providers and transferred into a Microsoft Access database with modules containing:

i) contextual information on the exposure situations in which individual measurements were obtained or to which aggregated data were assigned;
ii) the related exposure measurements;
iii) coded input parameters for all of the tools; and
iv) procedures for applying the various Tier 1 exposure tools to specific exposure situations and logging the resulting exposure estimates.

To facilitate handling of the large numbers of exposure situations and reduce the risk of data entry errors during manual transfer of input parameters from the database into the tools, semi-automated methods of implementing the various tools within the database were developed. For EMKG-EXPO-TOOL the decision tree was incorporated into the eteam database. For STOFFENMANAGER the algorithm to calculate the semi-quantitative exposure score was included in the eteam database. The STOFFENMANAGER score generated by the algorithm was then converted to an exposure estimate using the physical-form dependent equations given in Schinkel et al. (2009). For the Microsoft Excel-based MEASE and ECETOC TRAv2 tools routines were developed to run the tools in batch mode. This involved exporting the data from the database in a batch, single-line Excel format, then run through the tools and re-imported the estimates back into the eteam database.

The ECETOC TRAv3 tool contained an in-built batch-run facility which accepted data in batches of up to 60 situations, with 15 situations per substance. A Microsoft Access query was used to extract data in the input format of the tool from the eteam database. The data were then reformatted and run through the ECETOC TRAv3 tool in batch mode. Following completion, the results were copied from the tool output screens back into the database and stored with the situation description.

To verify the results obtained for EMKG-EXPO-TOOL and STOFFENMANAGER, a number of randomly-chosen test situations (10%) were run through the original tools for verification of the in-database tool method. As the original tools were used for ECETOC TRAv2, ECETOC TRAv3 and MEASE, any internal safeguards and checks still operated and resulted in the tool programme flagging up any inconsistencies which were then addressed through a review of the input parameters. To verify correct operation of these tools, cross-checks of 10% of the situations were run through the original ECETOC TRA and MEASE tools to confirm that the system was functioning correctly in terms of the export and import mechanisms.

The completed database was then utilised in the external validation process as outlined in Chapter 4 below.

3.5 Conclusions

The collection of a comprehensive set of measured data with which to compare the tool estimates was a primary aim of the eteam project. To provide as complete a picture as possible of the tools' performance, it was desirable that comparator data were collected across the range of applicability of the maximum number of tools. As discussed with, and agreed by, the project Advisory Board, data collection was therefore concentrated on situations that were applicable under the majority of the tools, to maximise the usefulness of all of the information collected. Measurement data covering a number of PROC codes as used under REACH were not therefore included in the validation process, as they did not fall into the common/ cross tool applicability categories.

It has been observed previously that the sourcing and collation of detailed contextual information on workplace situations is difficult. In the context of exposure assessment tool validation, with its requirement to ensure that the relevant input parameters are addressed, this difficulty is magnified (Maidment, 1998; Koppisch et al. 2012; Schinkel et al.; 2010). Whilst much of the data supplied was usable, limited contextual information required allocation of agreed default parameters during input of a number of exposure situation into the tools, for example in relation to concentration or dustiness.

From the initial returns by the providers, the data identified covered a variety of industries and categories of use, including upstream and downstream processes across the chemical and other manufacturing and service sectors. The submissions received were predominantly from EU countries, in particular Germany, the Netherlands and the United Kingdom with additional data from the United States of America also used.

The majority of the available data related to measurements of personal inhalation exposures, with comparatively few dermal measurements identified for a limited range of substance categories. Comparison of the limited number of dermal estimates of exposure was further complicated, and ultimately precluded, by the range of measurement technique used for sample collection and absence of conversion factors between results from different methods.

The potential inhalation dataset was predominantly comprised of exposures to vapours and, to a slightly lesser extent, dusts. Of these vapour exposures, the vast majority relate to the use of organic solvents, with smaller numbers of exposures to other non-solvent substances. Within the dust exposures (including powders;

granules; fumes and droplets), many were to a range of non-ferrous metals, with the remainder comprising agent-specific or generic inhalable dusts. Detailed information on dustiness was not generally provided. The dataset included measurements of long-term (> 4 hour) shift average, short-term and task-based exposures.

Despite a large effort to develop a comprehensive exposure measurement database for the comparison exercise, there remained important gaps. Sufficient varied and well-described dermal data could not be collected to allow a comprehensive evaluation of the dermal exposure assessment tools. Relatively few inhalation measurement results were available for non-volatile liquids, aqueous solutions and exposure to metals during abrasive and hot processes. The results and observations made within this report should therefore be considered in the light of these limits.

4 Dataset evaluation and comparison with tool estimates

4.1 Introduction

In this chapter, which summarises WP I.5 (Data evaluation/ comparison with tools), we describe the external validation process for the Tier 1 exposure assessment tools, i.e. the methods by which we compared the tool-generated estimates of exposure with measurement data from workplaces for specific situations. The Tier 1 tools are designed to allow users to identify situations where exposures may pose a risk to health. The tools are therefore expected to be both quick and simple to use, whilst also being conservative, i.e. overestimating the potential exposure and thus erring on the side of safety. The aim of the external validation process was to determine the degree of conservatism of the tools and identify circumstances where the tools may not be sufficiently conservative.

In a review of the control banding COSHH Essentials toolkit, Tischer et al. (2003) noted that there was no scientific consensus regarding the methods used to validate exposure assessment tools. Their work did, however, suggest two main aspects of the process: internal, or conceptual, validation; and external validation, i.e. comparison of tool predictions with an independent data set.

A general paucity of evaluation studies was highlighted by Kromhout (2002), who criticised a tendency for tools to be launched and used widely without adequate prior validation. There have since been a number of relatively small-scale comparisons of Tier 1 tool exposure estimates with measurement data for a limited number of substance types, activities and industry sectors (Lee et al., 2009; Lee et al., 2011; Tischer et al., 2003; Jones and Nicas, 2006; Schinkel et al., 2010; Koppisch et al., 2011; Kupczewska-Dobecka et al., 2011; Hofstetter et al., 2012). The results from these studies suggest that, although the tools appear to be conservative for many situations, there are also circumstances where this is not the case. To date, there have been no systematic validations of the tools carried out across different agents and covering their ranges of applicability.

WP I.5 of the eteam project aimed to collect sufficient contextual information and workplace measurement data from a variety of situations, and within the range of applicability of the tools, with which to compare the tool estimates of exposure. The majority of these workplace data were provided by the eteam Project Advisory Board, the IOM, the ITEM and other interested parties including the National Institute for Occupational Safety and Health (NIOSH) in the US. The measurement data included both individual measurements associated with a particular situation as well as aggregated data. Two types of aggregated data were obtained

- “Type 1 aggregated data“ covering multiple workers within an exposure situation ,and
- “Type 2 aggregated data“ which had been grouped across similar situations and operational conditions.

The data aggregation and grouping methods are described in the full eteam Project Report: D16: Final report on external validation exercise (Lamb et al., 2014).

The evaluation and comparison methods used for these individual and aggregated data with the tool estimates are summarised below.

4.2 Method

4.2.1 Overview

The purpose of the external validation was to compare the exposure estimates generated by the Tier 1 exposure assessment tools used under REACH with measurement data for a comprehensive range of situations. Exposure estimates were generated using the following tools:

- ECETOC TRAv2
- ECETOC TRAv3
- EMKG-EXPO-TOOL
- MEASE
- STOFFENMANAGER

To carry out the evaluation, a relational Microsoft Access database was developed, as detailed previously in Chapter 3. The exposure estimates obtained from the tools were subsequently compared with the corresponding measurement data for the specific situation.

4.2.2 Translation of situation descriptions into tool parameters

The external validation process required the generation of tool estimates from the collated exposure situations with which to compare the workplace measurement data. It was therefore necessary to interpret the contextual information given in the exposure situation descriptions and then input, or “code”, the required parameters into the tools.

Coding was done by a team of coders, consisting of a number of experienced exposure scientists from the IOM. The coding team (n=5) were allocated particular datasets to enter into the tools, on the basis of their previous knowledge of the tasks and/ or substances, or familiarity with the situations from the data collection work package. Initial and follow up training sessions were provided to the coders, combined with regular discussions about the input process.

Coders were requested to allocate the most appropriate option within the tool parameters. In the absence of clear descriptive information from either the situation itself or other reputable source e.g. manufacturers, coders followed the guidance in the eteam Project Quality Control Manual in relation to selection of default values. The guidance and default values are described in the Quality Control Manual following discussion with the Advisory Board. The manual is provided as an appendix to eteam Project Report Deliverable D16: Final report on external validation exercise.

4.2.3 Descriptive analysis of exposure situations

Descriptive and quantitative analyses were carried out for all of the collected measured exposure data. The aim of these analyses was to provide initial information about the exposure levels, and the availability of different items of metadata by which the measurements could be analysed, alone and in combination. It also provided a further check on the quality of the data. The methods used included tabular and graphical data summaries.

4.2.4 Quantitative analyses of exposure measurement data

The workplace exposure data were summarised using standard descriptive statistics for each of the datasets by a range of parameters. These included PROC code and the “exposure category” (i.e. physical form/ emission generation process), defined as follows:

- Non-volatile liquids, with vapour pressure $\leq$ 10 Pa at room temperature
- Volatile liquids, with vapour pressure > 10 Pa at room temperature
- Powder handling
- Metal abrasion (e.g. grinding, polishing or other mechanical treatment)
- Metal processing (e.g. hot metal processes such as welding or smelting)
- Wood processing (e.g. sawing and sanding)

4.2.5 Comparison of Tier 1 tool outputs and measured exposure data

For each situation considered, there were measured exposure data points together with exposure estimates from between one and four inhalation assessment tools available. Only comparisons for situations which were within the scope of applicability of the particular tool are reported.

For the EMKG-EXPO-TOOL, which predicts an exposure range rather than a single value, the upper range was used for the comparison with the measurement data. This is in accordance with the REACH guidance which suggests using the upper limit of the band for exposure assessment. In the case of the EMKG-EXPO-TOOL where the tool assigned an exposure of >10 mg m^{-3} (for solids) or >500 ppm (for liquids), a value of 20 mg m^{-3} or 1000 ppm was used, respectively. The maxima of the exposure predictions from the EMKG-EXPO-TOOL are similar to many international exposure limits for volatile liquids and match those for dust. To accommodate this tool feature, further evaluations with high tool estimates excluded were undertaken (see Section 4.3.2.4 below).

The STOFFENMANAGER tool generates estimates in the form of an exposure distribution, from which specific percentiles can be selected. The 75th and 90th percentiles of the STOFFENMANAGER exposure estimates were used for comparison with the measured data.

A variety of comparisons between the measured data and the tool estimates for a particular situation were carried out, which are detailed below. All tool exposure estimates were expressed in mg m^{-3}, to facilitate inter-tool comparisons.

4.2.5.1 Comparison of individual measurement data with tool estimates of exposure

For exposure situations containing individual measurement points, these values were plotted against the associated tool estimate, with the 1:1 line indicating full agreement between the two values. The number of values above the 1:1 line was counted and expressed as a percentage of the total, to illustrate the degree of over- and underestimation by the tool. "High", "medium" and "low" conservatism were defined as where ≤10%; 11≤25% and >25% of the measurements exceeded the tool estimate, respectively. Pearson correlation coefficients between the log-transformed measurement results and log-transformed tool estimates were calculated.

The ratio of the measurement value over the tool estimate was then calculated for each pair, with a ratio of <1 indicating a conservative prediction. Summaries of the ratios (arithmetic and geometric means) were calculated by tool, physical form and PROC. Overall conservatism for a particular comparison was further indicated by the geometric mean of the ratios of the measurement value over the tool estimate being <1.

4.2.5.2 Comparison of aggregated measurement data with tool estimates of exposure

Similar comparisons were made between the aggregated measurement data and the corresponding tool estimates. For the Type 1 aggregated data, the exposure estimate from the tool for the situation was compared with the corresponding arithmetic mean of the aggregated measurement data. For the Type 2 aggregated data, the arithmetic mean of the relevant group was compared with the arithmetic mean of the tool estimates from the group. The arithmetic means of the data and estimates were used in preference to the geometric means, as the use of geometric means would have reduced the impact of any high values of the measured exposure data. The ratio of the measurement value over the tool-based estimate was calculated for the two aggregated data sets as described previously and summarised by tool and exposure category. The proportion of the aggregated measurements predicted to have exceeded the tool estimate, (i.e. the number of measurements above the 1:1 line) was also estimated using Equation 4.1.

$$P(x_i > T) = 1 - \Phi\ \left\{Ln(T.GM^{-1}) \times \left(ln(GSD)\right)^{-1}\right\} \quad \textbf{Equation 4.1}$$

Where x_i is an individual measurement result; T is the estimate obtained from the tool; $\Phi\{t\}$ denotes the probability that a standard normal variate falls below T; and GM and GSD are the geometric mean and standard deviation from the measurements.

4.2.5.3 Impact of different data-specific and exposure-related factors on level of conservatism

The impact of different data-specific factors and exposure determinants on the comparison results was investigated by tabulation and examination of the percentage of measurements exceeding the tool estimates for particular combinations of factors. The determinants evaluated included the data provider; PROC code; dustiness; volatility; domain (i.e. professional or industrial setting); concentration of the substance in the preparation and the presence/ absence of local risk management controls/ LEV.

4.2.5.4 Dermal exposure

The quantity of dermal exposure data available was judged to be insufficient to allow for a reasonably comprehensive evaluation of the dermal exposure estimates from the tools. In addition, dermal measurements were obtained using different methods, leading to different results for which no consistent conversion factors exist (Gorman Ng et al., 2014). Hence, no results for dermal exposure are presented in this report.

4.3 Results

4.3.1 Description of workplace measurement data

The measurement results supplied and used in the external validation exercise are summarised by data type below. From this section onwards, for brevity and simplicity of tables, physical forms of the substances and emission generation processes (e.g. metal abrasion) are referred to collectively as “exposure category” or “exposure categories”.

4.3.1.1 Overview of individual measurement data

In total, the eteam database contained results from 2098 inhalation exposure measurements. These included long-term shift average measurements, short term and task based data. The majority of the measurements were for volatile liquids with vapour pressures higher than 10 Pa. An overview of the individual measurement data collected and used for the comparisons with the tool estimates of exposure are summarised in Table 4.1 by exposure category. It should be noted that Table 4.2 gives a generalised overview across the whole data set, i.e. all exposure situation types, and including full shift, short term and task-based measurements, with additional information on the data collected for each of the exposure categories given later in the report.

Table 4.1 Summary of individual measurement data used for comparison with tool estimates

Exposure category	N meas	GM (mg m^{-3})	GSD	Min (mg m^{-3})	Max (mg m^{-3})
Non-volatile liquid[1)]	316	0.07	15	<0.001	36
Volatile liquid[2)]	1356	7.1	26	<0.001	1949
Metal Abrasion	87	0.21	6.5	0.001	8.0
Metal Processing	71	0.28	7.3	0.003	22
Powder Handling	254	0.13	56	<0.001	446
Wood Processing	14	1.2	4.7	0.34	39
TOTAL	**2098**				

[1)]non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) <10 Pa. [2)]volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa. N meas: number of measurements; GM: geometric mean of measurement results; GSD: geometric standard deviation of measurement results; Min: lowest measurement result; Max: highest measurement result.

As shown in Table 4.2, a broad spectrum of measurements was collected for each of the categories, ranging from very low to very high values. The highest values for exposure related to workplaces with lower levels of control, however did not include accidental releases or deliberate misuse of the relevant substances. The data were therefore considered to be appropriate for comparison with the tool estimates, which under REACH should also reflect a full range of possible exposures.

The individual measurement data are also summarised by PROC code in Table 4.3. As noted in Section 3.2.1.1, and as agreed with the Advisory Board, data collection was focussed on PROC codes which were common to the majority of the tools, thus the full range of available PROC use descriptors was not covered.

Table 4.2 Individual measurement data by allocated PROC code

Exposure category	PROC codes																	
	3	4	5	7	8a	8b	9	10	11	13	14	15	19	21	22	23	24	25	Total
Non-volatile liquids[1)]	0	0	0	7	1	0	0	26	262	10	2	4	4	0	0	0	0	0	316
Volatile liquids[2)]	4	59	60	195	70	250	76	245	41	130	178	1	47	0	0	0	0	0	1356
Metal Abrasion	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	87	0	87
Metal Processing	0	0	0	0	0	0	0	0	0	0	0	0	0	0	16	14	0	41	71
Powder handling	0	1	63	8	74	54	30	0	0	0	24	0	0	0	0	0	0	0	254
Wood Processing	0	0	0	0	0	0	0	0	0	0	0	0	0	14	0	0	0	0	14
Total	4	60	123	210	145	304	106	271	303	140	204	5	51	14	16	14	87	41	2098

1) non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) $\leq$10 Pa.
2) volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.

4.3.1.2 Overview of Type 1 aggregated measurement data

Table 4.3 provides a summary of the Type 1 aggregated measurement data available for comparison with tool estimates by exposure category. A large number of measurements were available for powder handling from 29 different exposure situations. For metal processing, a relatively large number of measurements were available, but for only 7 exposure situations (although these exposure situations were amalgamations from similar situations).

Table 4.3 Summary of Type 1 aggregated measurement data used for comparison with tool estimates

Exposure Category	N Sit	N meas	GM (mg m^{-3})	GSD	Min AM (mg m^{-3})	Max AM (mg m^{-3})
Non-volatile liquid[1)]	2	42	0.01	1.5	0.01	0.01
Volatile liquid[2)]	39	262	0.17	12	<0.01	92
Metal Abrasion	3	47	0.01	1.5	0.01	0.01
Metal Processing	7	249	0.01	14	<0.01	0.31
Powder handling	29	757	0.02	9.3	<0.01	0.64
TOTAL	**80**	**1357**				

[1)]non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) $\leq$10 Pa. [2)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa. N Sit: number of exposure situations; N meas: number of measurements; GM: geometric mean of measurement results; GSD: geometric standard deviation of measurement results; Min AM: lowest arithmetic mean of aggregated data in the exposure category; Max AM: highest arithmetic mean of aggregated data in the exposure category.

The Type 1 aggregated data are shown in Table 4.4 by physical form and PROC code. As for the individual measurements, the PROC codes identified for pre-selection by the providers were based on those common to the majority of tools as agreed previously during WP I.1 (Conceptual basis of the models) and WPI.4 which included the data gathering exercise.

Table 4.4 Summary of Type 1 aggregated data (across all providers)

Physical form	PROC Code	Number of exposure situations	Number of measurements
Solid(1)	1	1	6
	3	2	102
	5	1	2
	8a	3	36
	8b	17	563
	9	3	24
	14	1	14
	21	3	41
	22	4	128
	23	2	92
	24	1	16
	27a	1	29
Liquids(2)	3	1	14
	4	1	28
	5	11	100
	7	1	7
	8a	1	3
	8b	3	10
	9	23	142
	TOTAL	**80**	**1357**

[1] includes powder handling, metal abrasion and metal processing
[2] includes non-volatile and volatile liquids

4.3.1.3 Overview of Type 2 aggregated data

The Type 2 aggregated data are summarised by exposure category and PROC code/ physical form in Tables 4.5 and 4.6, respectively. Additional Provider C exposure situations had been coded by the project team (total= 632). The grouping process resulted in some measurements from the original total being excluded, as the numbers per group (i.e. n<3) were insufficient to maintain the required level of confidentiality. Further to the grouping process, a final total of 486 measurements were used in the validation exercise.

Table 4.5 Summary of Type 2 aggregated measurement data used for comparison with tool estimates

Exposure category	N grouped situations	N meas	GM (mg m^{-3})	GSD	Min AM (mg m^{-3})	Max AM (mg m^{-3})
Non-volatile liquid[1)]	4	23	<0.01	2.0	<0.01	0.01
Volatile liquid[2)]	30	243	19	8.2	0.1	242
Metal Abrasion	7	51	0.06	3.84	0.01	0.8
Metal Processing	18	79	0.1	5.7	<0.01	1.2
Powder Handling	16	90	0.7	11	0.02	52
TOTAL	**75**	**486**				

[1)]non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa.
[2)]volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; GM: geometric mean of measurement results; GSD: geometric standard deviation of measurement results; Min AM: lowest arithmetic mean of the grouped data; Max AM: highest arithmetic mean of the grouped data.

Table 4.6 Type 2 aggregated data by PROC Code and physical form

Physical form	PROC code	Number of exposure situations/ measurements[(3)]
Solids[(1)]	5	49
	7	13
	8a	4
	8b	41
	9	8
	22	9
	23	17
	24	51
	25	28
Liquids[(2)]	4	6
	5	10
	7	25
	8b	13
	10	83
	11	3
	13	120
	15	3
	19	3
TOTAL		**486**

[1] includes powder handling, metal abrasion and metal processing;
[2] includes non-volatile and volatile liquids
[3] each situation contained a single measurement

4.3.2 Comparisons of tool estimates of exposure with individual measurement data

The following section describes the comparisons between measurement results and the tool estimates. For each tool, we will first summarise both the available measurement data that were used for the comparison for that particular tool and the corresponding tool estimates. We will then compare the tool estimates with the measurement results by plotting the data. Finally, we will summarise the ratios of the measurement result over the tool estimate and percentage of measurements exceeding the corresponding estimate.

4.3.2.1 ECETOC TRAv2

Table 4.7 shows a summary of the available measurement data for comparison with estimates from ECETOC TRAv2, by exposure category (but not by chemical agent). Most data were available for liquids with vapour pressure > 10 Pa (referred to henceforth as "volatile liquids") with 1337 measurement results from 283 situations, followed by powders (257 measurements from 32 situations). Only 82 measurements from 25 exposure situations were available for metal abrasion, giving a relatively limited set of comparator data for the validation. The results show a wide spread in the results as expressed by the geometric standard deviations (GSDs).

Table 4.7 Summary of measurement data available for comparison with ECETOC TRAv2 (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
Volatile liquids[1)]	283	1337	108	7.8	24	0.001	1949
Metal abrasion	25	82	0.8	0.2	6.6	0.001	8
Powder handling	31	254	19	0.1	56	< 0.001	446

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of measurement results; GM: geometric mean of measurement results; GSD: geometric standard deviation of measurement results; Min: lowest measurement result; Max: highest measurement result.

Table 4.8 summarises the tool estimates for ECETOC TRAv2 available for comparison with measurement results. The ECETOC TRAv2 estimates for metal abrasion are similar to the measurement results. The AM of the ECETOC TRAv2 estimates is higher than that for the measurement results for volatile liquids, but lower for powder handling. However, the GSDs for the tool estimates are much lower, and consequently the geometric means (GM) for the tool estimates are higher for all three exposure categories compared to the measurement results.

Table 4.8 Summary of the ECETOC TRAv2 tool estimates available for comparison with measurement data (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
Volatile liquids[1)]	283	1337	142	56	4.0	0.5	1878
Metal abrasion	25	82	0.7	0.5	2.4	0.2	3
Powder handling	31	254	6.2	2.4	3.8	0.005	50

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of tool estimates; GM: geometric mean of tool estimates; GSD: geometric standard deviation of tool estimates; Min: lowest tool estimate; Max: highest tool estimate.

Figures 4.1 to 4.3 show scatter plots of the measurement results versus the tool estimates for volatile liquids, metal abrasion and powders, respectively. The diagonal represents the 1:1 line, i.e. where the tool estimate is identical to the corresponding measurement value.

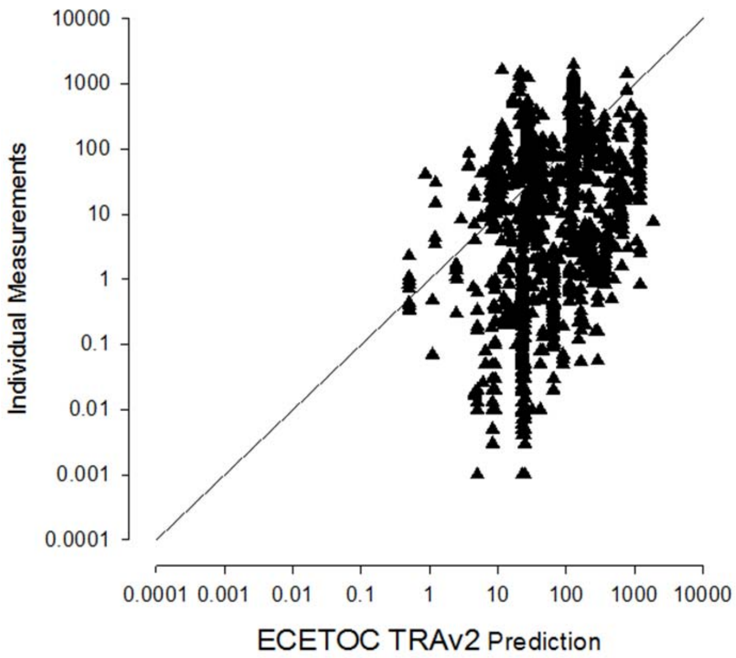


Figure 4.1 Measured data vs ECETOC TRAv2 estimates of exposure to volatile liquids (vapour pressure >10 Pa) (mg m^{-3})

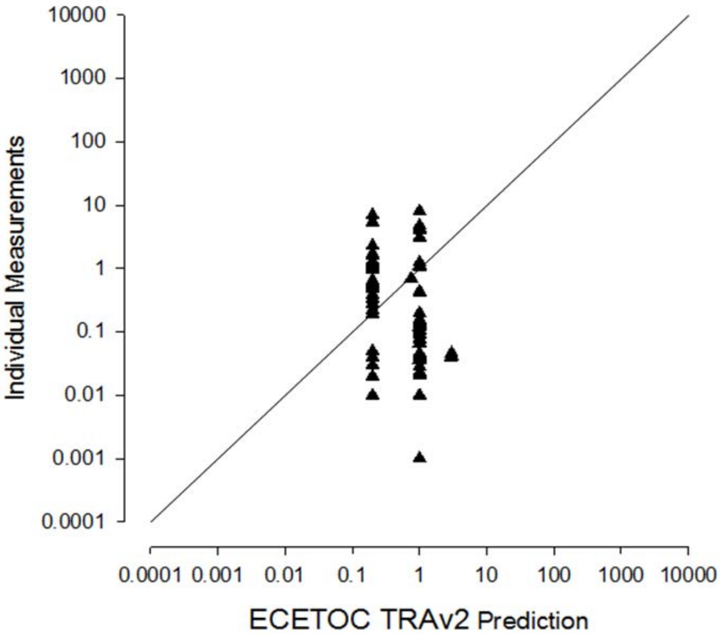


Figure 4.2 Measured data vs ECETOC TRAv2 estimates of exposure during metal abrasion (mg m^{-3})

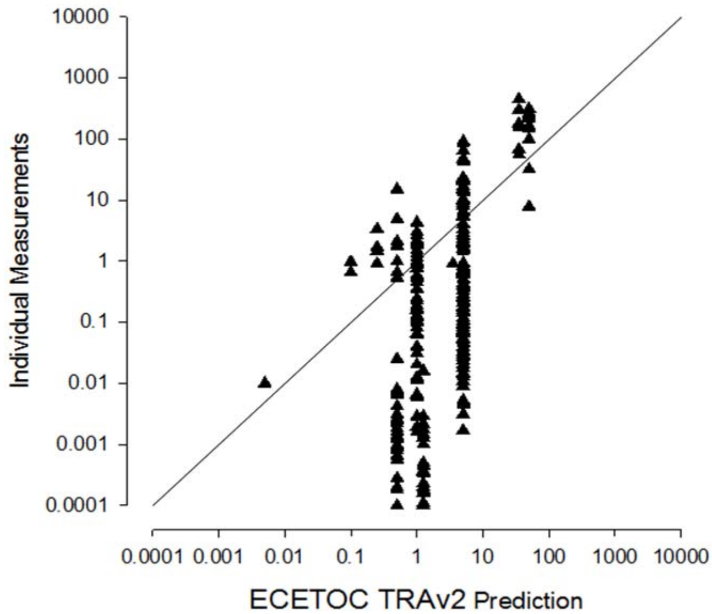


Figure 4.3 Measured data vs ECETOC TRAv2 estimates of exposure during powder handling processes (mg m^{-3})

A moderate positive correlation between the (log-transformed) tool predictions of exposure and the (log-transformed) measurement data was observed for volatile liquids (r= 0.35, p<0.001). For powder handling situations a relatively strong correlation (r=0.59, p <0.001) was observed between the tool estimates and the measured data. A negative correlation was observed between the ECETOC TRAv2 predictions and the measured exposures during metal abrasion.

Table 4.9 provides a summary of the ratios of the measurement results over the tool estimates together with the percentage of measurements that were higher than the tool estimates. As can be seen from the table, the AM of the ratio was greater than one, while the GM of the ratio was lower than 1.

Table 4.9 Summary of the ratios of the measurement results over the ECETOC TRAv2 estimates and the percentage of measurements exceeding the tool estimate

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max	%M >T
Volatile liquids[1)]	283	1337	2.2	0.1	20	<0.001	143	30%
Metal abrasion	25	82	2.5	0.4	10	0.001	35	43%
Powder handling	31	254	1.4	0.05	30	<0.001	30	27%

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of the ratios of the measurement over the tool estimates; GM: geometric mean of the ratios of the measurement results over the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest measurement/tool estimate ratio; Max: highest measurement/tool estimate ratio: %M>T: percentage of the measurements that exceed the relevant tool estimate.

Although the majority of the measurements are below the tool estimates: a sizeable fraction of the measurement results exceeded the tool estimates: 30% for volatile liquids, 43% for metal abrasion and 27% for powder handling. The tool guidance and discussions with the tool developer indicated that the exposure estimates generated correspond to values between the 75th and 90th percentile of the exposure distribution depending on the PROC, with the 90th percentile representative of a reasonable worst case exposure. As such, the tool seems to underestimate exposure compared with the assumed prediction level for each of the categories.

4.3.2.2 ECETOC TRAv3

The same measurement data were available for comparison with the ECETOC TRAv3 as for ECETOC TRAv2, hence Table 4.10 is identical to Table 4.8.

Table 4.10 Summary of measurement data available for comparison with ECETOC TRAv3 (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
Volatile liquids[1)]	283	1337	108	7.8	24	0.001	1949
Metal abrasion	25	82	0.8	0.2	6.6	0.001	8
Powder handling	31	254	19	0.1	56	<0.001	446

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of measurement results; GM: geometric mean of measurement results; GSD: geometric standard deviation of measurement results; Min: lowest measurement result; Max: highest measurement result.

The tool estimates for ECETOC TRAv3 are, however, on average somewhat lower compared to those of ECETOC TRAv2 (Table 4.11). The GMs for the ECETOC TRAv3 estimates are 35, 0.3 and 1.2 mg m^{-3}, for volatile liquids, metal abrasion and powder handling, respectively, compared to 56, 0.5, 2.4 mg m^{-3}, respectively, for ECETOC TRAv2 (Table 4.8).

Table 4.11 Summary of the ECETOC TRAv3 tool estimates available for comparison with measurement data (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
Volatile liquids[1)]	283	1337	98	35	4.4	0.3	1878
Metal abrasion	25	82	0.5	0.3	2.7	0.04	1
Powder handling	31	254	4.7	1.2	5.2	0.005	50

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of tool estimates; GM: geometric mean of tool estimates; GSD: geometric standard deviation of tool estimates; Min: lowest tool estimate; Max: highest tool estimate.

Figures 4.4 – 4.6 show the scatterplots of the measurement results versus the ECETOC TRAv3 predictions, which are fairly similar to those plots for ECETOC TRAv2, with nearly identical correlation coefficients (volatile liquids r=0.34, p<0.001; metal abrasion r=-0.32, p=0<0.05; powder handling r=0.69, p<0.001).

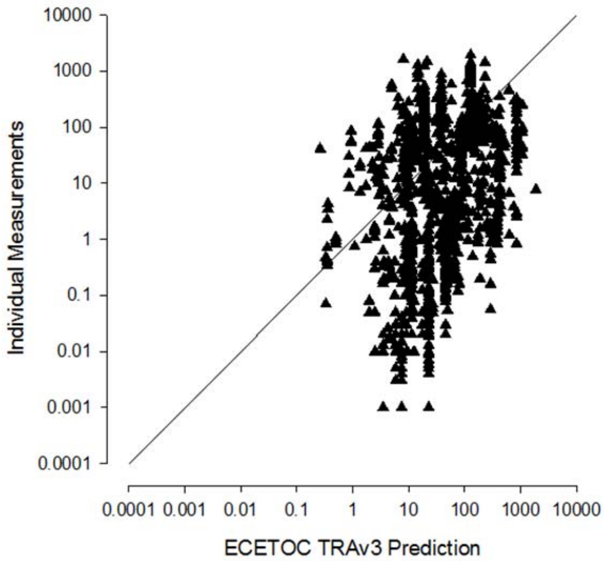


Figure 4.4 Measured data vs ECETOC TRAv3 estimates of exposure to liquids with vapour pressure >10 Pa (mg m^{-3})

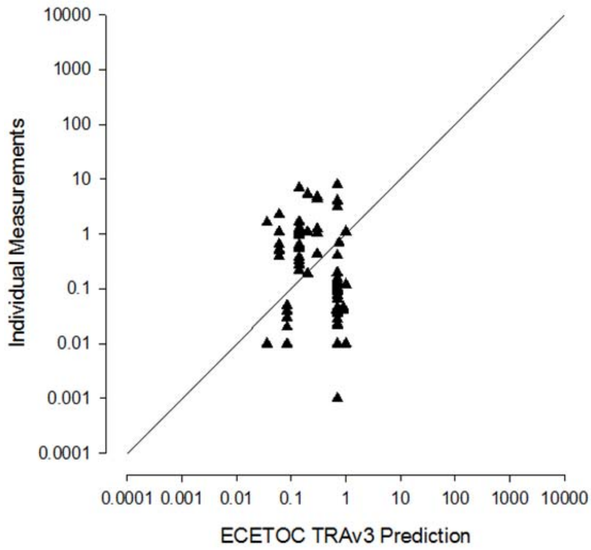


Figure 4.5 Measured data vs ECETOC TRAv3 estimates of exposure during metal abrasion (mg m^{-3})

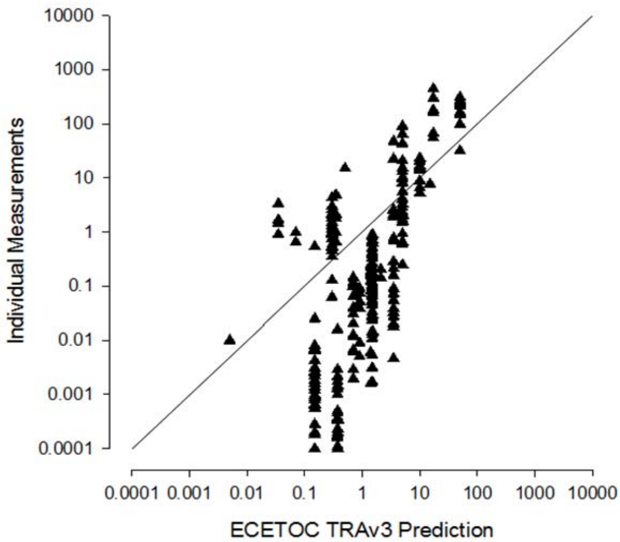


Figure 4.6 Measured data vs ECETOC TRAv3 estimates of exposure during powder handling processes (mg m^{-3})

However, the ratios of the measurement values over the relevant ECETOC TRAv3 estimates (Table 4.12) are higher than for ECETOC TRAv2 (Table 4.10). Similarly, the percentage of measurement results which exceed the corresponding tool prediction is increased compared to ECETOC TRAv2, albeit only marginally for metal abrasion and powder handling.

Table 4.12 Summary of the ratios of the measurement results over the ECETOC TRAv3 estimates and the percentage of measurements exceeding the tool estimate.

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max	%M >T
Volatile liquids[1)]	283	1337	3.7	0.2	20	< 0.001	204	35%
Metal abrasion	25	82	4.7	0.6	11	0.001	50	44%
Powder	31	254	2.6	0.1	23	< 0.001	96	28%

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of the ratios of the measurement over the tool estimates; GM: geometric mean of the ratios of the measurement results over the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest measurement/tool estimate ratio; Max: highest measurement/tool estimate ratio: %M>T: percentage of the measurements that exceed the relevant tool estimate.

This suggests that the version 3 tool, as applied in practice, can be less conservative than the ECETOC TRAv2. This may be a consequence of the greater flexibility of operation in version 3 arising from a wider range of input options, for example in relation to ventilation rates.

4.3.2.3 MEASE

For MEASE we were able to compare tool estimates with measurement data for liquids with vapour pressure ≤ 10 Pa (“non-volatile liquids”), metal abrasion, metal processing and powders. However, the quantity of data points was limited for non-volatile liquids, metal abrasion and metal processing (Table 4.13).

Table 4.13 Summary of measurement data available for comparison with MEASE (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
Non-volatile liquids[1)]	8	18	4.0	0.05	50	< 0.001	31
Metal abrasion	26	84	0.9	0.2	6.5	0.001	8
Metal processing	33	71	1.4	0.3	7.3	0.003	22
Powder handling	29	234	20	0.1	61	< 0.001	446

[1)]non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa. N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of measurement results; GM: geometric mean of measurement results; GSD: geometric standard deviation of measurement results; Min: lowest measurement result; Max: highest measurement result.

The GM of the MEASE estimates tended to be higher than those from the measurements, with the exception of the non-volatile liquids where the GM for the measurement results is very similar to the GM of the MEASE estimates (Table 4.14).

Table 4.14 Summary of the MEASE tool estimates available for comparison with measurement data (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
Non-volatile liquids[1)]	8	18	6.4	0.04	132	0.001	20
Metal abrasion	26	84	1.2	1.0	2.0	0.3	3
Metal processing	33	71	1.0	0.8	2.3	0.1	3
Powder handling	29	234	9.0	5.1	2.9	0.2	96

[1)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) $\leq$10 Pa. N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of tool estimates; GM: geometric mean of tool estimates; GSD: geometric standard deviation of tool estimates; Min: lowest tool estimate; Max: highest tool estimate.

Figures 4.7 to 4.10 plot the measurements against the MEASE estimates for non-volatile liquids, metal abrasion, metal processing and powder handling, respectively. For the non-volatile liquids a strongly positive correlation of 0.89 between the log-transformed tool estimates and the log-transformed measurements was observed ($p<0.001$), while for metal processing a statistically significant positive correlation of 0.31 was observed ($p=0.01$). For metal abrasion and powder handling negative correlations were observed.

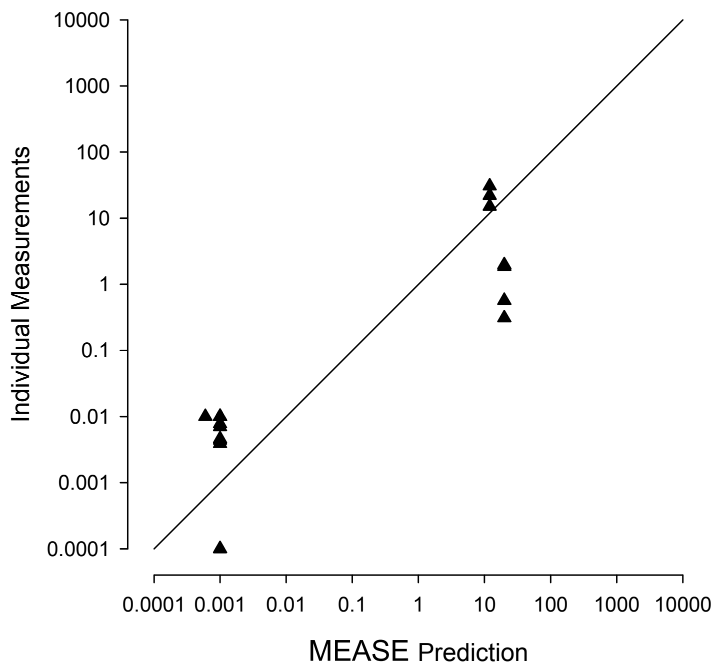


Figure 4.7 Measured data vs MEASE estimate of exposure to liquids with vapour pressure ≤10 Pa (mg m^{-3})

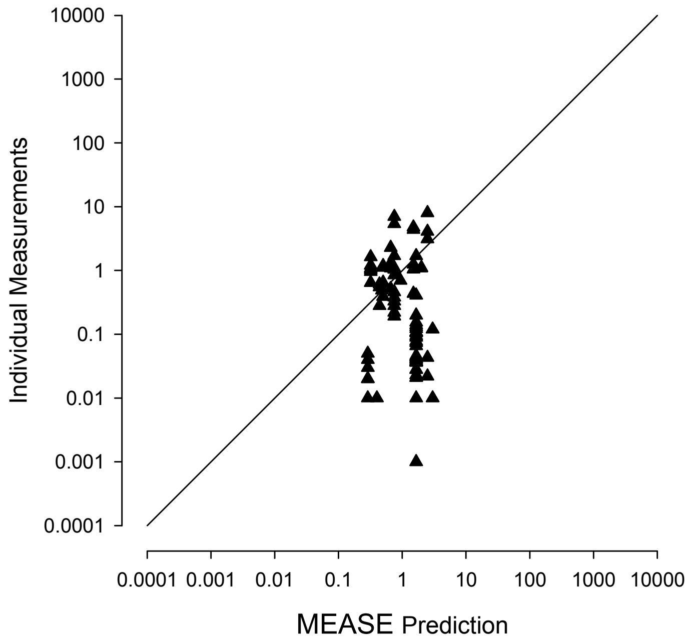


Figure 4.8 Measured data vs MEASE estimate of exposure during metal abrasion (mg m^{-3})

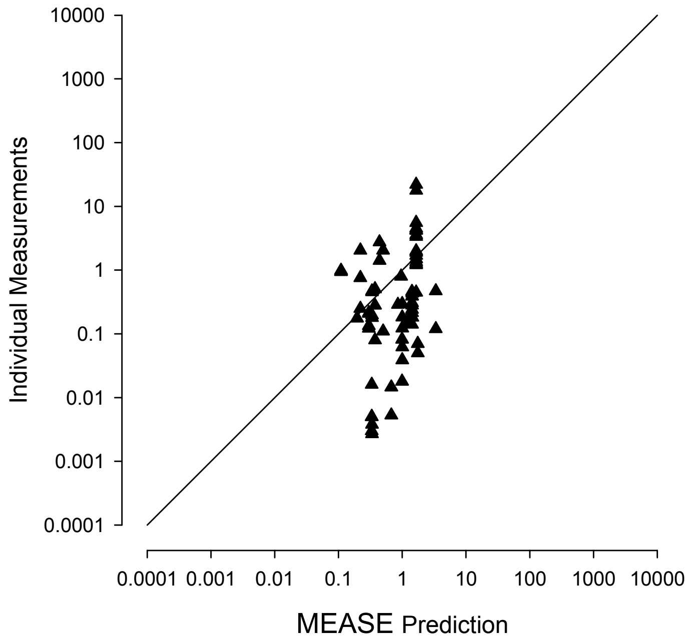


Figure 4.9 Measured data vs MEASE estimate of exposure during metal processing (mg m^{-3})

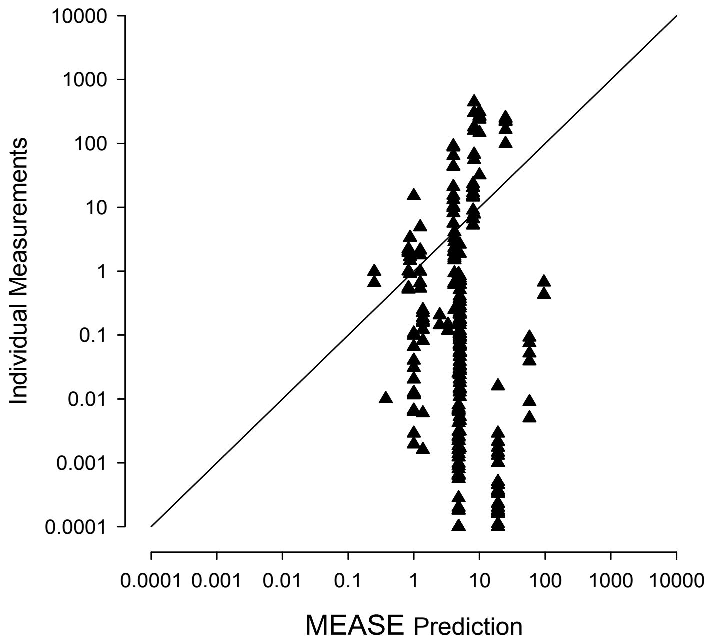


Figure 4.10 Measured data vs MEASE estimates of exposure during powder handling processes (mg m^{-3})

The ratios of the measurement data over the MEASE estimates are shown in Table 4.15, together with the percentage of cases in which the measurement was greater than the tool prediction.

Table 4.15 Summary of the ratios of the measurement results over the MEASE estimates and the percentage of measurements exceeding the tool estimate (%M>T).

Exposure Category	N Sit	N meas	AM	GM	GSD	Min	Max	%M >T
Non-volatile liquids[1)]	8	18	4.5	1.2	10	0.016	17	67%
Metal abrasion	26	84	1.0	0.2	8.3	0.001	9	33%
Metal processing	33	71	1.5	0.4	6.7	0.008	13	31%
Powder handling	29	234	2.3	0.02	80	< 0.001	54	23%

[1)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) $\leq$10 Pa. N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of the ratios of the measurement over the tool estimates; GM: geometric mean of the ratios of the measurement results over the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest measurement/tool estimate ratio; Max: highest measurement/tool estimate ratio: %M>T: percentage of the measurements that exceed the relevant tool estimate.

The AM and GM of the ratios for non-volatile liquids were both greater than 1, indicating that in comparison with this small data set MEASE did not generate conservative estimates. This is also reflected by the high percentage of measurements that exceeded the MEASE estimate (67%). However, it should be noted that the number of non-volatile liquid situations (n=8) and associated measurements (n=18) used for the comparison was very limited. For metal abrasion and metal processing, the GM of the ratio of the measurement results over the

MEASE predictions was below 1. The percentage of measurements greater than the corresponding tool estimates was around 30% for metal abrasion and metal processing. Powder handling resulted in the lowest GM of the ratios (0.02), but still with 23% of the measurement results exceeding the MEASE estimate.

4.3.2.4 EMKG-EXPO-TOOL

For the EMKG-EXPO-TOOL only measurement data relating to estimates of exposure during handling of powders and volatile liquids could be used for external validation. The situations involving non-volatile liquids related to open spray processes, which are out with the scope of this tool and were therefore excluded.

For volatile liquids, both the AM and GM of the tool estimate are much higher than the corresponding measurements (Table 4.16 and 4.17). For powder handling the AM for the tool estimates is lower than the measurement results (3.4 mg m^{-3} vs 19 mg m^{-3}), but the GM is higher (0.2 mg m^{-3} vs 0.1 mg m^{-3}).

Table 4.16 Summary of measurement data available for comparison with EMKG-EXPO-TOOL (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
Volatile liquids[1)]	209	905	86	13	17	0.001	1645
Powder handling	29	246	19	0.1	59	< 0.001	446

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of measurement results; GM: geometric mean of measurement results; GSD: geometric standard deviation of measurement results; Min: lowest measurement result; Max: highest measurement result.

Table 4.17 Summary of the EMKG-EXPO-TOOL estimates available for comparison with measurement data (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
Volatile liquids[1)]	209	905	1003	373	6.5	0.6	5462
Powder handling	29	246	3.4	0.2	13	0.01	20

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of tool estimates; GM: geometric mean of tool estimates; GSD: geometric standard deviation of tool estimates; Min: lowest tool estimate; Max: highest tool estimate.

Figures 4.11 and 4.12 again provide the scatterplots for volatile liquids and powder handling, respectively. From Figure 4.11, it is clear that relatively few data points (7%) were above the 1:1 line, suggesting that EMKG-EXPO-TOOL is conservative for volatile liquids (see also Table 4.18). The Pearson correlation coefficient between the log-transformed tool estimates and log-transformed measurement results was 0.28 ($p<0.001$).

A reasonably strong correlation coefficient of 0.7 ($p<0.001$) was observed between the EMKG-EXPO-TOOL estimates of exposure and the measurement results for powder handling. However, as can be seen from Figure 4.12, a large number of points lay above the 1:1 line.

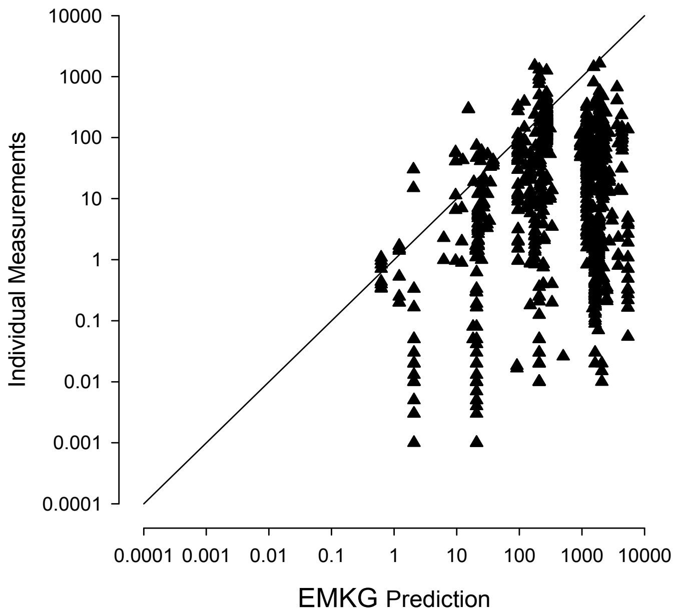


Figure 4.11 Measured data vs EMKG-EXPO-TOOL estimates of exposure to liquids with vapour pressure >10 Pa (mg m^{-3})

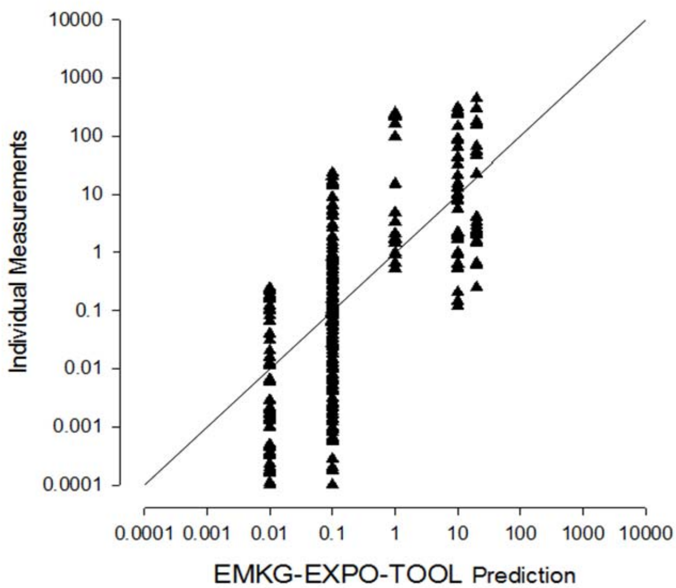


Figure 4.12 Measured data vs EMKG-EXPO-TOOL estimates of exposure during powder handling processes (mg m^{-3})

The ratios of the measurement values over the relevant EMKG-EXPO-TOOL estimates are presented in Table 4.18, together with the percentage of measurement results which exceed the corresponding tool prediction.

Table 4.18 Summary of the ratios of the measurement results over the EMKG-EXPO-TOOL estimates and the percentage of exceeding the tool estimate (%M>T)

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max	%M>T
Volatile liquids[1)]	209	905	0.4	0.04	19	< 0.001	19	7%
Powder handling	29	246	15	0.6	18	0.001	253	44%

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of the ratios of the measurement over the tool estimates; GM: geometric mean of the ratios of the measurement results over the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest measurement/tool estimate ratio; Max: highest measurement/tool estimate ratio: %M>T: percentage of the measurements that exceed the relevant tool estimate.

The results in Table 4.18 confirm that for volatile liquids, the EMKG-EXPO-TOOL was sufficiently conservative in comparison with this data set, as only 7% of the measurements exceeded the tool estimates. The high level of conservativeness and lack of a correlation for the volatile liquids for the EMKG-EXPO-TOOL may be at least partly explained by the fact that this tool does not allow for a correction of the concentration based on the percentage of the agent of interest in a mixture, but provides an estimate of exposure to the whole mixture. Correction of the concentration in the mixture should provide a better correlation with the measurement results, although is likely to reduce the observed level of conservatism of the tool.

From Table 4.18, it appears that around half of the measurements for powder handling exceeded the EMKG-EXPO-TOOL estimates. Hence, within this data set, there was no evidence that EMKG-EXPO-TOOL provides sufficiently conservative estimates for powders.

However; the maximum EMKG-EXPO-TOOL estimate for powder handling is given as “> 10 mg m^{-3}”, whilst for volatile liquids, it is “> 500 ppm”. As such, all cases where the tool assigns this category can be judged to be correct when compared with measurements in excess of 10 mg m^{-3} or 500 ppm. It should be noted that EMKG-EXPO-TOOL estimates of > 10mg m^{-3} and >500 ppm are out of the scope of the tool and are therefore not recommended according to REACH guidance document Chapter R.14.

The analyses were therefore repeated after exclusion of those exposure situations where the EMKG-EXPO-TOOL estimate was either >10 mg m^{-3} (for powders) or > 500 ppm (for volatile liquids) to examine the impact of using the tool for situations outside of its accepted range of applicability. A summary of the EMKG-EXPO-TOOL estimates for this restricted data set are shown in Table 4.19.

Table 4.19 Summary of the EMKG-EXPO-TOOL estimates available for comparison with measurement data (mg m^{-3}) (high values excluded)

Exposure category	N meas	AM	GM	GSD	Min	Max
Volatile liquids[1)]	692	563.5	215.6	6.1	0.6	3038.4
Powder handling	222	1.58	0.14	8.8	0.01	10.00

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N meas: number of measurements; AM: arithmetic mean of measurement results; GM: geometric mean of measurement results; GSD: geometric standard deviation of measurement results; Min: lowest measurement result; Max: highest measurement result.

Using this restricted dataset, the recalculated ratios of measurement values to the EMKG-EXPO-TOOL estimates and the percentage of measurements which exceed the corresponding tool estimates are shown in Table 4.20.

Table 4.20 Summary of the ratios of the measurement results over the EMKG-EXPO-TOOL estimates and the percentage of exceeding the tool estimate (%M>T) (restricted dataset)

Exposure category	N meas	AM	GM	GSD	Min	Max	%M>T
Volatile liquids[1)]	692	0.5	0.07	12.7	< 0.0001	19.4	9%
Powder handling	222	15.8	0.6	19.5	0.001	252.7	45%

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N meas: number of measurements; AM: arithmetic mean of the ratios of the measurement over the tool estimates; GM: geometric mean of the ratios of the measurement results over the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest measurement/tool estimate ratio; Max: highest measurement/tool estimate ratio: %M>T: percentage of the measurements that exceed the relevant tool estimate.

The removal of these values thus seems to have very little impact on the percentage of measurements that exceed the tool estimate for either volatile liquids or powders. Excluding high EMKG-EXPO-TOOL estimates for powders resulted in an almost identical correlation coefficient of 0.7 ($p < 0.0001$). For volatile liquids exclusion of the high estimates resulted in an improved correlation coefficient (0.47; $p < 0.0001$).

4.3.2.5 STOFFENMANAGER

STOFFENMANAGER generates estimates of different percentiles of the exposure distribution, e.g. the 50th, the 75^{th,} 90th and 95th percentiles of the exposure distribution. Following discussion with the Advisory Board, it was decided to use the 75th and the 90th percentiles for the comparisons with the measurement results. The use of the 90th percentile is considered appropriate in ECHA guidance document Chapter R14, and is considered to represent a reasonable worst case exposure in assessments under REACH. In the case of STOFFENMANAGER, comparisons could be carried out with measurement results for non-volatile liquids, volatile liquids, powder handling and wood dust (Table 4.21).

Table 4.21 Summary of measurement data available for comparison with STOFFENMANAGER (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
Non-volatile liquids[1)]	36	287	1.1	0.08	16	< 0.001	36
Volatile liquids[2)]	284	1349	106	7.0	26	< 0.001	1949
Powder handling	31	254	19	0.1	56	< 0.001	446
Wood dust	6	14	5.2	1.2	4.7	0.3	39

[1)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa. [2)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa. N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of measurement results; GM: geometric mean of measurement results; GSD: geometric standard deviation of measurement results; Min: lowest measurement result; Max: highest measurement result.

Table 4.22 shows the STOFFENMANAGER predictions using the 75th and the 90th percentile. The AM and GM estimates for the 90th percentile are approximately between 2.5 and 4 times higher than the 75th percentile. The AM and GM of the tool estimates for STOFFENMANAGER are generally higher than the summaries of the measurement results. Exceptions are non-volatile liquids (for which the AM of the 75th percentile is lower than that for the measurement results whilst the GM is similar), and powders, where the AM of the 75th percentile tool estimate is lower than that for the measured data, but the GM of the 75th percentile is higher than the GM of the measurement results.

Table 4.22 Summary of the STOFFENMANAGER tool estimates (75th and 90th percentile) available for comparison with measurement data (mg m^{-3})

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max
75th percentile							
Non-volatile liquids[1)]	36	287	0.7	0.2	7.0	0.008	5
Volatile liquids[2)]	284	1349	172	74	4.2	1.3	1619
Powder handling	31	254	12	3.7	3.7	0.3	164
Wood dust	6	14	8.9	7.0	2.3	1.6	22
90th percentile							
Non-volatile liquids[1)]	36	287	2.8	0.7	7.0	0.03	19
Volatile liquids[2)]	284	1349	488	209	4.2	3.6	4581
Powder handling	31	254	34	11	3.7	0.8	469
Wood dust	6	14	22	17	2.3	3.9	55

[1)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa. [2)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa. N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of tool estimates; GM: geometric mean of tool estimates; GSD: geometric standard deviation of tool estimates; Min: lowest tool estimate; Max: highest tool estimate.

Figures 4.13 to 4.16 give the scatterplots between STOFFENMANAGER estimates and measurement results for both the 75th and the 90th percentiles. For non-volatile liquids it can be seen that even when using the 90th percentile estimate, a relatively large number of measurement results are higher than the tool estimates (16%, see Table 4.23). It should be noted that whilst in this study, the 90th percentile was used for the comparisons in accordance with the REACH guidance, when generating estimates from the tool for general and REACH purposes, users can select a 95th percentile estimate, which would give additional conservatism.

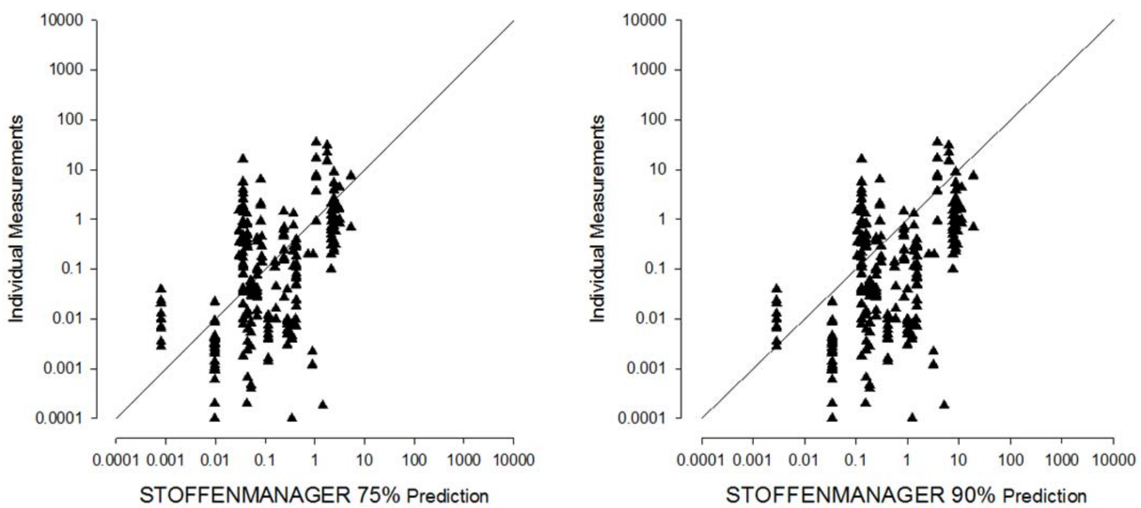


Figure 4.13 Measured data vs STOFFENMANAGER estimate of the 75th and 90th percentile of the exposure distribution- non-volatile liquids with vapour pressure ≤10 Pa (mg m^{-3})

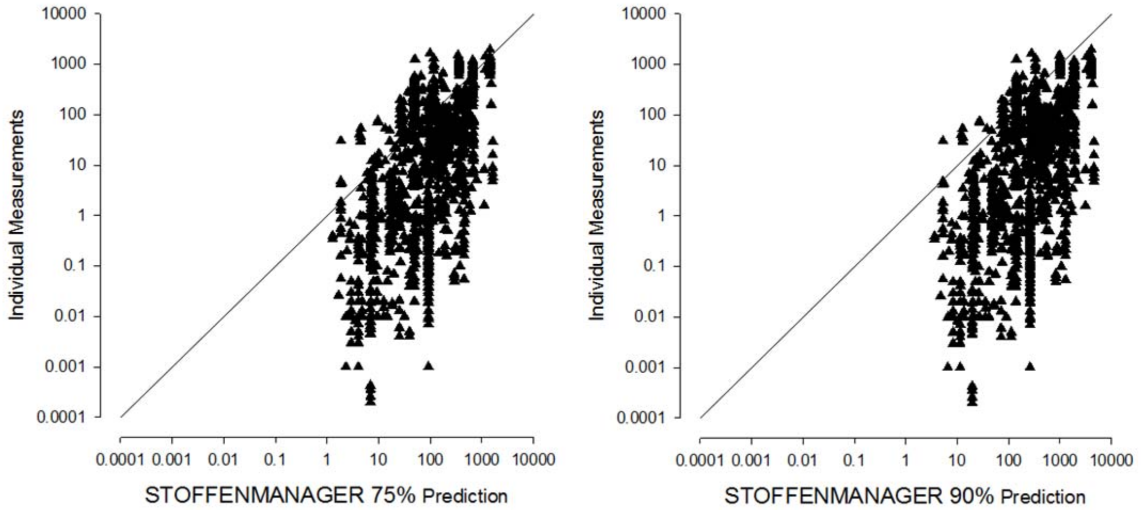


Figure 4.14 Measured data vs STOFFENMANAGER estimate of 75th and 90th percentile of the exposure distribution – volatile liquids with vapour pressure >10 Pa (mg m^{-3})

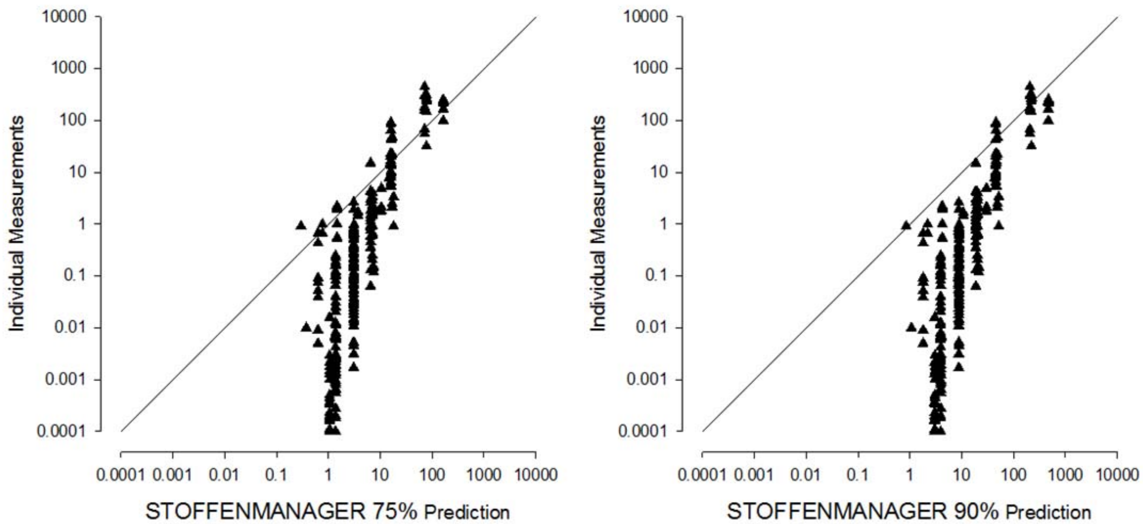


Figure 4.15 Measured data vs STOFFENMANAGER estimate of 75th and 90th percentile of exposure distribution during powder handling processes (mg m^{-3})

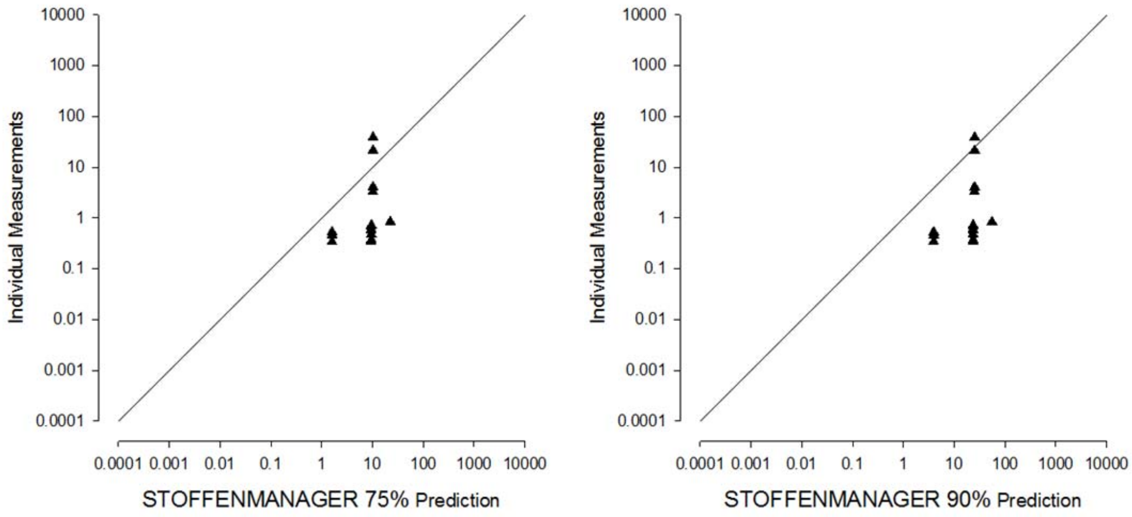


Figure 4.16 Measured data vs STOFFENMANAGER estimate of 75th and 90th percentile of exposure distribution during wood processing (mg m^{-3})

There was a strong positive correlation between the STOFFENMANAGER estimates of exposure and the measurement data for powder handling (r=0.83, p<0.001), whilst there was a moderate correlation for volatile liquids (r= 0.55, p<0.001) and non-volatile liquids (r=0.62, p<0.001), respectively. Within the very limited dataset for wood dust, no correlation was observed between the tool estimates and measurement results.

Table 4.23 shows the summaries of the ratios of the measurement results over the STOFFENMANAGER estimates (75th and 90th percentile). These results suggest that for non-volatile liquids, both the 75th and 90th percentiles obtained from STOFFENMANAGER somewhat underestimate the exposure compared to the measurements. When using the 75th percentile for comparison, the AM of the ratios is greater than 1 (2.6), whilst the GM of the ratios is below 1 (0.4). A high percentage of measurements in this dataset for non-volatile liquids (31%) exceeded the STOFFENMANAGER 75th percentile estimate. When the 90th percentile is used for the comparison, the AM of the ratios was reduced to 0.7, while the GM of the ratios reduced to 0.1. However, the percentage of measurements in this dataset that was above the STOFFENMANAGER estimate was 16%, which is higher than would be expected for a 90th percentile estimate. As noted previously, in actual use of the tool, the choice of the 95th percentile would increase the conservatism for this exposure category.

For volatile liquids, the ratios and the percentage of measurements above the 75th and 90th percentiles are lower than for non-volatile liquids. For the 90th percentile, both the AM and GM of the ratios were less than 1.

For powders and wood processing the AM and GM of the ratios are below 1 and the percentage of measurements above the STOFFENMANAGER estimates are somewhat lower than would have been expected on the basis of the percentile that it aims to predict.

Table 4.23 Summary of the ratios of the measurement results over the STOFFENMANAGER estimates (75th and 90th percentile) and the percentage of measurements exceeding the tool estimate (%M>T)

Exposure category	N Sit	N meas	AM	GM	GSD	Min	Max	%M >T
75th percentile								
Non-volatile liquids[1)]	36	287	2.6	0.4	9.0	< 0.001	79	31%
Volatile liquids[2)]	284	1349	0.9	0.1	16	< 0.001	25	22%
Powder handling	31	254	0.5	0.04	21	< 0.001	6	13%
Wood dust	6	14	0.6	0.2	4.4	0.04	4	14%
90th percentile								
Non-volatile liquids[1)]	36	287	0.7	0.1	9.0	< 0.001	22	16%
Volatile liquids[2)]	284	1349	0.3	0.03	16	< 0.001	9	13%
Powder handling	31	254	0.2	0.01	21	< 0.001	2	4%
Wood dust	6	14	0.2	0.07	4.4	0.02	2	7%

[1)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa. [2)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa. N Sit: number of exposure situations; N meas: number of measurements; AM: arithmetic mean of the ratios of the measurement over the tool estimates; GM: geometric mean of the ratios of the measurement results over the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest measurement/tool estimate ratio; Max: highest measurement/tool estimate ratio: %M>T: percentage of the measurements that exceed the relevant tool estimate.

4.3.3 Ratio of individual measurements to tool estimates by data provider

Table 4.24 shows the comparison of the geometric means of the measurement to tool estimate ratios together with the percentage of measurements that were above the tool estimates by tool and data provider. There appeared to be some considerable differences in the percentage of measurements above the tool estimates between the data providers. For example, for volatile liquids percentage of measurements above the tool estimates were much lower for data provider M compared to others.

It is unclear from the data what caused these differences in the ratios and percentage exceedances between the data providers. However, the data providers with lower and higher ratios and percentage exceedances coincide with the overall spread of the measurement levels for the different providers by exposure category. Hence, it is likely that the differences in the ratios are caused by differences in the way the data have been collected (e.g. as part of a specific survey campaign for a particular substance rather than routine/ reassurance sampling), or use of measurement methods (e.g. the use of long versus short-term measurements).

Table 4.24 Geometric mean of ratios of individual measurement results over the tool estimates and percentage of measurements above the tool estimates (%M>T) by tool and data provider

Exposure category	Data Provider																				
	A			B			D			E			G			K			M		
	N	GM	%M >T	N	GM	%M >T	N	GM	%M >T	N	GM	%M >T	N	GM	%M >T	N	GM	%M >T	N	GM	%M >T
ECETOC TRAv2																					
Volatile liquids[1]	258	0.1	32	592	0.5	46	19	0.1	21		-		16	0.5	13	110	0.3	25	342	<0.1	2
Metal abrasion	35	1.6	74	43	0.1	16	2	17	100		-		2	<0.1	0		-			-	
Powder handling	39	0.4	44		-			-			-		2	7.8	100		-		213	<0.1	23
ECETOC TRAv3																					
Volatile liquids[1]	258	0.3	43	592	0.8	52	19	0.2	21		-		16	0.7	25	110	0.7	43	342	<0.1	1
Metal abrasion	35	3.0	74	43	0.2	19	2	25	100		-		2	<0.1	0		-			*	
Powder handling	39	1.1	51		-			-			-		2	7.8	100		-		213	0.1	23
MEASE																					
Non-volatile liquids[2]		-			-			-		3	1.8	100	11	3.4	82		-		4	<0.1	0
Metal abrasion	40	0.8	53	40	0.1	13	2	4.6	100		-		2	<0.1	0		-			-	
Metal processing	44	0.5	39	27	0.2	19		-			-			-			-			-	
Powder handling	35	0.2	37		-			-			-		2	0.6	50		-		197	<0.1	20
EMKG-EXPO-TOOL																					
Volatile liquids[1]	215	<0.1	8	483	0.1	6	19	<0.1	16		-		15	0.1	13	76	<0.1	8	97	<0.1	4
Powder handling	31	0.3	29					-			-		2	1.2	50		-		213	0.7	46
STOFFENMANAGER 90th-%-ile																					
Non-volatile liquids[2]	9	0.4	44	49	0.1	2		-		33	0.3	36	14	<0.1	0		-		182	0.1	15
Volatile liquids[1]	259	<0.1	6	585	0.1	27	19	0.1	21		-		16	0.3	0	110	<0.1	2	360	<0.1	1
Powder handling	39	0.1	3		-			-			-		2	0.1	0		-		213	<0.1	5
Wood processing	5	0.2	20		-		9	<0.1	0		-			-			-			-	

[1] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa
[2] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa

4.3.4 Ratio of individual measurements to tool estimates by PROC code

Table 4.25 shows the percentage of measurements that were above the tool estimate by tool and PROC code. For the volatile liquids, both ECETOC TRAv2 and v3 only appeared to be sufficiently conservative (i.e. <10% measurements > tool estimate) for PROCs 8b, 9 and 11. In particular for PROCs 7 and 14, the percentage of measurements that exceeded the ECETOC TRA estimates was very high. For powder handling, both ECETOC TRA tools and MEASE appeared to underestimate the exposure for PROCs 8a and 14, while for PROCs 5, 7, 8b and 9 the tools were sufficiently conservative.

The results from the EMKG-EXPO-TOOL for volatile liquids appeared to be sufficiently conservative for most PROCs, with the exception of PROC 4 and perhaps PROC 3 (although for the latter only 4 measurements were available). For powder handling, EMKG-EXPO-TOOL appeared to be sufficiently conservative only for PROC 9.

For STOFFENMANAGER the vast majority of the measurements available for non-volatile liquids were available for PROC 11 (233 out of 285 measurements). The results suggest that for this PROC, STOFFENMANAGER was not sufficiently conservative for non-volatile liquids. For volatile liquids, STOFFENMANAGER underestimated the exposure compared to the measurement results for PROC 14. Finally, for powder handling, STOFFENMANAGER was highly conservative for PROCs 5, 7, 8b, 9 and 14, but was perhaps less conservative for PROC 8a.

These results suggest that the performance of the tools may depend on the activity or process type, although other factors, such as data provider, could also play a role in this. For example, about 50% of measurements from Provider M for volatile liquids (for which only a small fraction of measurements were observed to be higher than the tool estimates) were for PROC 8b.

Table 4.25 Percentage of measurements above the tool estimate (%M>T) by tool and PROC code.

	PROC Code																	
Exposure category	3	4	5	7	8a	8b	9	10	11	13	14	15	19	21	22	23	24	25
ECETOC TRAv2 (%M>T)/ (number of measurements)																		
Volatile liquids[1]	25 (n=4)	19 (n=59)	23 (n=60)	62 (n=195)	16 (n=70)	6 (n=249)	1 (n=76)	18 (n=245)	0 (n=23)	14 (n=130)	85 (n=178)	100 (n=1)[3]	21 (n=47)	*	*	*	*	*
Metal abrasion	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	43 (n=82)	*
Powder handling	*	0 (n=1)[3]	10 (n=63)	0 (n=8)	61 (n=74)	9 (n=54)	0 (n=30)	*	*	*	50 (n=24)	*	*	*	*	*	*	*
ECETOC TRAv3 (%M>T)/ (number of measurements)																		
Volatile liquids[1]	50 (n=4)	25 (n=59)	32 (n=60)	74 (n=195)	19 (n=70)	7 (n=249)	3 (n=76)	22 (n=245)	0 (n=23)	25 (n=130)	88 (n=178)	100 (n=1)[3]	36 (n=47)	*	*	*	*	*
Metal abrasion	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	43 (n=82)	*
Powder handling	*	0 (n=1)[3]	10 (n=63)	0 (n=8)	54 (n=74)	9 (n=54)	0 (n=30)	*	*	*	88 (n=24)	*	*	*	*	*	*	*
MEASE (%M>T)/ (number of measurements)																		
Non-volatile liquids[2]	*	*	*	*	100 (n=1)[3]	*	*	*	43 (n=7)	80 (n=10)	*	*	*	*	*	*	*	*
Metal abrasion	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	33 (n=84)	*
Metal processing	*	*	*	*	*	*	*	*	*	*	*	*	*	*	31 (n=16)	7 (n=14)	*	39 (n=41)
Powder handling	*	0 (n=1)[3]	5 (n=63)	0 (n=8)	57 (n=70)	7 (n=54)	0 (n=30)	*	*	*	75 (n=8)	*	*	*	*	*	*	*
EMKG-EXPO-TOOL (%M>T)/ (number of measurements)																		
Volatile liquids[1]	25 (n=4)	24 (n=33)	0 (n=60)	*	0 (n=44)	0 (n=73)	1 (n=68)	5 (n=244)	*	11 (n=130)	12 (n=178)	0 (n=1)[3]	11 (n=47)	*	*	*	*	*
Powder handling	*	100 (n=1)[3]	51 (n=63)	*	68 (n=74)	20 (n=54)	0 (n=30)	*	*	*	63 (n=24)	*	*	*	*	*	*	*
STOFFENMANAGER 90th %-ile (%M>T)/ (number of measurements)																		
Non-volatile liquids[2]	*	*	*	0 (n=7)	0 (n=1)	*	*	4 (n=26)	17 (n=233)	0 (n=10)	*	100 (n=4)	0 (n=4)	*	*	*	*	*
Volatile liquids[1]	25 (n=4)	3 (n=59)	15 (n=60)	6 (n=188)	1 (n=70)	8 (n=250)	8 (n=76)	6 (n=245)	0 (n=41)	2 (n=130)	75 (n=178)	0 (n=1)[3]	0 (n=47)	*	*	*	*	*
Powder handling	*	100 (n=1)[3]	0 (n=63)	0 (n=8)	14 (n=74)	0 (n=54)	0 (n=30)	*	*	*	0 (n=24)	*	*	*	*	*	*	*
Wood processing	*	*	*	*	*	*	*	*	*	*	*	*	*	7 (n=14)	*	*	*	*

[1] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa [2] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa [3] NB single data point only: included for completeness

4.3.5 Comparison of aggregated measurement data with tool estimates

Within this section, we describe the results of comparisons of tool estimates with those exposure situations for which aggregated data were provided. For the purposes of this process, the Type 1 and 2 aggregated data were merged into a single data set, with which the tool predictions of exposure could be compared.

4.3.5.1 ECETOC TRAv2

Table 4.26 summarises the aggregated measurement data available for comparison with the ECETOC TRAv2 estimates. The table gives the mean of the arithmetic means (AM) available for aggregated measurement data.[1] Table 4.27 shows the relevant mean, minimum and maximum estimates from ECETOC TRAv2. Comparison of the summaries from both tables shows that the mean ECETOC TRAv2 estimates are higher than the mean of the corresponding measurements.

Table 4.26 Summary of aggregated measurements available for comparison with ECETOC TRAv2 estimates by exposure category (mg m^{-3})

Exposure category	N Sit	N meas	Mean AM	Min AM	Max AM
Volatile liquids[1)]	69	505	31.10	<0.01	241.60
Metal abrasion	10	98	0.11	0.01	0.78
Powder handling	45	847	2.24	0.00	51.98

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; Mean AM: mean of the arithmetic means of measurement results for the exposure situations; Min AM: lowest arithmetic mean of the grouped measurement results; Max AM; highest arithmetic mean of grouped measurement results.

Table 4.27 Summary of the ECETOC TRAv2 estimates by exposure category available for comparison with aggregated measurement data (mg m^{-3})

Exposure Category	N Sit	Mean TRAv2	Min TRAv2	Max TRAv2
Volatile liquids[1)]	69	119.82	0.42	1502.29
Metal abrasion	10	0.81	0.20	3.00
Powder handling	45	6.07	0.01	35.00

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa
N Sit: number of exposure situations; Mean TRAv2: mean of ECETOC TRAv2 estimates for the exposure situations; Min TRAv2: lowest ECETOC TRAv2 estimate; Max TRAv2: highest ECETOC TRAv3 estimate.

Figures 4.17- 4.19 give the scatterplots of the AM of the aggregated measurement data vs the ECETOC TRAv2 estimates. The arithmetic means of the Type 2 aggregated data were plotted. As can be seen the majority of means of the

[1] Arithmetic means were not always available for the aggregated data. If the AM was not available, the geometric mean and geometric standard deviation were used to estimate the AM using the following equation: $AM=\exp\{m+(0.5s^2) \times ((N-1)/N)\}$, where m=ln(GM), s=ln(GSD) and N is the number of measurements.

aggregated data are below the mean of the ECETOC TRAv2 predictions, but there are also points above the 1:1 line.

There appeared to be no association between the ECETOC TRAv2 predictions and the estimates based on measurements when using the aggregated dataset for volatile liquids, metal abrasion or powder handling.

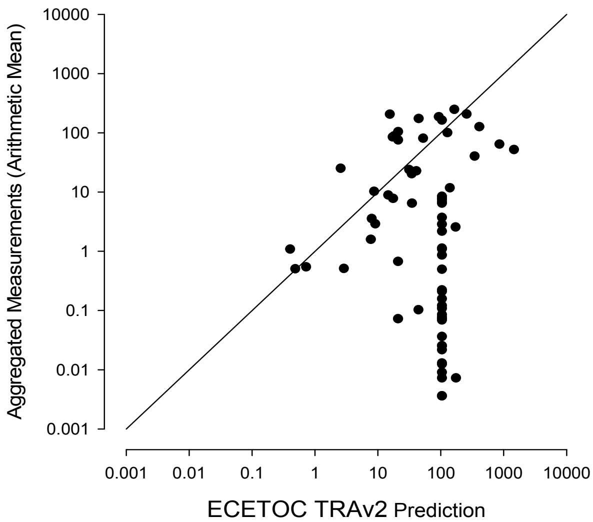


Figure 4.17 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv2 predictions (volatile liquids) (mg m^{-3})

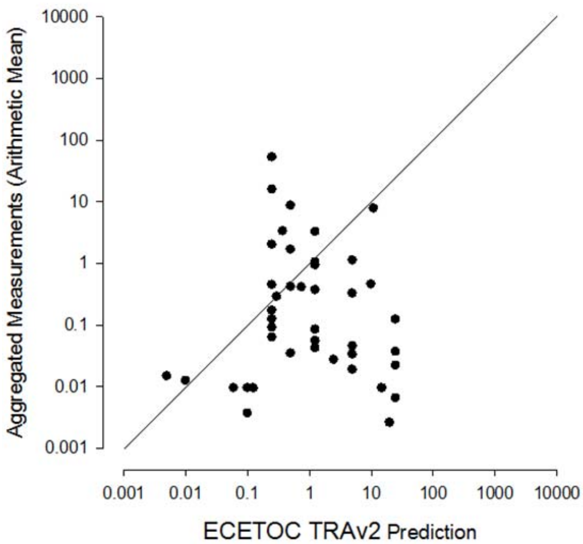


Figure 4.18 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv2 predictions (powders) (mg m^{-3})

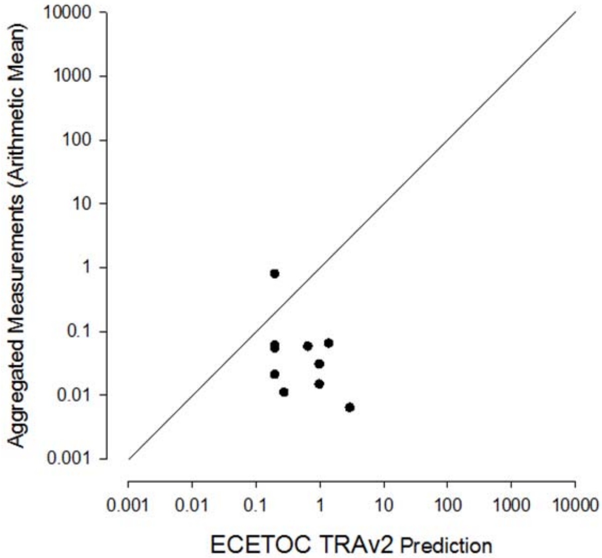


Figure 4.19 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv2 predictions (metal abrasion) (mg m^{-3})

Table 4.28 gives a summary of the ratios of the means of the aggregated data over the (means) of the ECETOC TRAv2 estimates for the situations. The ratios were highest for powder handling. The percentage of measurements predicted to have exceeded the ECETOC TRAv2 estimate was 17% for volatile liquids, 8% for metal abrasion and 13% for powder handling, respectively.

Table 4.28 Summary of the ratios of the mean of the aggregated measurement results over the mean of the ECETOC TRAv2 estimates, and predicted percentage of measurements exceeding the tool estimates (%M>T)

Exposure category	N Sit	N meas	AM ratio	GM ratio	Min ratio	Max ratio	%M >T
Volatile liquids[1)]	69	505	0.89	0.03	<0.01	12.58	17
Metal abrasion	10	98	0.48	0.07	<0.01	3.88	8
Powder handling	45	847	7.19	0.09	<0.01	207.9	13

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM ratio: arithmetic mean of the ratios of the arithmetic mean of measurement results over arithmetic mean of the tool estimates; GM: geometric mean of the ratios of the arithmetic mean of the measurement results over the arithmetic mean of the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest arithmetic mean of measurement over arithmetic mean of tool estimate ratio; Max: highest arithmetic mean of measurement over arithmetic mean of tool estimate ratio: %M>T: estimated percentage of the measurements that exceed the relevant tool estimate.

4.3.5.2 <u>ECETOC TRAv3</u>

The available aggregated measurement results for comparison with ECETOC TRAv3 (Table 4.29) were the same as for the ECETOC TRAv2 (Table 4.26). Table 4.30 gives the summary of the ECETOC TRAv3 estimates, which again shows that on average the estimates for ECETOC TRAv3 are lower than for ECETOC TRAv2 (see Table 4.27).

Table 4.29 Summary of aggregated measurements available for comparisons with ECETOC TRAv3 estimates by exposure category (mg m^{-3})

Exposure category	N Sit	N meas	Mean AM	Min AM	Max AM
Volatile liquids[1)]	69	505	31.10	<0.01	241.60
Metal abrasion	10	98	0.11	0.01	0.78
Powder handling	45	847	2.24	<0.01	51.98

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; Mean AM: mean of the arithmetic means of measurement results for the exposure situations; Min AM: lowest arithmetic mean of the grouped measurement results; Max AM; highest arithmetic mean of grouped measurement results.

Table 4.30 Summary of the ECETOC TRAv3 estimates by exposure category available for comparison with (aggregated) measurement data (mg m^{-3})

Exposure category	N Sit	Mean TRA3	Min TRA3	Max TRA3
Volatile liquids[1)]	69	82.54	0.38	1051.06
Metal abrasion	10	0.68	0.07	3.00
Powder handling	45	3.63	0.01	35.00

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; Mean TRAv3: mean of ECETOC TRAv3 estimates for the exposure situations; Min TRAv3: lowest ECETOC TRAv3 estimate; Max TRAv3: highest ECETOC TRAv3 estimate.

Figures 4.20- 4.22 show plots of the aggregated measurements versus the ECETOC TRAv3 predicted values, where, compared to the ECETOC TRAv2, a higher number of means of the aggregated data are above the 1:1 line.

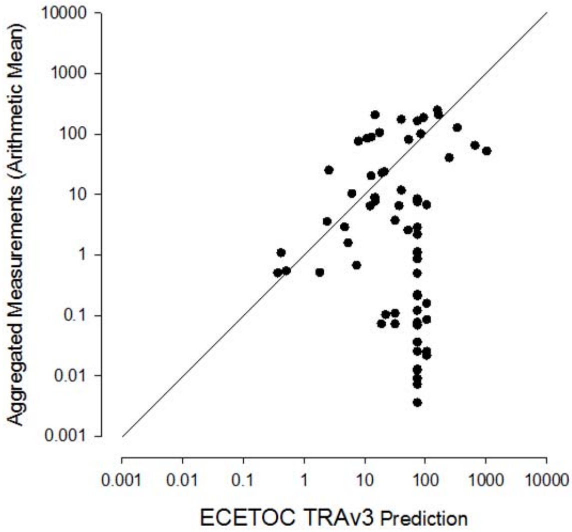


Figure 4.20 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv3 predictions (volatile liquids) (mg m^{-3})

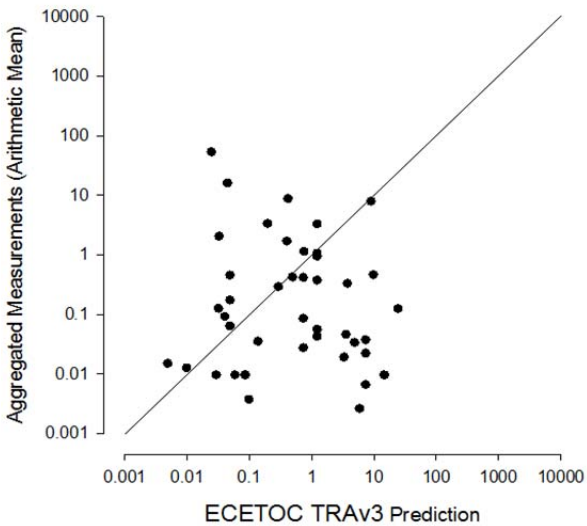


Figure 4.21 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv3 predictions (powders) (mg m^{-3})

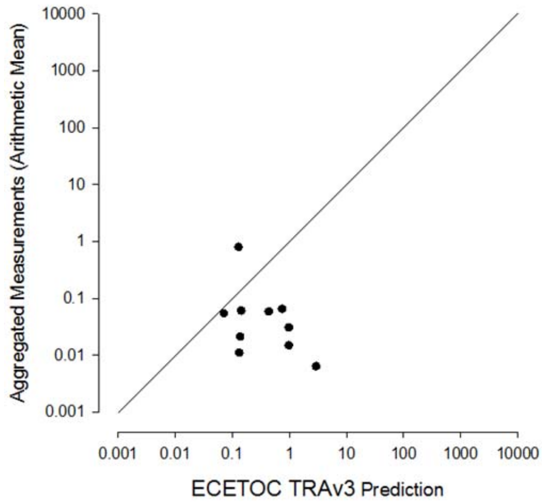


Figure 4.22 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv3 predictions (metal abrasion) (mg m^{-3})

The AM and GM of the ratios of the measured over the predicted levels were also higher than for the ECETOC TRAv2 comparisons, as were the predicted percentages of measurements that exceeded the ECETOC TRAv3 predictions (Table 4.31).

Table 4.31 Summary of the ratios of the mean of the aggregated measurement results over the mean of the ECETOC TRAv3 estimates and the predicted percentage of measurements exceeding the tool estimates (%M>T)

Exposure category	N Sit	N meas	AM ratio	GM ratio	Min ratio	Max ratio	%M>T
Volatile liquids[1)]	69	505	1.17	0.04	<0.01	13.20	22
Metal abrasion	10	98	0.75	0.11	<0.01	5.89	10
Powder handling	45	847	56.86	0.17	<0.01	2079	19

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM ratio: arithmetic mean of the ratios of the arithmetic mean of measurement results over arithmetic mean of the tool estimates; GM: geometric mean of the ratios of the arithmetic mean of the measurement results over the arithmetic mean of the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest arithmetic mean of measurement over arithmetic mean of tool estimate ratio; Max: highest arithmetic mean of measurement over arithmetic mean of tool estimate ratio: %M>T: estimated percentage of the measurements that exceed the relevant tool estimate.

An estimated 22% of the measurements available for comparison exceeded the ECETOC TRAv3 predictions for the volatile liquids, while for powders this was 19%. For metal abrasion, the estimated percentage of measurements exceeding the tool estimate was 10%. As was seen for ECETOC TRAv2, the log-transformed tool estimates were not correlated with the log-transformed AM of the measurement results.

4.3.5.3 MEASE

Tables 4.32 and 4.33 and Figures 4.23-4.26 show the aggregated measurement data and tool estimates available for MEASE and the comparisons between these values. On average, the MEASE estimates are higher than the mean of the measurement results. However, for non-volatile liquids, the AM as well as the GM of the ratios of the measurement based estimates over the MEASE estimates are higher than 1. The estimated percentage of measurements that have exceeded the MEASE estimates was 54% (Table 4.34). For the other exposure categories, the ratios and estimated percentage of measurements above the MEASE predictions are lower.

For metal abrasion there was a non-statistically significant correlation between the log-transformed AM of the measurement results and the log-transformed tool estimates (r=0.46, p=0.1963). However, for metal processing and powder handling there was no evidence of a correlation between measurement results and tool estimates.

Table 4.32 Summary of aggregated measurements available by exposure category for comparisons with MEASE estimates (mg m^{-3})

Exposure Category	N Sit	N Meas	Mean AM	Min AM	Max AM
Non-volatile liquids[1)]	2	42	0.02	0.02	0.02
Metal abrasion	10	98	0.11	0.01	0.78
Metal processing	25	328	0.35	<0.01	2.25
Powder handling	45	847	2.24	<0.01	51.98

[1)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa N Sit: number of exposure situations; N meas: number of measurements; Mean AM: mean of the arithmetic means of measurement results for the exposure situations; Min AM: lowest arithmetic mean of the grouped measurement results; Max AM; highest arithmetic mean of grouped measurement results.

Table 4.33 Summary of the MEASE estimates by exposure category available for comparison with (aggregated) measurement data (mg m^{-3})

Exposure Category	N Sit	Mean MEASE	Min MEASE	Max MEASE
Non-volatile liquids[1)]	2	0.01	<0.01	0.01
Metal abrasion	10	0.71	0.04	5.5
Metal processing	25	0.73	0.05	6.72
Powder handling	45	3.98	0.01	22.00

[1)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa N Sit: number of exposure situations; Mean MEASE: mean of MEASE estimates for the exposure situations; Min MEASE: lowest MEASE estimate; Max MEASE: highest MEASE estimate.

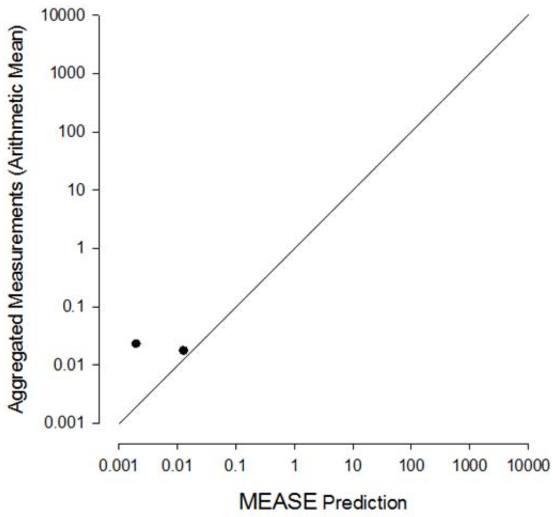


Figure 4.23 Comparison of the AM of the aggregated measurement data compared with the AM of the MEASE predictions (non-volatile liquids) (mg m^{-3})

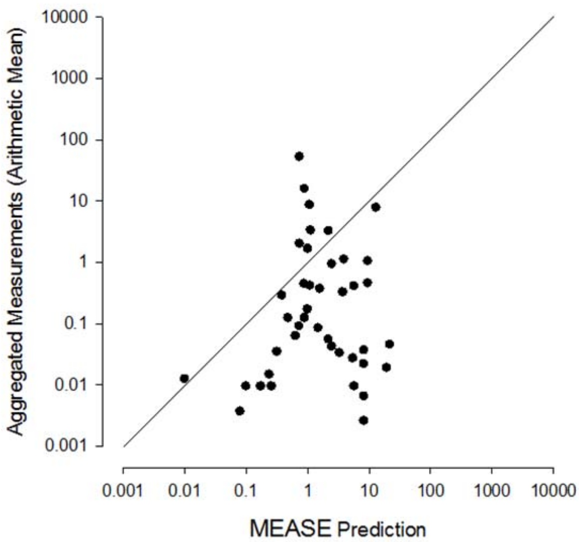


Figure 4.24 Comparison of the AM of the aggregated measurement data compared with the AM of the MEASE predictions (powders) (mg m^{-3})

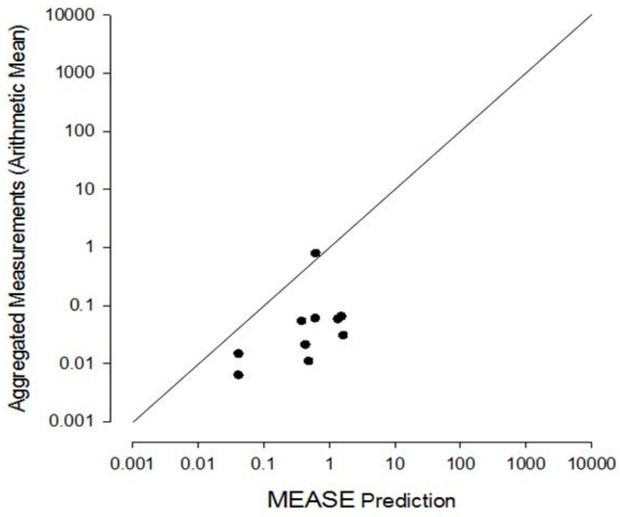


Figure 4.25 Comparison of the AM of the aggregated measurement data compared with the AM of the MEASE predictions (metal abrasion) (mg m^{-3})

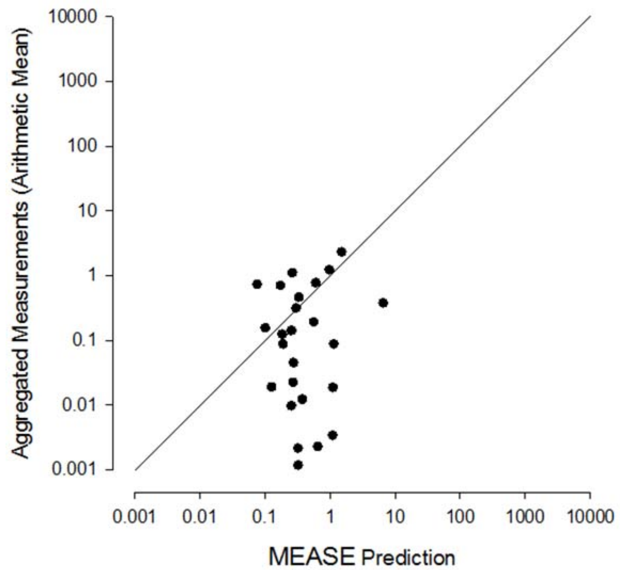


Figure 4.26 Comparison of the AM of the aggregated measurement data compared with the AM of the MEASE predictions (metal processing) (mg m^{-3})

Table 4.34 Summary of the ratios of the mean of the measurement results over the mean of the MEASE estimates, as well as the predicted percentage of measurements exceeding the tool estimates (%M>T)

Exposure Category	N Sit	N Meas	AM ratio	GM ratio	Min ratio	Max ratio	%M>T
Non-volatile liquids[1)]	2	42	6.32	3.88	1.33	11.30	54
Metal abrasion	10	98	0.21	0.09	0.02	1.23	5
Metal processing	25	328	1.09	0.19	<0.01	9.16	10
Powder handling	45	847	2.44	0.06	<0.01	69.87	7

1) non- volatile liquids are defined as liquids with a vapour pressure (at room temperature) $\leq$10 Pa. N Sit: number of exposure situations; N meas: number of measurements; AM ratio: arithmetic mean of the ratios of the arithmetic mean of measurement results over arithmetic mean of the tool estimates; GM: geometric mean of the ratios of the arithmetic mean of the measurement results over the arithmetic mean of the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest arithmetic mean of measurement over arithmetic mean of tool estimate ratio; Max: highest arithmetic mean of measurement over arithmetic mean of tool estimate ratio: %M>T: estimated percentage of the measurements that exceed the relevant tool estimate.

4.3.5.4 EMKG-EXPO-TOOL

The aggregated measurements used for comparison with estimates from the EMKG-EXPO-TOOL are summarised in Table 4.35. The corresponding tool estimates are shown in Table 4.36. The mean value of the tool estimates for exposure to volatile liquids is much higher than that for the comparator measurements. The mean EMKG-EXPO-TOOL estimate for powder exposure was closer to that of the comparator measurements.

Table 4.35 Summary of measurements available by exposure category for comparisons with EMKG-EXPO-TOOL estimates (aggregated data) (mg m^{-3})

Exposure category	N Sit	N Meas	Mean AM	Min AM	Max AM
Volatile liquid[1)]	62	476	33.53	<0.01	241.60
Powder handling	42	817	2.40	<0.01	51.98

1) volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; Mean AM: mean of the arithmetic means of measurement results for the exposure situations; Min AM: lowest arithmetic mean of the grouped measurement results; Max AM; highest arithmetic mean of the grouped measurement results.

Table 4.36 Summary of the EMKG-EXPO-TOOL estimates by exposure category available for comparison with (aggregated) measurement data (mg m^{-3}).

Exposure category	N Sit	Mean EMKG	Min EMKG	Max EMKG
Volatile liquid[1)]	62	1312.49	1.22	3608.01
Powder handling	42	4.87	0.01	15

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; Mean EMKG: mean of EMKG-EXPO-TOOL estimates for the exposure situations; Min EMKG: lowest EMKG-EXPO-TOOL estimate; Max EMKG: highest EMKG-EXPO-TOOL estimate.

The results of the comparisons between EMKG-EXPO-TOOL estimates and the measurement data are illustrated in Figures 4.27 and 4.28.

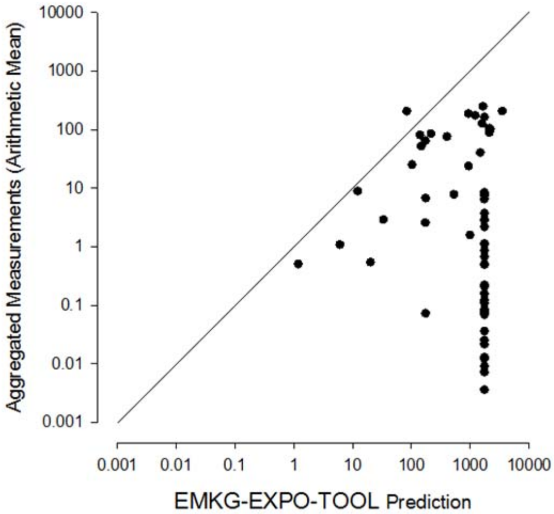


Figure 4.27 Comparison of the AM of the aggregated measurement data compared with the AM of the EMKG-EXPO-TOOL predictions (volatile liquids) (mg m^{-3})

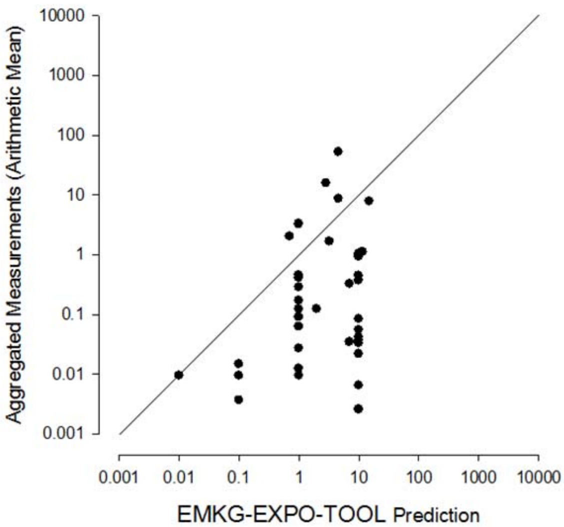


Figure 4.28 Comparison of the AM of the aggregated measurement data compared with the AM of the EMKG-EXPO-TOOL predictions (powders) (mg m^{-3})

The ratios of measurements to tool estimates were low for both volatile liquids and powder handling.

Table 4.37 Summary of the ratios of the mean of the measurement results over the mean of the EMKG-EXPO-TOOL estimates, as well as the predicted percentage of measurements exceeding the tool estimates (%M>T)

Exposure category	N Sit	N meas	AM ratio	GM ratio	Min ratio	Max ratio	%M>T
Volatile liquid[1)]	62	476	0.11	<0.01	<0.01	2.36	2
Powder handling	42	817	0.76	0.05	<0.01	11.30	9

[1)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.
N Sit: number of exposure situations; N meas: number of measurements; AM ratio: arithmetic mean of the ratios of the arithmetic mean of measurement results over arithmetic mean of the tool estimates; GM: geometric mean of the ratios of the arithmetic mean of the measurement results over the arithmetic mean of the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest arithmetic mean of measurement over arithmetic mean of tool estimate ratio; Max: highest arithmetic mean of measurement over arithmetic mean of tool estimate ratio: %M>T: estimated percentage of the measurements that exceed the relevant tool estimate.

The EMKG-EXPO-TOOL estimates for powders were somewhat closer to the measurement results, but the ratios were still relatively low. No statistically significant correlation between measurement results and tool estimates were observed. The estimated percentage of measurement exceeding the EMKG-EXPO-TOOL estimate was 2% for volatile liquids and 9% for powder handling.

4.3.5.5 STOFFENMANAGER

The aggregated measurement data available for comparison with the STOFFENMANAGER estimates (75th and 90th percentiles) are summarised in Table 4.38.

Table 4.38 Summary of measurements available by exposure category for comparison with STOFFENMANAGER estimates (aggregated data) (mg m^{-3})

Exposure category	N Sit	N Meas	Mean AM	Min AM	Max AM
Non-volatile liquids[1)]	5	37	0.01	<0.01	0.02
Volatile liquids[2)]	69	505	31.10	<0.01	241.60
Powder handling	45	847	2.24	<0.01	51.98

[1)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa.
2) volatile liquids are defined as liquids with a vapour pressure (at room temperature) of > 10 Pa
N Sit: number of exposure situations; N meas: number of measurements; Mean AM: mean of the arithmetic means of measurement results for the exposure situations; Min AM: lowest arithmetic mean of the measurement results; Max AM; highest arithmetic mean of measurement results.

On average, the 75th and 90th percentile estimates from STOFFENMANAGER are higher than the measurement results (Table 4.39).

Table 4.39 Summary of the STOFFENMANAGER estimates (75th and 90th percentiles) by exposure category available for comparison with (aggregated) measurement data (mg m^{-3})

Exposure category	N Sit	Mean STM75	Min STM75	Max STM75
Non-volatile liquids[1)]	5	0.17	0.01	0.53
Volatile liquids[2)]	69	82.92	2.67	500.81
Powder handling	45	5.61	0.13	21.58
		Mean STM90	Min STM90	Max STM90
Non-volatile liquids[1)]	5	0.60	0.02	1.90
Volatile liquids[2)]	69	234.60	7.57	1416.85
Powder handling	45	16.03	0.37	61.62

[1)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa. [2)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa. N Sit: number of exposure situations; Mean STM75: mean of STOFFENMANAGER 75th percentile estimates for the exposure situations; Min STM75: lowest STOFFENMANAGER 75th percentile estimate; Max STM75: highest STOFFENMANAGER 75th percentile estimate; Mean STM90: mean of STOFFENMANAGER 90th percentile estimates for the exposure situations; Min STM90: lowest STOFFENMANAGER 90th percentile estimate; Max STM90: highest STOFFENMANAGER 90th percentile estimate.

This can also be seen in the scatterplots of aggregated measurement data versus the STOFFENMANAGER estimates (Figures 4.29 – 4.31).

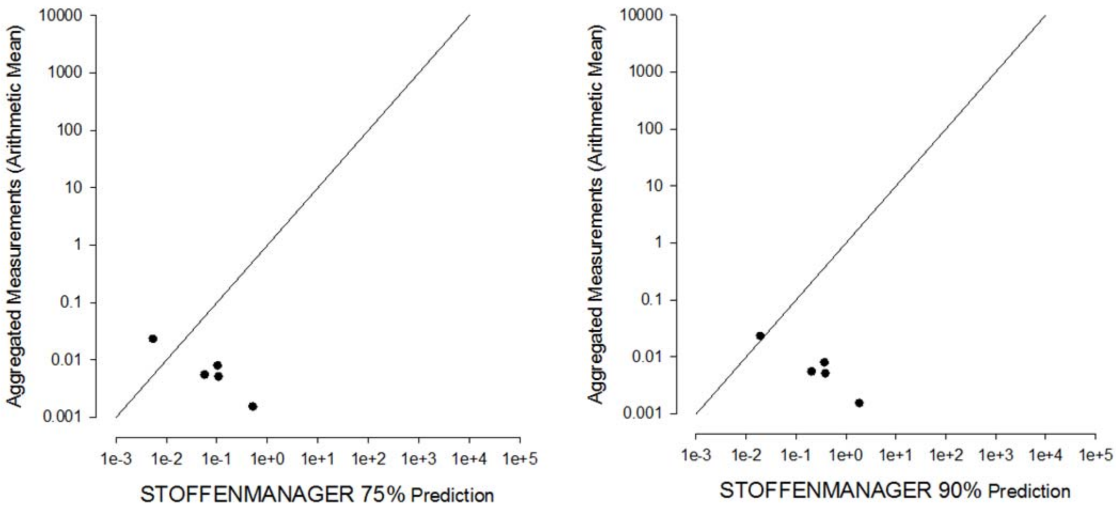


Figure 4.29 Comparison of the AM of the aggregated measurement data compared with the AM of the STOFFENMANAGER predictions 75th and 90th percentiles) – non-volatile liquids (mg m^{-3})

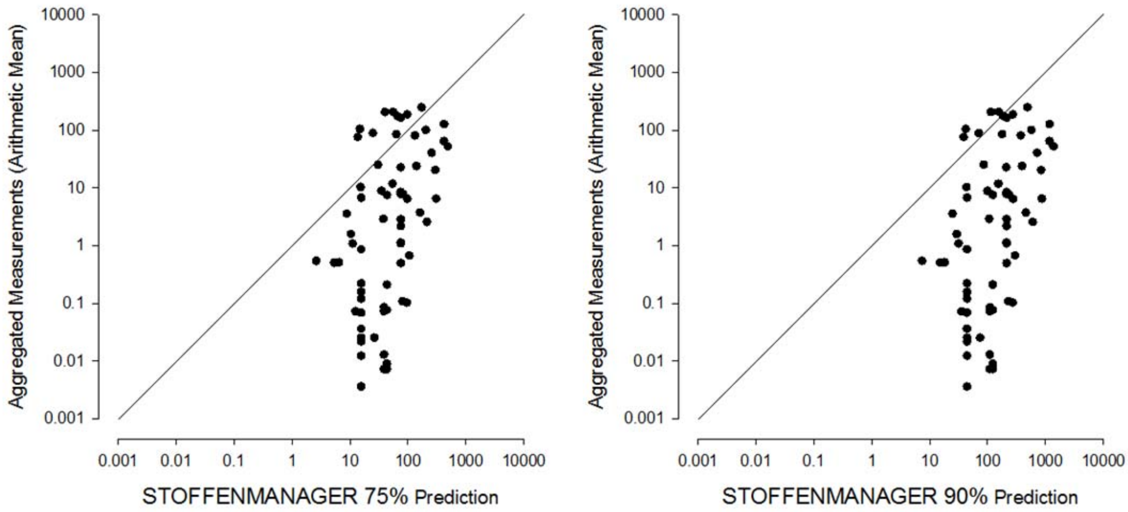


Figure 4.30 Comparison of the AM of the aggregated measurement data compared with the AM of the STOFFENMANAGER predictions (75^{th} and 90^{th} percentiles) –volatile liquids (mg m^{-3})

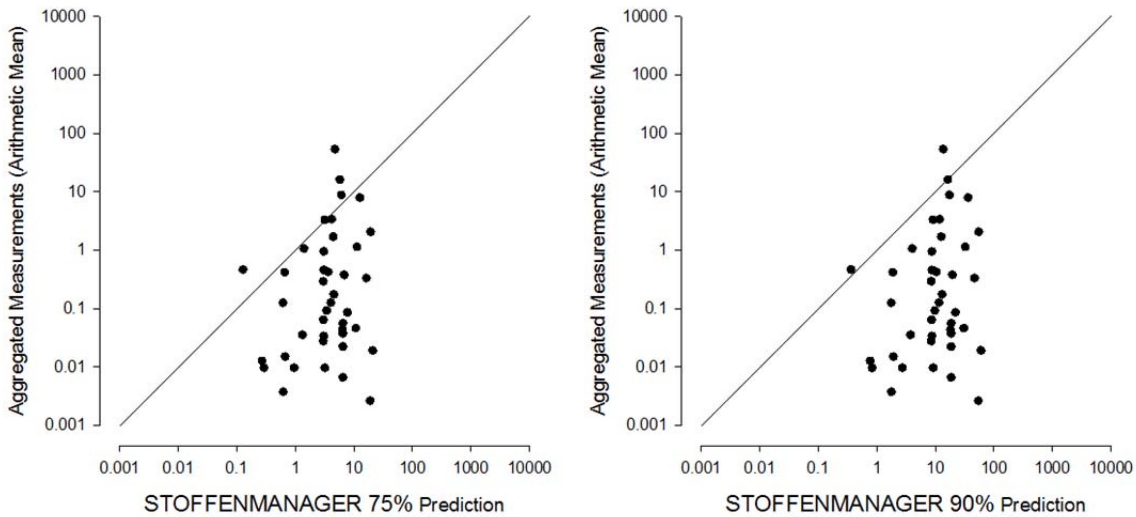


Figure 4.31 Comparison of the AM of the aggregated measurement data compared with the AM of the STOFFENMANAGER predictions (75^{th} and 90^{th} percentiles) –powder handling (mg m^{-3})

Table 4.40 the ratios of the measurements over the STOFFENMANAGER estimates for the aggregated data set and the percentages of measurements that exceeded the corresponding tool estimates.

Table 4.40 Summary of the ratios of the mean of the measurement results over the mean of the STOFFENMANAGER estimates (75th and 90th percentiles) and predicted percentage of measurements exceeding the tool estimates (%M>T)

Exposure category	N Sit	N meas	AM ratio	GM ratio	Min ratio	Max ratio	%M>T
75th percentile							
Non-volatile liquids[1)]	5	37	0.85	0.08	<0.01	4.06	30
Volatile liquids[2)]	69	505	0.56	0.04	<0.01	6.69	12
Powder handling	45	847	0.53	0.03	<0.01	10.67	7
90th percentile							
Non-volatile liquids[1)]	5	37	0.24	0.02	<0.01	1.14	13
Volatile liquids[2)]	69	505	0.20	0.01	<0.01	2.36	6
Powder handling	45	847	0.18	0.01	<0.01	3.74	3

[1)] non- volatile liquids are defined as liquids with a vapour pressure (at room temperature) ≤10 Pa [2)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa
N Sit: number of exposure situations; N meas: number of measurements; AM ratio: arithmetic mean of the ratios of the arithmetic mean of measurement results over arithmetic mean of the tool estimates; GM: geometric mean of the ratios of the arithmetic mean of the measurement results over the arithmetic mean of the tool estimates; GSD: geometric standard deviation of the ratios; Min: lowest arithmetic mean of measurements over arithmetic mean of tool estimate ratio; Max: highest arithmetic mean of measurements over arithmetic mean of tool estimate ratio: %M>T: estimated percentage of the measurements that exceed the relevant tool estimate.

As was seen for the results based on the individual measurements, it appears that the STOFFENMANAGER estimates for non-volatile liquids are less conservative than for the other exposure categories. A statistically significant correlation between the log-transformed AM of the measurement data and the log-transformed tool estimates was observed for volatile liquids (r=0.5, p<0.001), while for powders the Pearson correlation coefficient was 0.2, which was not significant (p=0.15). There was no (positive) correlation between measurements and tool predictions for the non-volatile liquids.

4.3.6 Impact of tool parameters on ratios of measurements to tool estimates

Table 4.41 provides the level of conservatism (as percentage of measurement results above the corresponding tool estimates) by a number of model parameters: dustiness, vapour pressure, concentration in mixture, domain and presence of LEV. The results presented in Table 4.41 suggest that the domain, i.e. whether it is an industrial or professional setting has an impact on the level of conservatism for the ECETOC TRA tools, as well as for MEASE. For these tools, the percentage of measurements that exceeded the tool estimates was consistently higher for the industrial domain. Although the EMKG-EXPO-TOOL and STOFFENMANAGER tools do not explicitly include domain as an input, for STOFFENMANAGER the level of conservatism was also lower for the industrial domain. Such differences were not observed for the EMKG-EXPO-TOOL.

Table 4.41 Percentage of (individual) measurements above the tool estimates (%M>T) by tool input parameter factors

	Factor															
	Dustiness			Vapour pressure			Domain		LEV				Concentration in mixture			
Exposure Category	High	Med	Low	High	Med	Low	Professional	Industrial	LEV	LEV/ out [1]	No LEV	No LEV/ out[1]	<1%	1-5%	6-25%	>25%
ECETOC TRAv2 (%M>T)/ (number of measurements)																
Volatile liquids	*	*	*	37 (n=320)	29 (n=886)	18 n=(131)	5 (n=374)	40 (n=963)	67 (n=542)	0 (n=15)	5 (n=772)	0 (n=8)	43 (n=7)	2 (n=296)	30 (n=364)	42 (n=670)
Metal abrasion	*	66 (n=41)	20 (n=41)	*	*	*	0 (n=4)	45 (n=78)	74 (n=35)	*	19 (n=47)	*	*	*	0 (n=7)	47 (n=75)
Powder handling	35 (n=51)	25 (n=194)	100 (n=1)	*	*	*	13 (n=92)	35 (n=162)	13 (n=107)	*	37 (n=147)	*	*	*	0 (n=8)	28 (n=246)
ECETOC TRAv3 (%M>T)/ (number of measurements)																
Volatile liquids	*	*	*	43 (n=320)	35 (n=886)	21 (n=131)	6 (n=374)	47 (n=963)	74 (n=542)	0 (n=15)	9 (n=772)	0 (n=8)	57 (n=7)	3 (n=296)	43 (n=364)	45 (n=670)
Metal abrasion	*	68 (n=41)	20 (n=41)	*	*	*	0 (n=4)	46 (n=78)	74 (n=35)	*	21 (n=47)	*	*	*	0 (n=7)	48 (n=75)
Powder handling	35 (n=51)	27 (n=194)	100 (n=1)	*	*	*	8 (n=92)	40 (n=162)	13 (n=107)	*	39 (n=147)	*	*	*	0 (n=8)	29 (n=246)
MEASE (%M>T)/ (number of measurements)																
Non-volatile liquids	*	*	*	*	*	*	43 (n=7)	82 (n=11)	100 (n=6)	100 (n=3)	33 (n=9)	*	*	*	86 (n=14)	0 (n=4)
Metal abrasion	*	53 (n=43)	12 (n=41)	*	*	*	0 (n=1)	34 (n=83)	56 (n=39)	*	13 (n=45)	*	*	*	0 (n=7)	36 (n=77)
Metal processing	31 (n=29)	46 (n=13)	24 (n=29)	*	*	*	0 (n=8)	35 (n=63)	35 (n=31)	*	28 (n=40)	*	0 (n=4)	0 (n=4)	13 (n=15)	42 (n=48)
Powder handling	37 (n=51)	20 (n=174)	0 (n=1)	*	*	*	9 (n=92)	32 (n=142)	9 (n=107)	*	34 (n=127)	*	*	*	0 (n=8)	23 (n=226)
EMKG-EXPO-TOOL (%M>T)/ (number of measurements)																
Volatile liquids	*	*	*	5 (n-=191)	7 (n=608)	8 (n=106)	8 (n=249)	6 (n=656)	14 (n=381)	0 (n=10)	2 (n=514)	0 (n=2)	0 (n=7)	5 (n=75)	5 (n=282)	8 (n=541)
Powder handling	39 (n=51)	46 (n=194)	0 (n=1)	*	*	*	60 (n=92)	35 (n=154)	25 (n=99)	*	57 (n=147)	*	*	*	0 (n=2)	45 (n=244)
STOFFENMANAGER. 90th *%ile* (%M>T)/ (number of measurements)																
Non-volatile liquids	*	*	*	*	*		16 (n=257)	17 (n=30)	17 (n=30)	*	11 (n=105)	18 (n=152)	13 (n=71)	33 (n=79)	7 (n=68)	7 (n=69)
Volatile liquids	*	*	*	3 (n=313)	18 (n=905)	5 (n=131)	1 (n=393)	19 (n=956)	30 (n=536)	0 (n=15)	2 (n=790)	0 (n=8)	0 (n=25)	0 (n=296)	4 (n=365)	25 (n=663)
Powders	14 (n=510	2 (n=194)	0 (n=-1)	*	*	*	0 (n=92)	7 (n=162)	1 (n=107)	*	7 (n=147)	*	*	*	0 (n=8)	4 (n=246)
Wood processing	13 (n=8)	0 (n=3)	0 (n=3)	*	*	*	*	7 (n=14)	13 (n=8)	*	0 (n=6)	*	*	*	*	*

(1) outdoors

Presence of LEV also appeared to have an impact on the level of conservatism of the tools. For volatile liquids the percentage of measurements above the tool estimates was consistently higher across all the tools for those exposure situations where LEV was present. A similar effect was observed for metal abrasion (ECETOC TRAv2 and v3 and MEASE). Interestingly, for powder handling the opposite appeared to be the case, with a higher percentage of measurements exceeding the tool estimate for situations with LEV. For non-volatile liquids (which were only assessed using MEASE and STOFFENMANAGER) there did not appear to be any major differences observed between situations with and without LEV.

The dustiness of powders appeared to affect the level of conservatism for STOFFENMANAGER, with a higher level of exceedance (14%) when handling powders that were judged to be of high dustiness compared to medium and low dustiness powders.

With regard to vapour pressure, there appeared to be a trend of decreasing level of conservatism with increasing vapour pressure when applying the ECETOC TRA tools. When using STOFFENMANAGER, 18% of measurements exceeded the tool estimate when handling volatile liquids with a medium vapour pressure, compared to 3% and 5% for higher and lower volatility liquids, respectively.

Finally, when considering the concentration in the mixture no consistent trends could be observed. For volatile liquids, the ECETOC TRA tools appeared to be much more conservative for the 1-5% mixtures compared to the other concentration categories. For metal abrasion, metal processing and powder handling the highest percentage of measurements exceeding the tool estimates were observed for >25% mixtures, although the number of measurements in the other concentration categories were often too low to make any firm conclusions. For non-volatile liquids, the STOFFENMANAGER estimates appeared to be less conservative for the 1-5% category compared to others.

In summary, some of the input parameters appear to have an impact on the level of conservatism of the tools, in particular domain and presence of LEV.

4.3.7 Impact of use of default parameters

When coding some situations into the tools, a lack of clear contextual information necessitated the use of agreed mid-range default parameters for dustiness, concentration and duration of task. The impact of these choices on the ratios of measurements to the tool estimates was again investigated using linear mixed effects statistical modelling. Table 4.42 provides the percentage of measurements exceeding the tool estimate by use of default parameters. Clearly, for each situation, in addition to the parameters for which defaults were used, there are a number of other relevant parameters of potential influence on the level of conservatism, for example the presence/ absence of LEV, which are discussed elsewhere in this report.

Table 4.42 Percentage of individual measurements exceeding the tool estimates (%M>T) by use of default parameters

Tool/ exposure category	Factor					
	Default concentration used		Default dustiness used		Default duration used	
	Yes	No	Yes	No	Yes	No
ECETOC TRAv2 (%M>T)/ (number of measurements)						
Volatile liquids	31 (n=292)	29 (n=1045)	-	-	16 (n=120)	31 (n=1217)
Metal abrasion	50 (n=2)	43 (n=80)	100 (n=3)	41 (n=79)	-	43 (n=82)
Powder handling	0 (n=6)	27 (n=248)	57 (n=30)	23 (n=224)		27 (n=254)
ECETOC TRAv3 (%M>T)/ (number of measurements)						
Volatile liquids	47 (n=292)	32 (n=1045)	-	-	31 (n=120)	35 (n=1217)
Metal abrasion	50 (n=2)	44 (n=80)	100 (n=3)	42 (n=79)	-	44 (n=82)
Powder handling	0 (n=6)	29 (n=248)	67 (n=30)	23 (n=224)	-	28 (n=254)
MEASE (%M>T)/ (number of measurements)						
Non-volatile liquids	43 (n=7)	82 (n=11)	-	-	-	67 (n=18)
Metal abrasion	50 (n=2)	33 (n=82)	67 (n=3)	32 (n=81)	-	33 (n=84)
Metal processing	0 (n=7)	34 (n=64)	-	-	-	31 (n=71)
Powder handling	0 (n=6)	23 (n=228)	54 (n=26)	19 (n=208)	-	23 (n=234)
EMKG-EXPO-TOOL (%M>T)/ (number of measurements)						
Volatile liquids	6 (n=217)	7 (n=688)	-	-	5 (n=96)	7 (n=809)
Powder handling	-	44 (n=246)	33 (n=30)	46 (n=216)	-	44 (n=246)
STOFFENMANAGER 90th %-ile (%M>T)/ (number of measurements)						
Non-volatile liquids	5 (n=22)	17 (n=265)	-	-	-	16 (n=287)
Volatile liquids	16 (n=293)	5 (1056)	-	-	2 (n=120)	14 (n=1229)
Powder handling	0 (n=6)	7 (n=248)	3 (n=30)	7 (n=224)	-	4 (n=254)

On the whole, there was little evidence that the use of default parameters would have affected the overall results. Some differences were noted, but often these were relatively small and the use of default parameters was limited. Perhaps the only example where the use of a default value could have affected the overall conclusion is for STOFFENMANAGER when estimating exposure from volatile liquids and a default value for concentration of the mixture was used. When using the default value for the mixture concentration 16% of the measurements exceeded the STOFFENMANAGER 90th percentile estimate, compared to 5% when information on the concentration was available. The overall percentage of exceedance for volatile liquids for STOFFENMANAGER (90th percentile) was 13%, hence excluding the use of default parameters would have reduced the percentage of exceedance to below the 10% level.

There were some other examples where the use of default values appears to be related to an increased percentage of measurements exceeding the tool estimates.

In case of powder handling, the use of a default dustiness level was associated with an increase in exceedance level for the ECETOC TRA tools and MEASE from approximately 20% to 50-60%. However, when comparing the corresponding results in Tables 3.16, 3.19 and 3.22, excluding the situations where a default dustiness level was used only reduced the exceedance from 27% to 23% for ECETOC TRAv2; from 28% to 23% for ECETOC TRAv3 and from 23% to 19% for MEASE respectively. This would not have affected the overall conclusion of the results.

4.4 Discussion

4.4.1 Overview

This chapter described the methods used for, and results from, a comparison of Tier 1 exposure assessment tool estimates with inhalation measurements obtained from a variety of sources. The comparison focussed on i) the level of conservatism of the tool estimates compared to the measurement results and ii) the correlation between the measurement results and tool estimates.

The level of conservatism was expressed in two ways. Firstly, the percentage of measurements that were higher than the corresponding tool estimate was examined, with the level of conservatism defined in this case as follows:

- High – where ≤10% of measurements exceeded the tool estimate
- Medium- where 11≤25% of measurements exceeded the tool estimate
- Low- where >25% of the measurements exceeded the tool estimate

As reported elsewhere in Chapter 2 the limited number of input parameters required for first tier exposure assessment using the tools being evaluated can give rise to considerable levels of inherent uncertainty. We therefore considered the tools to be sufficiently conservative if the estimates of the tools were comparable with the 90th percentile of an exposure distribution. For STOFFENMANAGER, which generates an exposure distribution, the estimates for the 75th and 90th percentiles were used in the comparisons. STOFFENMANAGER estimates were considered to be sufficiently conservative if the percentage of measurements above the tool estimates were less than 25% or 10%, respectively. For EMKG-EXPO-TOOL, the upper estimate of the exposure range was used. In cases where the EMKG-EXPO-TOOL assigned an exposure of >10 mg m^{-3} (for solids) or >500 ppm (for liquids), values of 20 mg m^{-3} or 1000 ppm were used respectively.

We also considered the ratio of the measurement results to the tool estimate, where a geometric mean of the ratios below 1 was taken as an additional indicator that the tool was conservative to some degree for that situation.

4.4.2 Overall level of conservatism

The overall level of conservatism was evaluated using the percentage of measurements exceeding the tool estimates. Table 4.44 provides an overview of

Table 4.43 Proportion of measurements exceeding the tool estimate, by exposure category (individual and aggregated measurements combined)

Tool	Non-volatile liquids			Volatile liquids			Metal abrasion			Metal processing			Powder handling		
	nM	nM >T	%M >T	nM	nM >T	%M >T	nM	nM >T	%M >T	nM	nM >T	%M >T	nM	nM >T	%M >T
ECETOC TRAv2	0	-	-	1842	485	26	180	42	23	-	-	-	1101	180	16
ECETOC TRAv3	0	-	-	1842	585	32	180	46	26	-	-	-	1101	231	21
MEASE	60	35	58	-	-	-	182	33	18	399	54	14	1081	115	11
EMKG-EXPO-TOOL	0	-	-	1372	70	5	-	-	-	-	-	-	1063	184	17
STM 75th percentile	324	101	31	1854	359	19	-	-	-	-	-	-	1101	90	8
STM 90th percentile	324	50	15	1854	209	11	-	-	-	-	-	-	1101	33	3

nM= number of measurements
nM>T= number of measurements exceeding the tool estimate;
%M>T= Percentage of measurements exceeding the tool estimate

proportion of measurements that exceeded the tool estimates for the combined individual and aggregated datasets. The largest number of measurement results available for comparison with tool estimates was for volatile liquids. When considering the combined individual and aggregated datasets (Table 4.43), the EMKG-EXPO-TOOL was the only tool that appears to be highly conservative for this exposure category, when using the criterion of <10% measurements above the tool estimate. This is most likely to have arisen because the concentration of the substance in the mixture is not taken into account within the EMKG-EXPO-TOOL. If the estimates were to be adjusted for the mixture content, the level of conservatism will clearly be reduced. There was only a moderate correlation between individual measurement results and tool estimates for the EMKG-EXPO-TOOL for this exposure category, but not for the aggregated data. The degree of correlation may however increase if concentration is taken into account.

STOFFENMANAGER is also conservative for this category, with 11% of measurements for exposure to volatile liquid vapours exceeding the 90th percentile tool estimate.

The ECETOC TRAv2 and ECETOC TRAv3 were observed to be less conservative in comparison with the overall dataset for volatile liquids, with 26% and 32% of the measurements exceeding the tool estimate.

A relatively high overall number of data points were collected for powder handling, with differences again noted between the tools in terms of both level of conservatism and the degree of correlation with the measured values.

For powder handling, STOFFENMANAGER appears to provide very conservative estimates when using both the 90th and 75th percentiles. Furthermore, MEASE could also be considered conservative, with around 11% of measurements exceeding the tool estimates. However, ECETOC TRAv2 and v3 are judged to have only a medium level of conservatism for this category, with 16% and 21% of the estimates exceeded by the measurement value. A similar finding was observed for the EMKG-EXPO-TOOL.

In relation to exposures during abrasion of metals, the ECETOC TRAv2 (24% of the measurements exceeding the tool estimate) and MEASE (18% of measurements in exceedance) were of medium conservatism, with the ECETOC TRAv3 judged to be of a low level of conservatism (exceedance in 26% of cases). It should be noted that there were very few data points for certain of the metal abrasion and metal processing process codes. For example, no individual measurements were available for PROC 21, only aggregated data. Similarly, the metal processing data available were primarily from welding/ brazing and cutting tasks, rather than basic metal production activities such as furnace operation.

Metal processing activities were assessed only using MEASE, as, in agreement with the relevant developers, none of the other tools were considered applicable. In relation to this dataset, the tool was observed to be of a medium level of conservatism (14% of measurements > tool estimates).
In comparison with this dataset, limited evidence of conservatism was found for STOFFENMANAGER and MEASE in relation to prediction of exposures to non-

volatile liquids. For STOFFENMANAGER, 15% of the measurements exceeded the tool 90^{th} percentile estimate, whilst for MEASE the tool exposure prediction was exceeded in 58% of cases.

A concern was raised by a member of the Advisory Board that exposure situations associated with multiple measurements could have had an unduly large impact on the overall results when expressed as the %M>T. For example if the multiple measurement situations originated from less controlled workplaces, and so reflected higher exposure levels, then the level of conservatism of the tools may be underestimated. The amount of data available for each exposure situation varied from 1 measurement to 137 measurements.

We investigated this possibility by calculating the percentage of situations which exceeded the tool estimate as follows.

$$\%S > T = \frac{\sum_{i=1}^{N} \frac{\sum_{j=1}^{n_i} P_{ij}}{n_i}}{N} \quad \textbf{Equation 4.2}$$

where

$$P_{ij} = \begin{cases} 1, & M_{ij} > T_i \\ 0, & M_{ij} < T_i \end{cases}$$

N = Number of exposure situations
ni = Number of measurements for exposure situation i
Mij = measurement j from exposure situation i
Ti = tool estimate for exposure situation i

This provided a weighted percentage of measurements exceeding the tool estimate, with the results presented in Table 4.44 together with %M>T as reported previously.

Table 4.44 Comparison of percentages of individual measurement values (%M>T) and exposure situations (%S>T) exceeding the tool estimates

Tool	Exposure category	%M>T	%S>T
ECETOC TRAv2	Volatile liquids	30	27
	Metal abrasion	43	59
	Powder handling	27	46
ECETOC TRAv3	Volatile liquids	35	41
	Metal abrasion	44	60
	Powder handling	28	48
MEASE	Non-volatile liquids	67	75
	Metal abrasion	33	48
	Metal processing	31	31
	Powder handling	23	36
EMKG-EXPO-TOOL	Volatile liquids	7	10
	Powder handling	44	45
STM 90th percentile	Non-volatile liquids	16	16
	Volatile liquids	13	6
	Powder handling	4	8

As can be seen from the table, the above results suggest that the number of comparator measurements per situation appears to have some impact on the likelihood of the measurement exceeding the corresponding tool estimate. For most of the exposure category-tool combinations, the level of conservatism decreased (i.e. the percentage of measurements higher than the tool estimate increased). In a small number of cases, (estimation of exposure to volatile liquids by the ECETOC TRAv2 and STOFFENMANAGER), the level of conservatism improved somewhat. It is thus felt that the impact of multiple measurement exposure situations does not affect the overall project findings.

4.4.3 Differences in level of conservatism between data types and providers

Table 4.43 provides a useful overview of the overall level of conservatism across the entire dataset. However, different results were observed based on the individual data and aggregated data. The tools were generally found to be more conservative when compared with the aggregated data than when the individual measurement results were used.

There are a number of possible reasons for this. Statistically significant differences were observed between data providers in the geometric means of the ratios of individual measurements to tool estimates.

As reported above, when examining the data from each of the providers, the sets with outlying mean levels of exposure are those which also exhibit higher geometric mean ratios and higher percentages of measurements in excess of the tool estimates. Hence, the differences in the ratios between the data providers are considered likely to arise from differences in the reasons for, and the methods and strategies by which the measurement data were collected. For example, Provider G relates to measurements from visits carried out by a regulatory body. Samples may therefore have been taken for enforcement purposes, or in workplaces with lower levels of exposure control for a particular campaign, whilst those from Provider M reflect a wider range of sampling purposes, with very specific task and substance information given.

The aggregated data originated from different providers, thus the differences between these comparisons and those with the individual measurements may result from these differences in data collection between providers rather than any differences in data analyses and interpretation. The two main aggregated data sets were taken for routine compliance or research purposes, rather than regulatory/ enforcement purposes.

4.4.4 Differences in level of conservatism between PROC code/ activity type

Differences in the percentage of exceedances were observed between PROC codes and exposure categories, suggesting that the tools may predict with varying levels of conservatism for different process/ activity types.

For example, for volatile liquids, both ECETOC TRAv2 and v3 were considered to be sufficiently conservative (i.e. <10% measurements > tool estimate) for PROCs 8b, 9 and 11, whilst for PROCs 7 and 14, high percentages of measurements exceeded the estimates from both of the ECETOC TRA tools. These results suggest that in comparison with the project dataset, both of the ECETOC TRA may not be sufficiently conservative for these types of situation.

For powder handling, both ECETOC TRA tools and MEASE appeared to provide insufficiently conservative estimates of exposure for PROCs 8a and 14, while for PROCs 5, 7, 8b and 9 the tools were sufficiently conservative.

Although neither EMKG-EXPO-TOOL nor STOFFENMANAGER use PROC codes as an input, using the PROC as a proxy for activity type for these tools also gave rise to differences in conservatism. The EMKG-EXPO-TOOL appeared to generate sufficiently conservative estimates of exposure to volatile liquids for most PROC codes, with the exception of PROC 4 and perhaps PROC 3 (although for the latter only 4 measurements were available). For powder handling, EMKG-EXPO-TOOL appeared to be sufficiently conservative only for PROC 9, which relates to controlled filling/ transfer processes.

For STOFFENMANAGER, the vast majority of the measurements available for non-volatile liquids were available for PROC 11 (233 out of 285 measurements). The results suggest that for this PROC, which covers non-industrial spraying activities, STOFFENMANAGER was not sufficiently conservative for non- volatile liquids. For volatile liquids, STOFFENMANAGER underestimated the exposure compared to the measurement results for PROC 14. Finally, for powder handling, STOFFENMANAGER was highly conservative for PROCs 5, 7, 8b, 9 and 14. As for the ECETOC TRA tools and MEASE, STOFFENMANAGER was less conservative for PROC 8a, which relates to less controlled powder transfer processes at non-dedicated facilities.

These results suggest that the performance of the tools may depend on the activity or process type, either singly or in combination with other factors, such as data provider, as outlined below. For example, about 50% of measurements from Provider M for volatile liquids (for which only a small fraction of measurements were observed to be higher than the tool estimates) were for PROC 8b.

4.4.5 Differences in level of conservatism associated with input parameters

To investigate more fully where tool performance differed from expectations, i.e. where the tools were less or more conservative than predicted, parameters of potential interest and their impact on the comparisons with individual measurement data were considered. These were the fugacity (i.e. dustiness and volatility); domain; presence/absence of LEV and concentration in mixture. The impact of the use of default parameters for dustiness, duration, concentration and on the ratios of measurement data to tool estimate and percentage of measurements exceeding the tool estimates was also evaluated.

4.4.5.1 Fugacity

For all of the tools, the percentages of measurements exceeding the tool estimates for powder handling and metal abrasion were generally higher for the high and medium dustiness categories respectively compared with low dustiness, suggesting that there may be less conservatism for these types of situation. The use of the default dustiness (i.e. “medium”) level also generated higher percentages of exceedances for the ECETOC TRA tools and MEASE. However, the number of situations where this was the case was relatively low compared with those where the default had not been selected; hence, excluding the situations using default values did not appear to have a major impact on the results.

When considering the impact of vapour pressure, there were differences for the ECETOC TRAv2 and ECETOC TRAv3 tools, where larger numbers of measurements of high vapour pressure substances exceeded the tool estimates compared with less volatile materials. This suggests that the level of conservatism in tool estimates may be lower for substances with vapour pressures > 10 kPa compared with substances of lower volatility. For STOFFENMANAGER, more exceedances were noted for the medium vapour pressure category, again suggesting that the tool is comparatively less conservative for this category.

4.4.5.2 Domain

Differences in the percentage of measurements exceeding the tool estimates were observed between different settings for the ECETOC TRA and MEASE tools across all of the exposure categories. This suggests that whether exposure occurs in an industrial or professional setting may have an impact on the level of conservatism for the ECETOC TRA tools, as well as for MEASE. For these tools, in comparison with this dataset, the percentage of measurements that exceeded the tool estimates was consistently higher for the industrial domain option. Hence, based on these results, the ECETOC TRAv2 and ECETOC TRAv3 appear to provide less conservative estimates of exposure in industrial settings compared to professional environments. The ECETOC TRAv3 tool allows greater choice of options for the industrial setting, for example in relation to ventilation controls, which may be partly reflected in the observed lower level of conservatism.

For non-volatile liquids, the total number of data points used for the comparison with MEASE was very low, (11 industrial and 7 professional measurements), making analysis of differences between domains difficult.

For the MEASE, ECETOC TRAv2 and ECETOC TRAv3 tools, which allow allocation of the domain as a parameter, the observed differences in conservatism between settings may relate to the base exposure estimates for each type of setting to which modifiers are applied. In many cases, the base estimates for the industrial settings are lower than those for professional ones, on the assumption that the exposures of industrial workers are generally better controlled. Alternatively, or indeed in addition, the observed differences may be linked to the exposure modifiers themselves, for example the tool-inherent assumptions about relative control efficiencies for each domain, where effectiveness is assumed to be higher in industrial settings.

The percentage of measurements exceeding the STOFFENMANAGER predictions was also higher for situations which had been described as industrial, although neither this tool nor the EMKG-EXPO-TOOL incorporate the exposure setting in their estimation processes. For STOFFENMANAGER the level of conservatism was thus considered to be lower for the industrial domain. The domain did not affect the percentage of exceedances for the EMKG-EXPO-TOOL.

4.4.5.3 Local exhaust ventilation (LEV)

A possible link between tool-inherent exposure modifiers and the level of conservatism was also observed in relation to use of LEV as a local control. The level of conservatism was different for situations with and without LEV for volatile liquids for the ECETOC TRAv2, ECETOC TRAv3 and EMKG-EXPO-TOOL. Situations with LEV had higher percentages of measurements exceeding the estimates, suggesting that in these circumstances the tools were less conservative. Similarly, higher percentages of measurements for metal abrasion exceeded the corresponding ECETOC TRAv2, ECETOC TRAv3 and MEASE estimates where LEV was present compared with those without localised control.

All of the tools incorporate different assumptions about the effectiveness of the available control measure input options. In some tools the applied level of effectiveness is explicit, for example MEASE, whilst for the ECETOC TRA tools it is provided in look-up tables. Assumed control efficiencies are given in the background literature for STOFFENMANAGER, wherein a lower level of efficiency is generally assumed than that used in the ECETOC TRA tools. The assumptions made in the EMKG-EXPO-TOOL regarding control efficiency were not identifiable for each approach, but rather as a relative efficiency between control approaches for a particular situation. For the vast majority of the workplace data collected, there was no or very limited specific information provided about measured efficiencies for LEV and general or mechanical ventilation systems.

It may therefore be that these tools overestimate the efficiency of LEV, when compared with measurements of exposure to vapours and dust from metal abrasion in real workplaces. However, as the tools are used under REACH to specify risk control measures (to be implemented only with the assigned efficiency), in theory higher levels of control should be achieved than those in the many and very varied workplaces from which the comparator data arose. Achievement of the tool-predicted exposures would self-evidently depend on the performance of the LEV system being maintained indefinitely at the expected level defined in the tool. This point is also obviously of relevance in the implementation and maintenance of all tool-specified measures used in the REACH assessment.

Conversely, for powder handling activities, the geometric means of the ratios and the percentages of measurements greater than the tool estimates were higher for those situations where no LEV had been used compared with those where it was present. This was observed for all of the tools, suggesting that for these situations, which may involve lower general levels of control, exposures may generally be underestimated.

It is also possible that a mixture of (unrecorded) exposure controls were in place in some of the workplaces, for example good general ventilation plus a degree of process containment may have been described as “indoors with LEV”. In such situations, the tools may have underestimated the combined impact of the control measures. Equally, a number of the tools also include exposure modifiers related to the level of process enclosure. In practice, the level of control achievable may be lower than that assumed by the tools because of unrecorded breaches of containment during process sampling or maintenance- in such circumstances the tool may underestimate the exposure.

The observed differences in conservatism related to exposure controls are in accordance with findings by previous researchers, for example in relation to COSHH Essentials by Lee et al (2009), Jones and Nicas (2006) and Kindler and Winteler (2010) for the EMKG-EXPO-TOOL and EASE, and for STOFFENMANAGER (Koppisch et al (2011) where in some cases the efficiency of control measures appears to be overestimated by the tools.

4.4.5.4 Concentration in mixture

When considering the impact of concentration in the mixture on the degree of conservatism, no consistent trends were observed. For volatile liquids, the ECETOC TRA tools appeared to be much more conservative for the 1-5% mixtures compared to the other concentration categories. For metal abrasion, metal processing and powder handling the highest percentages of measurements exceeding the tool estimates were observed for >25% mixtures, although the number of measurements in the other concentration categories were often too low to draw any firm conclusions. For non-volatile liquids, the STOFFENMANAGER estimates appeared to be less conservative for the 1-5% category compared to others.

4.4.6 Differences in level of conservatism associated with specific input parameter combinations

To assist in identifying areas where the tools may be less conservative, the calculations of percentage exceedances were further stratified using different combinations of PROC and other input parameters: fugacity; domain; presence/ absence of LEV and concentration of substance in mixture. The stratification was restricted to those PROCs where the percentage of measurements that exceeded the tool estimate was greater than 20% and where the number of individual measurements was at least 50. The exception to this rule was the inclusion of PROC 11 to investigate the level of conservatism of STOFFENMANAGER for non-volatile liquids within this PROC, for which 17% of measurements exceeded the 90th percentile STOFFENMANAGER estimate. The identified appropriate combinations are discussed below by exposure category. In the following sections, only those combinations of PROC and input parameter which gave rise to observable differences in level of conservatism are discussed.

4.4.6.1 Powders

For powders, PROCs 5, 8a, 8b and 14 were selected for stratification according to the above criteria.

i) Dustiness

For PROC 8a, the high dustiness category generated higher percentages of measurements exceeding the tool estimate for all of the tools except for STOFFENMANAGER, where medium dustiness resulted in a higher degree of exceedance indicative of a lower level of conservatism.

For PROC 8b, analysis was possible for all of the tools except STOFFENMANAGER (for which no measurements exceeded the tool estimate). For the ECETOC TRAv2, ECETOC TRAv3, EMKG-EXPO-TOOL and MEASE the medium dustiness category led to higher percentage exceedances than the low dustiness category.

These results suggest that, with the exception of STOFFENMANAGER, the tools generate less conservative estimates for activities categorised under PROC 8a involving highly dusty materials than for substances with lower intrinsic dustiness. For PROC 8b, the ECETOC TRAv2, ECETOC TRAv3, EMKG-EXPO-TOOL and MEASE appeared less conservative for the medium dustiness category, suggesting that they may underestimate exposure to such materials during transfer processes at dedicated facilities.

ii) Domain

When assessing PROCs 5, 8a and 8b higher percentages of measurements exceeded the exposure predictions in industrial situations compared with those defined as professional. This was the case for all of the tools except for the EMKG-EXPO-TOOL, where the situation was reversed and professional settings appeared to generate less conservative predictions.

The results suggest that the ECETOC TRAv3, MEASE and STOFFENMANAGER are less conservative in industrial settings compared with professional environments.

The EMKG-EXPO-TOOL is less conservative in professional settings for PROC 8a which relates to transfer activities which take place at non-dedicated facilities, therefore may be less well controlled. This finding is therefore of interest in light of the EMKG-EXPO-TOOL's origin as a control banding tool for small and medium enterprises and other non-expert users.

The tools were more conservative for PROC 8b than PROC 8a; however, the ECETOC TRAv2, ECETOC TRAv3 and MEASE were again less conservative for industrial settings, with no exceedances for professional settings for any of the tools. The reverse was true for the EMKG-EXPO-TOOL with a larger proportion of measurements for professional settings exceeding the tool compared with those for industrial settings. No measurements exceeded the STOFFENMANAGER tool estimates for the combination of PROC 8b and either domain.

iii) Presence/ absence of LEV

For all of the tools except STOFFENMANAGER (where no predictions were less than the measurement value), higher percentages of measurements exceeded the tool predictions for PROC 5 powder handling activities where LEV was used compared with those where it was absent. This suggests that, for this PROC, the ECETOC TRAv2, ECETOC TRAv3, EMKG-EXPO-TOOL and MEASE are less conservative where local control is used, and may be result from tool-inherent assumptions about RMM efficiencies.

For PROC 8b, the percentages of measurements exceeding the estimates from the ECETOC TRAv2, ECETOC TRAv3, MEASE and STOFFENMANAGER were higher where LEV was present compared with those where it was absent. The opposite was true for the EMKG-EXPO-TOOL, whereby situations where LEV was not used were more conservative than those where it was present.

iv) Concentration in mixture

For PROC 5, all of the tools, in particular the EMKG-EXPO-TOOL, were less conservative for situations where the concentration was in the >25% band compared with those where concentration was 6-25%. As the number of points in the 6-25% band was very small, it is however difficult to draw firm conclusions regarding any impact of concentration in combination with PROC code.

4.4.6.2 Volatile liquids

Numbers of data were sufficient to allow further analysis of PROCs 4, 5, 7, 10, 13 and 14 in combination with vapour pressure, domain, presence/absence of LEV and concentration in mixture. MEASE was not evaluated for volatile liquids as this category is outwith its domain of applicability. PROC 7 is also outside of the scope of the EMKG-EXPO-TOOL.

i) Vapour pressure

For PROC 4 and PROC 7, higher percentages of measurements generally exceeded the estimates from the applicable tools for the low and high volatility categories compared with the medium category. For PROCs 5, 10, 13 and 14, the medium vapour pressure category tended to be more conservative.

ii) Domain

Where both domains were available for comparison (PROCs 4, 10 and 13), the estimates of exposure in industrial domains were generally less conservative than those for professional environments for all of the tools. A minor exception was the EMKG-EXPO-TOOL where the estimates from the tool for PROC 13 were more conservative in the industrial domain than for professional settings.

iii) Presence/ absence of LEV

The presence of LEV for processes described by PROCs 4, 7, 10, 13 and 14 was associated with higher levels of measurements in excess of the estimates from the ECETOC TRAv2, ECETOC TRAv3, EMKG-EXPO-TOOL and STOFFENMANAGER when compared with those where LEV was absent. The ECETOC TRAv2 and ECETOC TRAv3 were also less conservative than the EMKG-EXPO-TOOL and STOFFENMANAGER for each of the PROCs.

iv) Concentration in mixture

In PROCs 4 and 10, a higher proportion of measurements exceeded the tool estimates for the 6-25% category for the ECETOC TRAv2, ECETOC TRAv3 and STOFFENMANAGER tools compared with the other concentrations. In PROCs 7 and 14 the highest concentration band (>25%) appeared least conservative for each of the tools.

4.4.6.3 Non-volatile liquids

For non-volatile liquids, further analysis was only applicable to the combination of PROC 11 with presence/ absence of LEV and concentration in mixture for the STOFFENMANAGER tool.

i) Presence/ absence of LEV

STOFFENMANAGER appeared to be less conservative for PROC 11 in situations where LEV was present compared with those where it was not implemented.

ii) Concentration in mixture

STOFFENMANAGER was least conservative for PROC 11 for concentrations of 1-5% in comparison with the other concentration bands.

4.4.6.4 Metal abrasion

Only PROC 24 contained sufficient numbers of data to allow further stratification in combination with other input factors. This PROC is only applicable for the ECETOC TRAv2, ECETOC TRAv3 and MEASE tools.

i) Dustiness

For PROC 24, all of the tools evaluated were less conservative for situations where medium dustiness was chosen compared with those where low dustiness was selected.

ii) Domain

The tools were less conservative for industrial settings than those taking place in professional environments. The number of professional situations was however small (n=4) compared with those categorised as industrial, making a simple comparison of the effect of different domains difficult.

iii) Presence/ absence of LEV

For PROC 24, the three tools evaluated were less conservative where LEV was present compared with those where no local control was implemented. This suggests a degree of underestimation for the tools in relation to this type of activity, and may again be related to the assumptions made regarding LEV effectiveness when compared with this workplace measurement dataset.

iv) Concentration in mixture

The three tools were less conservative for concentrations of >25% than for the other mixture compositions. The concentration of the substance in the material may have some impact on the degree of conservatism.

4.4.6.5 Summary

In summary, from this limited stratification exercise, it would appear that although for each of the tools there are some specific combinations of input parameters and exposure category where the estimates are less conservative than might be expected, in general the patterns of conservatism are similar to those observed in the overall validation exercise. In particular, the impact on tool conservatism of domain and the presence/ absence of LEV observed in the stratification exercise are in accordance with the main comparison.

4.4.7 Correlation between tool estimates and measurement data

In the second part of the comparison process, correlations between the estimates of exposure and the measured values for the different exposure categories and for the data types were determined. Table 4.45 shows an overview of the Pearson correlation coefficients that were observed between the log-transformed tool estimates and log-transformed individual and aggregated measurement results.

Table 4.45 Pearson correlation coefficients between log-transformed measurement results and log-transformed tool estimates, by exposure category and data type

Tool	Exposure category									
	Non-volatile liquids		Volatile liquids		Metal abrasion		Metal processing		Powder handling	
	Ind	Aggr	Ind	Aggr	Ind	Aggr	Ind	Aggr	Ind	Aggr
ECETOC TRAv2	-	-	0.35	-0.05	-0.34	-0.47	-	-	0.59	-0.22
ECETOC TRAv3	-	-	0.34	-0.03	-0.32	-0.46	-	-	0.69	-0.24
MEASE	0.89	-	-	-	-0.17	0.45	0.32	0.05	-0.13	0.00
EMKG-EXPO-TOOL	-	-	0.28	-0.16	-	-	-	-	0.71	0.23
STM 90th percentile	0.62	-0.95	0.55	0.48	-	-	-	-	0.83	0.22

Ind: individual measurement data (log transformed)
Aggr: aggregated measurement data (log transformed arithmetic mean)

Differences in the level of correlation of the measurement data with the tool estimates were noted both between exposure categories and comparator data type.

Based on individual measurement results, strong (r=0.9) and moderate (r=0.5) correlations were observed for non-volatile liquids for MEASE and STOFFENMANAGER respectively. This suggests that, whilst the tools may underestimate exposure in some circumstances for this exposure category, they exhibit a degree of predictive potential in relation to exposure. A strong negative correlation was however noted between STOFFENMANAGER and the aggregated data for non-volatile liquids.

For volatile liquids, weak to moderate significant correlations were noted between the log transformed individual measurement data and estimates from the EMKG-EXPO-TOOL, ECETOC TRAv2, ECETOC TRAv3 and STOFFENMANAGER (r= 0.3- 0.6), suggesting that the tools predicted exposure to a certain degree. There were no correlations noted between aggregated data and the volatile liquid exposure estimates from the EMKG-EXPO-TOOL, ECETOC TRAv2 and ECETOC TRAv3. The STOFFENMANAGER estimates showed a moderate correlation with the aggregated volatile liquids data, suggesting that the tool had some predictive power in these cases.

No correlation was noted between the ECETOC TRAv2, ECETOC TRAv3 and MEASE estimates for metal abrasion and the individual measurements, however for MEASE a moderate correlation with the aggregated data was noted for this category.

A moderate correlation was observed between the MEASE estimates for metal processing and the individual measurements, although this was not observed for the equivalent aggregated data category.

Moderate to strong correlations between the tool estimates and individual measurements from powder handling were observed for all tools except MEASE. However, this was not observed when using the aggregated data.

In summary, the correlation between the tool estimates and measurement data was better for powders and non-volatile liquids, followed by volatile liquids then the other exposure categories. This suggests that the tools are better at predicting potential exposure in these categories compared with the metals-related situations.

4.4.8 Limitations of external validation

The project team aimed to carry out a full and comprehensive evaluation of the tools. To contextualise the validation exercise, a number of pertinent factors in relation to the method and datasets used are outlined below.

4.4.8.1 Dataset

i) General comments

The formation of a comprehensive set of measured data with which to compare the tool estimates was a primary aim of the eteam Project. To provide as complete a picture as possible of the tools' performance, it was desirable that comparator data were collected across the range of applicability of the tools. Data collection therefore concentrated on situations which were applicable under the majority of the tools. This focus on maximising the applicability of the data set however meant that the full range of PROC codes could not be included. The vast majority of data provided were collected for non-REACH purposes, however the dataset covered many common activity/task/process types, for example transfers, mixing, spraying and mechanical treatment. In addition, whilst a very useful descriptor for summarising the dataset, this parameter is not an input for either the STOFFENMANAGER or EMKG-EXPO-TOOL, which are also used for REACH assessments. Consideration of the types of activity and process covered within the dataset are perhaps therefore of more relevance in determining the scope of the validation exercise.

Our focus on collecting data which were relevant to the majority of the tools also had some impact on the exposure categories covered, for example project timescales did not allow for use of some of the non-volatile liquids data and metal processing from one provider.

It is also acknowledged that the use of data collected for non-REACH purposes may have resulted in a dataset primarily focussed on substances and activities which give rise to health concerns, whereas REACH requires assessment of all potential uses. We were however constrained by the data available to us, which, in common with most occupational hygiene measurements, were generally collected to determine exposure in situations where there may be a risk to health. For example, whilst there are several metals-related abrasion and processing PROC codes assessable using the MEASE tool under REACH, relatively few points were available for these activity types, and then only for a limited range. By way of illustration: no individual measurements were available for PROC 21, only aggregated data. Similarly, rather than being REACH-specific, the metal processing data available were primarily from relatively commonplace welding/ brazing and cutting tasks, as opposed to more specialised metal production activities such as furnace operation, casting and metal powder formation.

It has been observed previously that the sourcing and collation of detailed contextual information on workplace situations is difficult. In the context of tool validation, with its requirement to ensure that the relevant input parameters are addressed, this difficulty is magnified (Maidment, 1998; Koppisch et al, 2012; Schinkel et al, 2010). For example, detailed temperature information was not available for the many of the metal processing exposure situations within the individual measurement dataset. Comparisons with similar processes within the eteam database and appropriate external information sources were therefore carried out to identify likely temperatures. Similar methods were used to identify the level of dustiness for metal abrasion. Some uncertainty may have arisen from the assumptions made. The lack of detailed information on the type and efficiency of workplace exposure control measures was particularly evident, with the descriptions varying widely in terms of their level of detail.

Despite a large effort to develop a comprehensive exposure measurement database for the comparison exercise, the above constraints resulted in some gaps. Relatively few measurement results were available for non-volatile liquids, aqueous solutions and exposure to metals from abrasive and hot processes. The results and observations made within this report should therefore be considered in the light of the above limitations.

ii) Individual versus aggregated data

Measurement data were obtained in both individual and aggregated form, with summary statistics provided for a group of measurements. Two types of data aggregation were carried out. For Type 1 aggregation we had groups of measurement results for a single described exposure situation. For the aggregated data from Provider C, contextual information was available for all of the individual situations, thus allowing tool estimates to be generated for each one. The individual situations were then grouped as described previously. The grouped situations were thus identical in terms of tool input for PROC, presence of LEV and dustiness or volatility category. The summary statistics were calculated across all of the individual tool estimates generated for the situations in a particular group, which mitigated differences between other inputs, for example domain or additional risk management measures. A comparison was therefore possible between a single "group" tool estimate and the corresponding grouped measurement data.

The results of the comparisons based on individual measurements were somewhat different from the results based on the aggregated data. In general, the results based on the aggregated data suggested that tools were more conservative, but generally poor or no correlations were observed (with the exception of STOFFENMANAGER estimate for volatile liquids, the MEASE estimates for metal abrasion and the EMKG-EXPO-TOOL for powder handling).

There is no clear reason for this observed difference between the individual and aggregated data sets. However, as noted previously, large differences were also observed within the individual dataset between different providers. These may have resulted from differences in the reasons for measurements collection and measurement strategy. Hence, the differences between the individual and aggregated data could be due to the same underlying issues as the differences between the data providers. Aggregation of the data, and the resulting loss of individual detailed situation information, may however have had some impact, for example in relation to the level of correlation between the estimates and the measurement data.

4.4.8.2 Method of estimate generation

The ideal method of exposure assessment tool estimate generation would involve the inputting of the required parameters directly into the various tools, followed by extraction of the relevant values and import into the database. However, the limited amount of time allocated for coding and cross checking of the parameters, the number of situations collected and the time required for preparing, entering and recording the tool entries made this impossible. In addition, use of separate individual Excel worksheets for the tools for each situation would have hampered the identification of inconsistencies in coding: extraction of the inputs from various coders allowed quick comparisons to be made across multiple situations. Using individual spreadsheets would also have hampered future efforts to look at the effect of particular parameters (e.g. concentration, LEV, domain) on the study results. Multiple checks of the estimates obtained via the procedures and algorithms used in the eteam project database against results obtained directly from the original tools were carried out. These checks covered a selection of situation types. Any differences were investigated until we were confident that the procedures developed resulted in correct estimates. As such, it is not felt that the automated estimate generation process was a potential source of error in the validation process.

4.5 Conclusions

In conclusion, the comparison of the tool estimates with measurement data suggests that whilst the tools tend overall to be conservative, they may not be sufficiently conservative in all situations.

Of the exposure categories, most comparator data were available for volatile liquids, followed by powder handling. Fewer data from the other exposure categories could be included in the external validation. This arose from a necessity to maximise the applicability of the measurements to the maximum number of tools possible, whilst still covering specific categories of interest, for example metal processing.

Based on the combined results available in this study and presented in Table 4.42, with reference to the conservatism criteria mentioned above, ECETOC TRAv2 and v3 provided estimates that were of medium or low levels of conservatism across all of the exposure categories. The ECETOC TRAv3 tool appeared slightly less conservative than the earlier ECETOC TRAv2 tool which may be related to additional input option flexibility.

Similarly, for MEASE the level of conservatism was judged to be medium or low, although for powder handling the percentage of measurements exceeding the tool estimate was only 11%.

The EMKG-EXPO-TOOL was highly conservative for volatile liquids, although this may relate to the absence of a substance concentration adjustment factor. The EMKG-EXPO-TOOL was of medium conservatism for powder handling. STOFFENMANAGER and MEASE were of low and medium levels of conservatism for non-volatile liquids. For volatile liquids, the STOFFENMANAGER 75th and 90th percentile estimates were broadly comparable with the equivalent percentiles of the measurement data, whilst for powder handling the percentiles estimates generated by STOFFENMANAGER overestimated exposure.

Fewer data were valuable for the other exposure categories; however the results do not suggest that any of the tools are highly conservative in all cases evaluated or that they are strongly correlated with the measurement results.

Whilst acknowledging the limitations in the data set and methodologies as described before, it is felt that these results provide a good basis for identifying areas where tool performance may need to be improved. Consideration of the following areas may be of assistance in future tool development.

Although not incorporated as inputs for all of the evaluated tools, PROC codes were used to describe the tasks/ activities for the workplace situations used for comparison with the tool estimates. Differences were noted between the PROC codes for all of the tools, with variation also observed between exposure categories. The following PROC codes and exposure categories were associated with lower levels of conservatism, and so are worthy of further investigation.

- Exposures to volatile liquids for PROC 14 were generally underestimated by all of the tools. The ECETOC TRAv3 also produced less conservative estimates for industrial spray processes (PROC 7) for this exposure category, with the ECETOC TRAv2 more conservative but the percentage of measurements exceeding the corresponding estimates also relatively high.

- For handling of powders, some differences between PROC codes were observed for MEASE and STOFFENMANAGER, but not for ECETOC TRAv2, ECETOC TRAv3 and EMKG-EXPO-TOOL. All of the tools appeared less conservative for PROC 8a, which relates to less well controlled transfer processes, and with the exception of STOFFENMANAGER, PROC 14 associated powder handling exposures were also underestimated to a certain degree by the other tools.

- For non-volatile liquids, differences between PROC codes were observed for STOFFENMANAGER, with higher percentages of measurements exceeding the tool estimate for PROC 11 (non-industrial spraying). For MEASE, the tool appeared less conservative for PROC 13, although only a few comparator data (n=10) were available.

- There were also some differences observed between the numbers of measurements exceeding the tool estimates for the various PROC codes for metal processing (evaluated for MEASE only). Whilst around 30-40% of the measurements exceeded the tool estimate for PROCs 22 and 25, for PROC

23 the tool appeared to be very conservative with only 7% of the measured data greater than the corresponding prediction.

The numbers of data points available generally precluded further stratification of the analyses by PROC code in combination with other factors such as LEV, domain or dustiness. Some combinations did however include enough data to allow more detailed assessment of the impact of these factors together with PROC on the percentages of measurements exceeding the tool estimates, thus further clarifying those areas where the tools may be less conservative than expected.

The results from the stratification exercise were predominantly in accordance with those from the overall comparison. For volatile liquids the tools were less conservative where LEV was present. Consideration should therefore be given to the assumptions made about control efficiencies within the tools- the results suggest that these may be overestimated in comparison with the actual effectiveness in the workplaces from which the measurement data originated.

The level of conservatism varied by PROC for powder handling with LEV: for example, PROC 5 generated less conservative estimates where LEV was present compared with where it was absent, whilst for PROC 8b the converse was observed.

The observed impact of domain and LEV on the level of conservatism suggests that these two aspects of tool operation require review. In particular, the assumptions made in relation to domain regarding the initial base exposure estimates and the modifiers subsequently applied for LEV implementation should be re-evaluated.

Due to the limited availability of varied data types for non-volatile liquids and metal dusts or fumes, we cannot make any firm conclusions on the performance of the tools and further studies are required. However, the results suggest that the level of conservatism for these exposure categories may need to be improved.

In the second part of the comparison process, correlations between the estimates of exposure and the measured values for the different exposure categories and for the data types were determined. Differences in the level of correlation of the measurement data with the tool estimates were noted both between exposure categories and comparator data type.

The correlation between the tool estimates and measurement data was better for powders and volatile liquids, followed by non-volatile liquids then the other exposure categories. This suggests that the tools are better at predicting potential exposure in these categories compared with the metals-related situations. The predictive power of the tools could thus be further enhanced, for example by the inclusion and/ or revision of certain input parameters (e.g. concentration of the mixture for EMKG-EXPO-TOOL and effectiveness of control measures, all tools).

The above findings provide suggestions for areas which could be addressed by model developers to improve the tools so that they are appropriately conservative for all or the most important exposure situation types.

5 Operational analysis - evaluation of tool usability and reliability

5.1 Introduction

The nature of the interaction between the tool user and tool is an important factor in determining the validity and reliability of the exposure estimates obtained. In addition to external validation with measurement data, Tischer et al. (2003) also suggested that any evaluation of exposure assessment tools should include an evaluation of the uncertainty resulting from differences in application by different users and the user-friendliness of the systems.

WP I-6 of the project aimed to evaluate these operational aspects of the tools. The work package incorporated two main evaluation approaches:

- appraisal of the usability and user-friendliness of the tools, through the use of telephone and on-line questionnaires; followed by an

- assessment of the reliability of tool predictions of exposure, i.e. the between user variability and its impact on the estimates

The methods, results and conclusions from these evaluations are outlined and discussed below.

5.2 User- friendliness and usability of the tools

5.2.1 Background information

Part 1 of WP I-6 was developed to evaluate the usability and user-friendliness of the tools through the use of telephone interviews and an online questionnaire survey. The reader is referred to eteam Project Deliverable “D18: Report on User-Friendliness of Tier 1 Exposure Assessment Tools under REACH” (Crawford et al., 2012) for a comprehensive discussion of the evaluation process and findings.

Usability is defined as "the effectiveness, efficiency and satisfaction with which specified users can achieve specified goals in particular environments" (ISO 1998). ISO define effectiveness as the “extent to which a goal or task is achieved”. Efficiency is defined as the amount of effort required to achieve the task, whilst ISO relate satisfaction (the most subjective state) to the level of comfort and acceptability the user feels when using the product.

All three of these factors are important in relation to usability but the latter (satisfaction) may have a greater influence on individuals in relation to choosing (and continuing) to use a particular product. In the case of the Tier 1 tools evaluated in the eteam project, choice of a particular system will also be driven by the users’ technical requirements, for example whether the tool predicts dermal exposure, inhalation exposure or both for a particular situation. Furthermore, their choice will also be influenced by the degree to which a tool is supported by, and/ or is compatible with, commonly available systems and approaches for communicating use and exposure within their supply chains.

The primary aims of the evaluation process were to examine users' experience with the different tools and address the following questions:

- Is the tool understandable by (and of practical value to) the users?
- How good is the software- i.e. the design of the input mask/ system crash frequency/ 'bugs'/ interface with other software packages/ system requirements?
- How easily can the user translate a given use/exposure situation into the available tool input parameters?
- Does the documentation meet users' needs with regard to clarity, user-friendliness and their level of expertise?
- How well do the tools and their outputs meet user requirements for assessment of workplace exposure?

5.2.2 Methods

A group of experienced tool users were identified and recruited in consultation with the eteam Project Advisory Board. A series of telephone interviews was carried out with this group for each of the tools. This was followed up by the development and administration of an online automated SurveyMonkey questionnaire survey of a much larger tool-user population, recruited via the eteam Project website, postings on professional organisations' message boards, personal contacts and communication via the Tier 1 tool developers' networks. The online survey question set was based on the initial questions used in the telephone interviews with appropriate modifications to facilitate web-based completion by a wider range of participants.

The interviews and online surveys were designed to identify:

- participants' level of experience in exposure assessment and tool usage
- the purpose for which tool is used
- any difficulties experienced in installing and using the tool
- the relevance of the tool input parameters to their situation being assessed
- whether measured exposure data had been used as a comparison with the tool outputs and
- whether the participants had used any other tools.

Data from the interviews were collated and thematic analysis carried out to identify and examine common themes. The online survey responses were analysed using the MINITAB statistical software package. Statistical analyses of the questionnaire output focussed on each tool, and used frequency tables and chi-square tests to examine any associations between users' experiences of the tools and their personal characteristics. These included occupational hygiene experience, level of experience of using the tool, and the purpose for which they used the tool (i.e. whether it was used for REACH purposes or not).

Within this report, and this summary, participants in the telephone interviews are denoted “interviewees” whilst those people who participated in the online survey are called “respondents”.

5.2.3 Results

The results for both the telephone interviews and online survey are presented in the following sections.

5.2.3.1 Response rate/ demographic information

In total, 11 telephone interviews were carried out with experienced tool users. The interviewees were based in several EU countries and were involved in consultancy, REACH management, REACH regulation, occupational medicine, occupational hygiene and toxicology.

There were 295 respondents to the online survey, with the percentage of respondents shown by sector in Figure 5.1.

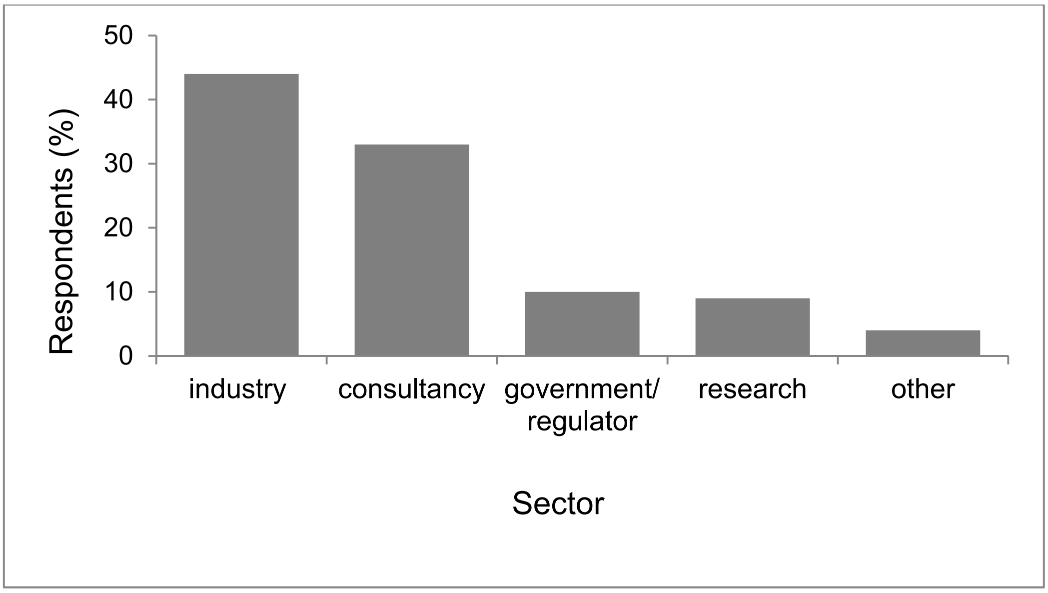


Figure 5.1 Percentage of respondents by sector

The respondents were primarily from a range of EU countries, had a wide range of experience in exposure assessment and most self-reported having intermediate computer skills and a high level of English language ability.

5.2.3.2 Respondents’ perceptions of tools

The respondents were asked a number of questions regarding their perception of the usability and user-friendliness of the tools.

- How easy is it to access and download the tool?
- How easy is it to understand the tool layout?
- How easy is it to learn how to use the tool?
- How easy is it to generate outputs from the tool?

- How easy is it to return to using the tool following a period of non-use?
- How easy is it for you to identify and rectify errors you have made in the tool?

The percentage of respondents reporting some level of difficulty regarding these aspects of the tools is summarised in Table 5.1.

Table 5.1 Percentage of respondents reporting difficulty by usability category and tool (inhalation and dermal exposures)

	ECETOC TRAv2		ECETOC TRAv3		EMKG-EXPO-TOOL	MEASE		RISKOF-DERM	STOFFEN-MANAGER
Usability category									
Accessing and downloading the tool		4		10	0		0	6	9
Understanding the screen layout		17		17	2		4	4	16
Learning how to use the tool		24		31	4		6	17	27
Generating the required tool output		21		19	4		4	15	23
Returning after a period of non-use		12		17	2		6	10	17
Fixing user-related problems in tool		21		22	4		2	8	21
Tool operation	Inh	Der	Inh	Der	Inh	Inh	Der	Der	Inh
Translating workplace situation into tool	12	20	12	12	20	9	6	21	19

In general, respondents reported little difficulty in finding and downloading the tools, with slightly more difficulty reported for STOFFENMANAGER and the ECETOC TRAv3. The majority of respondents found the layout of the tools easy to understand, however the layouts of STOFFENMANAGER, the ECETOC TRAv2 and ECETOC TRAv3 tools were found to be slightly harder to understand.
The respondents reported relatively more difficulty in learning to use the ECETOC TRAv2, ECETOC TRAv3 and STOFFENMANAGER tools compared with the others. Very few respondents had experienced difficulty in learning to use MEASE or the EMKG-EXPO-TOOL.

Entering input parameters and generating exposure estimates using the tools was found to be easy or neutral by most respondents. However, 5- 25% of respondents experienced some degree of difficulty in obtaining outputs from all of the tools, with the lowest levels reported for MEASE and EMKG-EXPO-TOOL.

Respondents generally found returning to use the tool after a period of non-use to be easy, or neither easy/ difficult, however slightly more difficulty was reported for ECETOC TRAv3, ECETOC TRAv2, STOFFENMANAGER and RISKOFDERM than for the other two tools.

Fixing user-related errors, for example incorrect input parameters, was considered a more difficult issue than other aspects of usability for all of the tools. Relatively more difficulty was reported for both the ECETOC TRA tools and STOFFENMANAGER.

The perceived usefulness of the help functions and supplementary guidance available for the tools was also investigated as part of the suitability assessment. The percentage of respondents describing the help functions and guidance as “unhelpful”/ “very unhelpful” is shown by tool in Table 5.2. The tools were very similar in terms of the perceived helpfulness of the in-tool and supplementary guidance, with a maximum of around 10% of users responding negatively.

Table 5.2 Percentage of respondents selecting “unhelpful/ very unhelpful” regarding the tool guidance and supplementary guidance.

Suitability Category	ECETOC TRAv2	ECETOC TRAv3	EMKG-EXPO-TOOL	MEASE	RISKOF-DERM	STOFFEN-MANAGER
Usefulness of Help Functions	12	12	10	2	4	5
Usefulness of Supplementary Guidance	6	10	not applicable	10	8	6

5.2.3.3 Tool-specific feedback

Feedback from the respondents in the form of direct quotations regarding their positive and negative perceptions of the individual tools is summarised in Table 5.3 below.

Table 5.3 Positive and negative aspects of tools highlighted by respondents (direct quotations given)

ECETOC TRAv2	ECETOC TRAv3	MEASE	EMKG-EXPO-TOOL	STOFFENMANAGER	RISKOFDERM
Positive aspects of tools					
Easy to learn and use	Availability of RMMs improved	Easy to use	Practical tool	Ease of use	Easy and simple to use
fast method of calculating estimates		Colour coding good for relevance	Easy to use but not as robust as other tools	Colour coding good for prioritising	More detailed and accurate compared to other tools
Allows prioritisation of exposure situation		Changes in parameter being immediately visible	Quick to achieve results	Takes into account control measures	Rapid solution
		Guidance helpful and easy to use		Results showing percentiles	
		Simplicity of the spreadsheet layout		Ability to explore a situation	
Negative aspects of tools					
Date entry time consuming	Date entry time consuming	Only being able to assess one substance at a time	Perceived its simplicity as a weakness	Takes time to learn	Hard to find tool
Slow	Not user friendly	Overestimation perceived as a problem		PROC alignment should be present in tool	Too conservative in its outputs
Layout difficult	Dislike of layout			A large amount of effort required to input data	Suggest fewer colours in its layout
Integrated tool perceived to be more complex	Advanced user manual would help			Layout difficult to manage	Prone to over-estimation
Needs more PPE and RMM input					

5.2.4 Discussion

Participants in the interviews were identified as users who had an interest in assisting the research project and who reported being experienced in one or more of the tools. The interviewees therefore represent experienced tool users, and this factor was considered in the assessment of the interviews and in comparison with the findings of the questionnaire survey.

Invitations to participate in the survey were widely distributed by various routes in order to REACH as many users as possible. However, as the total number of tool users contacted is ultimately unknown, an overall response rate for the survey cannot be calculated. It is likely however that proportionally more responses were attained from users of tools for which it is necessary to register before it can be downloaded or used, as publicity for the exercise and a direct request, sent via the tool providers, was then possible. Most respondents worked in industry or consultancy and they had a broad range of occupational exposure experience.

Six usability categories were assessed for each of the tools. For all of the tools accessing and downloading the tool was the category most often reported to be easy or very easy, followed by understanding the screen layout and returning after a period of non-use. Respondents had most difficulty with fixing a problem, learning how to use the tool, and generating the required tool output. For all six categories, a higher proportion of users of MEASE (63% to 92%) and of EMKG-EXPO-TOOL (66% to 91%) reported that the usability was easy or very easy than users of the other tools (38% to 88%). For all of the tools, there was evidence that users who were unfamiliar with the underlying concepts of a tool found it more difficult to use than users with more familiarity of the tool.

For five of the six tools, between 56% and 61% of respondents found the help functions helpful or very helpful; the exception was ECETOC TRAv3 where only 43% of respondents found the help functions to be helpful/ very helpful. For all tools, over half of all respondents found the guidance provided with the tool to be helpful/ very helpful, ranging from 51% for MEASE to 66% for ECETOC TRAv2.

For most of the tools, around half of the respondents perceived that it was easy or very easy to translate real-life exposure situations into the necessary inputs. The exception was RISKOFDERM where only 25% of respondents found this to be easy. For ECETOC TRAv2 and STOFFENMANAGER, respondents with less knowledge of the underlying concepts of the tool found this more difficult to do.

Around three-quarters of respondents for the ECETOC TRA tools, MEASE and STOFFENMANAGER reported that the tools fulfilled their requirements. The responses were less positive for the EMKG-EXPO-TOOL (46%) and RISKOFDERM (54%). The principal reasons given for both tools were that exposure estimates were not perceived as being realistic and that it was unclear how to translate workplace information into the required input parameters. RISKOFDERM users also felt that they had insufficient workplace exposure information to enter all required input parameters.

5.2.5 Conclusions

The interview and questionnaire survey data identified that interviewees and respondents were generally happy about the usability of the tools and supporting documentation. However, the use of the tools appears to be affected by knowledge of the underlying tool concepts and by levels of user experience. To ensure effective exposure estimates are generated, it is therefore essential that training is available for the tools and that there is ongoing support and guidance provided for the user (both within the tool interface and through additional material) that is fully understandable for all levels of users.

5.3 Evaluation of the between user reliability of the Tier 1 exposure assessment tools

5.3.1 Background information

When applying Tier 1 exposure assessment tools, users must select from a number of possible input parameters. Hence, results obtained with the tools could be affected by factors such as the professional experience and judgment of the tool user and level of available information. Studies of inter-rater reliability when grading subjects' occupational histories in epidemiological studies, and within other disciplines such as clinical medicine, have shown substantial variation between assessors (Friesen et al., 2011; Kunac et al. 2006). High levels of variation between users of higher tier exposure assessment tools have also been identified (Schinkel et al., 2014), thus some variation in Tier 1 tool estimates between different users when assessing exposure for the same situation should be expected.

This part of WP I.6 of the eteam project aimed to assess the between-user reliability of the exposure assessment tools to investigate how consistent tool users were in making input parameter choices in comparison with other users. Two complementary approaches were used in the study to evaluate tool user consistency: a remote completion Between User Reliability Exercise (BURE) and a focus group. Participants in the BURE were asked to assess inhalation and dermal exposure for a given set of workplace situations using the Tier 1 tools. The variation between the exposure estimates generated by the different users from these situation-tool combinations was determined and potential reasons for differences identified. The focus group session facilitated collection of more detailed information on potential sources of variation from a selected range of users. The findings from the focus group were used to supplement and complement the results from the BURE. The reader is referred to eteam Project Deliverable D22: Report on Between-User Reliability Exercise (BURE) and Workshop (Lamb et al., 2013) for additional information.

5.3.2 Method

The methods used in the BURE and focus group are outlined below, together with a description of the statistical analyses carried out.

5.3.2.1 BURE

Recruitment to the remote-completion exercise was undertaken using postings on professional organisations' message boards, personal contacts, communication via the Tier 1 tool developers' networks and through an email distribution list of respondents from the previous eteam project online tool user-friendliness questionnaire (Crawford et al., 2013). All individuals who had expressed an interest in participation were asked to complete a short background questionnaire, to gather information on a range of personal characteristics, including employment sector, location, English language ability, experience of exposure assessment and previous modelling tool use.

Individuals (n=160) who had returned the background questionnaire were provided electronically with an introductory pack containing simple guides to installing and operating the Tier 1 tools for the BURE. All participants were also issued with an individual online account for STOFFENMANAGER. To encourage completion, these accounts were pre-populated by the project team with essential supplier and substance information, e.g. vapour pressures and molecular weights. The pre-populated inputs did not impact on the generation of exposure estimates, for example participants were still required to select the activity description and allocate dustiness for solid materials.

A series of 20 exposure situation case studies were developed (Table 5.4) which described commonplace industrial and non-industrial uses of chemicals, for example spraying of liquids, object immersion and filling of containers with powders. The descriptions varied in their level of detail regarding exposure determinants. No measurement data for the exposure situations were provided to the participants.

Table 5.4 Summary of exposure situations used in BURE

Situation	Description	Substance	Exposure type	Use type	Descriptive information provided on task duration?	Descriptive information provided on LEV?	Descriptive information provided on general ventilation?	Descriptive information provided on RPE?	Descriptive information provided on glove use?	Overall level of detail given in situation description [(1)]
1	Use of Styrene-Resin in Fibre-Reinforced Plastics	Styrene	Vapour	Industrial	yes	yes	yes	no	no	medium
2	Cleaning of Floor Using Hand Brush	Magnesium stearate	Solid	Industrial	yes	yes	yes	yes	yes	high
3	Use of Toluene in Coatings- Spray painting in furniture manufacturing industry	Toluene	Vapour	Industrial	yes	yes	yes	yes	yes	high
4	Use of Xylene in Formulations- Mixing of chemicals in an Open Vessel	Xylene	Vapour	Industrial	yes	yes	yes	yes	yes	high
5	Use of Naphtha in Coatings- Solvent tank emptying and re-filling	Naphtha	Vapour	Industrial	yes	yes	yes	yes	yes	high
6	Use of Toluene in Adhesives- Manufacture of Rubber Garments	Toluene	Vapour	Industrial	yes	yes	yes	yes	yes	high
7	Use of N-methyl pyrrolidone in formulations- Changing of air filters in a vehicle paint spray booth	N-methyl pyrrolidone	Vapour	Industrial	yes	yes	no	yes	yes	medium
8	Cleaning of Endoscopy Equipment in a Hospital	Glutaraldehyde	Vapour	Professional	yes	yes	yes	yes	yes	high
9	Packaging of Sodium Resinate Powder in a Factory	Sodium Resinate	Solid	Industrial	yes	no	yes	yes	yes	medium
10	Dipping of Metal Parts during Manufacture of Electrical Connectors	Isopropanol	Vapour	Industrial	yes	yes	no	yes	yes	medium
11	Weighing of Powdered Pharmaceutical Products	Amoxicillin trihydrate	Solid	Industrial	no	yes	yes	yes	yes	medium
12	Re-filling of Dry Cleaning Equipment with 1-Bromopropane in Retail Premises	1-Bromopropane	Vapour	Professional	yes	no	yes	yes	yes	medium

Table 5.4 (continued)

Situation	Description	Substance	Exposure type	Use type	Descriptive information provided on task duration?	Descriptive information provided on LEV?	Descriptive information provided on general ventilation?	Descriptive information provided on RPE?	Descriptive information provided on glove use?	Overall level of detail given in situation description
13	Top loading of Tankers with Heavy Fuel Oil	Heavy fuel oil	Vapour	Industrial	yes	no	yes	yes	yes	medium
14	Use of Phenol in Adhesives: Gluing of Rotors	Phenol	Vapour	Industrial	yes	yes	yes	yes	yes	high
15	Packing of Nickel Metal Powder	Nickel	Solid	Industrial	yes	yes	yes	yes	yes	high
16	Filling of vessels with Isopropyl Benzene	Isopropyl benzene	Vapour	Industrial	yes	yes	yes	yes	yes	high
17	Cleaning of Solder Dross during Manufacture of Electronic Components	Lead	Solid (metal fume)	Industrial	yes	yes	yes	yes	yes	high
18	Use of hexabromocyclododecane (HBCD) additive during production of Extruded Polystyrene	Hexabromo-cyclododecane	Solid	Industrial	yes	yes	yes	yes	yes	high
19	Casting of Aluminium into Blocks	Aluminium	Solid (metal fume)	Industrial	no	no	no	no	no	low
20	Use of acetone in formulations-Batch Manufacture of Automotive Paints	Acetone	Vapour	Industrial	yes	no	yes	yes	yes	medium

(1) The level of detail provided in the exposure situations was graded as follows:

High: Information provided on task duration and all RMMs
Medium: No information provided on task duration and/or information missing on 1-2 RMMs
Low: No information provided on task duration and information missing on >2 RMMs

The content of the situation descriptions was such that either or both inhalation and dermal exposure routes were applicable. The following five tool combinations were applied to generate estimates for both routes for each situation: ECETOC TRAv2 (inhalation and dermal); ECETOC TRAv3 (inhalation and dermal); MEASE (inhalation and dermal); STOFFENMANAGER (inhalation) and RISKOFDERM (dermal); EMKG-EXPO-TOOL (inhalation) and RISKOFDERM (dermal).

Prior to the BURE starting, the distribution system, data harvesting routines and participant documentation were piloted successfully. Over a four week period, participants were issued weekly with five exposure situation/ tool combinations to complete. A separate email was issued for each combination, which contained details of the allocated exposure situation, a worksheet to record their results and a fresh copy of the Tier 1 tool to be used in the exercise and returned. In the event of STOFFENMANAGER being allocated, this was highlighted in the accompanying worksheet. Allocation of the 20 exposure situation/tool combinations to 20 participants was done using a 20*20 Latin square design, built using cyclic generation (John and Williams, 1995). The cyclical Latin square design gave balanced combinations by the end of a 20-participant replication, with order-related learning effects minimised by randomisation of situations and toolsets. The design was scaled up to the total number of participants.

On completion of the exercise, questionnaire-based feedback was requested from the participants on their experiences of using the tools for the given exposure situations. Returned emails and attachments were stored automatically by participant name in a Microsoft Access database and the assessment outputs harvested directly from the returned worksheets and questionnaires using an automated routine.

5.3.2.2 Focus group session

A focus group session was held over two days in February 2013 at the IOM premises in Edinburgh. Delegates had been selected from those who had completed all 20 allocated exposure situations in the BURE, with the group composition balanced between representatives from industry, research and regulatory bodies. The delegates had a range of experience of tool use and exposure assessment.

Following an introductory plenary session, the delegates were split into two groups for the focus group sessions (A and B). Group A participated in the dermal focus group in the first instance and Group B the inhalation focus group. The two groups then swapped over on the second day of the workshop so that all delegates were given the opportunity to discuss use of the Tier 1 tools for assessment of inhalation and dermal exposure.

A comprehensive written record of the focus group discussions was produced. This was used to identify the main themes and individual issues from the sessions, thus allowing their inclusion in the overall between-user reliability report.

5.3.2.3 Statistical analyses

A series of systematic and random manual data checking and cleaning exercises were undertaken for the returned BURE assessments, including checks of outliers and the highest, mid-range and lowest results for each tool-situation combination. All statistical analyses were undertaken using GenStat software.

The data were summarised and results cross-tabulated by various factors. The formal statistical analyses aimed to:

i) quantify the variation in results recorded for each tool applied to each situation assessed;
ii) examine and quantify the components of that variation due to systematic differences between and within participants in carrying out their assessments;
iii) examine systematic patterns within the components of variation relating to aspects of the situation assessed, the characteristics of the participants, and their recorded opinions regarding familiarity with the specific situation and their perceived difficulty/ uncertainty in making the assessment.

Analyses were carried out on the logarithms of the assessment results. Linear mixed models were fitted, with fixed effects for differences in level between situations, and a random distribution for differences between participants, assumed to follow the Normal distribution on the logarithmic scale. This resulted in the estimation of mean effects (corresponding to geometric means) for the situations, and a variance component (convertible to a geometric standard deviation [GSD]) for the participants' distribution. The remaining variation not explained by either of those components estimated, on that scale, the random within-participant variance.

Additional analyses attempted to investigate systematic structure in the components estimated as detailed above. Terms representing differences between participants, e.g. level of tool experience were added one at a time to the mixed models described above and the extent to which each explained structure in the relevant variance component assessed.

For each exposure situation, participants had been instructed to undertake both inhalation and dermal assessments using the specified tool, regardless of whether or not they considered the situation to be within the tool's scope of applicability. Initial analyses were undertaken with applicable and non-applicable situations included. Further specific analyses were then carried out with only those situations which were within the tool developer's stated range of applicability.

The fixed and random effects estimated were used to characterise the average differences in level in the assessed result, but could not highlight instances or characteristics that were associated with larger amounts of random variation. To investigate this, the standardised residuals from each analysis were extracted, and their variance cross-tabulated by situation and the factor(s) under investigation. The tabulated variances were expressed as GSDs for ease of interpretation.

The impact of a number of participant characteristics on variation in response was investigated. These included: type of organisation/ sector of employment; self-reported English language ability; years of experience in exposure assessment; and main reason for carrying out exposure assessments. The impact of situation-related factors was also considered: e.g. participant familiarity with the situation and their perceived level of uncertainty in input choice. Mixed statistical models were fitted, adding each of these factors, in turn to a base model containing factors for situation and participant, as described above. The variances of the standardised residuals were again tabulated, inspected and assessed as detailed previously.

5.3.3 Results

5.3.3.1 Response rate and participant demographics

From the original group of interested persons (n=160), an initial pool of participants (n=148) completed the BURE background questionnaire. From this group, a total of 146 participants then completed one or more assessments, with 70 participants completing all 20 situations. A demographic summary of these participants is given in Table 5.5.

Table 5.5 Summary of participant demographic information (n= 146)

Characteristic	Category	Number of Participants (%)
Sector	Consultancy	43 (29)
	Industry	41 (28)
	Research	24 (16)
	Government/ Regulator	22 (15)
	Other	16 (11)
Country	European Union	123 (84)
	United States/ Canada	9 (6)
	Asia/ Middle East	4 (3)
	Other	8 (5)
	Missing	22 (15)
Age (years)	<30	12 (8)
	30-49 years	93 (64)
	>50	40 (27)
	missing	1 (1)
Job Title	Chemical risk assessor	37 (25)
	Occupational hygienist	38 (26)
	Product stewardship expert	5 (3)
	REACH advisor	17 (12)
	Researcher/ scientist	21 (14)
	Toxicologist	11 (8)
	Other	17 (12)
English Language- Reading ability	Native	31 (21)
	Excellent/ Good/	107 (73)
	Average/ Poor	8 (5)
English language- Writing ability	Native	31 (21)
	Excellent/ good	101 (69)
	Average/ poor	14 (10)
Reason for Performing Exposure Assessments	REACH exposure assessment	58 (40)
	Compliance with OEL[(1)]	30 (21)
	Identification of RMMs	28 (19)
	Other	29 (20)
	Missing	1 (1)
Experience in Exposure Assessment (years)	< 1	22 (15)
	1-4	33 (23)
	5-9	33 (23)
	10-19	33 (23)
	>20	25 (17)

[(1)] Occupational Exposure Limit

The participants varied in their level of experience of the tools, as shown in Table 5.6.

Table 5.6 Participants' level of knowledge of exposure assessment tools

	Level of Knowledge of Exposure Assessment Tool (N/ %)				
Tool	**Full/ Good**	**Limited**	**None**	**Missing**	**Total**
ECETOC TRAv2	67 (46)	38 (26)	39 (27)	2 (1)	146
ECETOC TRAv3	58 (40)	36 (25)	49 (34)	3 (2)	146
EMKG-EXPO-TOOL	26 (18)	23 (16)	94 (64)	3 (2)	146
MEASE	27 (18)	30 (21)	86 (59)	3 (2)	146
RISKOFDERM	29 (20)	43 (29)	71 (49)	3 (2)	146
STOFFENMANAGER	50 (34)	35 (24)	59 (40)	2 (1)	146

The ECETOC TRAv3 and ECETOC TRAv2 were the most frequently used tools, followed by STOFFENMANAGER. A relatively high proportion of the participants had never used the EMKG-EXPO-TOOL, MEASE and RISKOFDERM, which may be associated with the more specialised nature of these three tools. The number of worksheets returned by situation ranged from 95 to 107, with a total of 4066 collected (inhalation, n= 2033; dermal, n= 2033). The numbers of completed tool-situation assessments harvested from the returned worksheets were similar across the range of inhalation tools (n=400 to 412). The numbers of returned dermal assessments were also balanced between the ECETOC TRAv3, ECETOC TRAv2 and MEASE (n=400 to 412), with more assessments being collected for RISKOFDERM (n=810) from its pairing with two different inhalation tools.

For each situation/ tool combination completed, participants were asked to record their previous experience of the situation and the level of uncertainty they experienced when selecting inputs. Lower levels of experience were reported for situations with exposure to powders and fumes from metals compared with those for liquids. Situations involving end uses of substances, for example in retail premises, were less familiar to participants than those describing larger scale industrial processes. The tool input parameters were grouped into four categories: Substance Characteristics e.g. dustiness; Operational Conditions e.g. general work environment; Task/ activity description and RMMs e.g. local exhaust ventilation, personal protective equipment. Over all of the situations and tools, more participants reported major uncertainty in allocating inhalation and dermal parameters relating to the task/ activity being carried out than for the other parameter groups. Higher numbers of participants reported major uncertainty in choosing dermal task/activity than for inhalation, which may be a reflection of lower general levels of experience in dermal exposure assessment. Participants also reported more uncertainty in selection of Substance Characteristics for solid substances compared with liquids, perhaps related to the absence of explicit information on dustiness in the descriptions.

The tools differ in their apparent level of complexity and thus participants were asked to indicate their overall ease of translation of the situation into the required inhalation and dermal tool input parameters. In general, participants did not report significant difficulty in translating situations into the tools, with the proportion choosing "difficult/ very difficult" being relatively small (6-10%) compared with the categories "very easy/ easy" (27- 49%) and "neither easy nor difficult" (16-29%). A slightly higher overall percentage (14%) of participants found translation of the situations into

STOFFENMANAGER more “difficult/ very difficult” than for the other tools. Moderately higher numbers of participants chose “difficult/ very difficult” to describe how they found translation of situations into the dermal tools, compared with the inhalation tools. Participants reported more difficulty in translating the situations into RISKOFDERM (21%) compared with the other tools (9-14%), although overall a substantial number of participants reported finding translation into the dermal tools as being “very easy/ easy” (23–47%). These results are similar to those found in the user-friendliness evaluation, where slightly higher percentages of respondents reported difficulty in generating estimates from STOFFENMANAGER, RISKOFDERM and the ECETOC TRA tools compared with MEASE and the EMKG-EXPO-TOOL.

The impact of level of uncertainty and ease of translation on the exposure estimates was assessed using statistical modelling, with residual variation and associated GSDs calculated. The GSDs for the residual variation were determined by tool for the various uncertainty levels associated with different groups of input parameters, with a high GSD reflecting higher variation in estimates. No consistent patterns could be observed to suggest that higher levels of perceived uncertainty were associated with higher levels of variation in tool outputs. The highest GSDs were observed as frequently for categories of low uncertainty as for categories where high uncertainty was reported. Results in relation to the impact of ease of translation on the spread of inhalation and dermal estimates were similarly inconclusive, with high GSDs associated both with situations which were considered difficult to translate, and those perceived as easy.

5.3.3.2 Exposure Estimates- Statistical Analyses of Variation

Table 5.7 summarises estimates of exposure to solids and vapours generated by the participants during the BURE. Estimates of GSDs, which express the total variation in exposure estimates obtained from the tools, are also presented. These combine variation due to differences in exposure between situations and differences between assessments of the same situation.

For the same group of situations, the estimates obtained thus varied significantly between different tools. Results for dermal exposure estimates cannot be compared directly, as the various tools generate results in different units; however, the estimates from the RISKOFDERM tool appear to be much higher than those from the other tools. After taking into account the default weight of an adult (70kg), it appears that the estimates from ECETOC TRAv2 and ECETOC TRAv3 are higher than those obtained by MEASE.

Table 5.7 Estimates of exposure generated by participants across all situations by tool and exposure route (solid and vapour)

	Solid						Vapour					
Tool Name/ Units	**N**	**AM**	**Min**	**Max**	**GM**	**GSD**	**N**	**AM**	**Min**	**Max**	**GM**	**GSD**
Inhalation exposure estimates												
ECETOC TRAv3 (mg m^{-3})	103	2.6	$7.0x10^{-4}$	21	0.3	12	247	130	$1.0\ x10^{-4}$	$1.3\ x10^{3}$	21	17
ECETOC TRAv2 (mg m^{-3})	129	2.9	$1.0\ x10^{-4}$	32	0.3	14	276	110	$8.2\ x\ 10^{-3}$	$1.1\ x10^{3}$	24	12
MEASE (mg m^{-3})	151	1.9	$5.0\ x10^{-4}$	41	0.3	12	247	120	$5.0\ x10^{-4}$	$1.9\ x\ 10^{3}$	9.0	53
EMKG-EXPO-TOOL (mg m^{-3})	144	107	$1.0\ x10^{-3}$	$4.3x10^{3}$*	2.1	17	253	$3.4\ x10^{3}$	$2.1\ x10^{-1}$	$9.3\ x10^{4}$	350	14
STOFFENMANAGER (mg m^{-3}) (1)	113	34	$1.5\ x10^{-5}$	470	4.4	11	196	480	$1.3\ x10^{-3}$	$7.2\ x10^{3}$	61	21
Dermal exposure estimates												
ECETOC TRAv3 (mg/ kg/ day)	104	6.2	$2.8\ x10^{-3}$	43	1.5	9.7	246	11	$1.4\ x10^{-3}$	110	2.8	7.6
ECETOC TRAv2 (mg /kg/ day)	129	8.7	$3.4\ x10^{-2}$	140	1.5	7.2	276	11	$3.4\ x10^{-2}$	140	4.5	5.1
MEASE (mg/ day)	151	37	$2.0\ x10^{-3}$	590	1.8	18	247	30	$5.0\ x10^{-4}$	240	0.4	35
RISKOFDERM hands (mg) (1)	260	$3.1\ x10^{4}$	$2.0\ x10^{-3}$	$6.5\ x10^{5}$	200	23	482	$4.1\ x10^{5}$	2.0	$8.7\ x10^{7}$	$6.6\ x10^{3}$	24
RISKOFDERM body (mg) (1)	42	$3.8\ x10^{4}$	2.0	$1.2\ x10^{6}$	$1.2\ x10^{3}$	11	269	$5.9\ x10^{5}$	$6.3\ x10^{-1}$	$7.4\ x10^{7}$	$6.6\ x10^{3}$	260

(1) tool-predicted 90^{th} percentile exposure estimate * Note: this value exceeds the upper limit for solids exposures in the tool (>10 mg m^{-3}). The participant had incorrectly assigned the physical form as liquid instead of solid, hence the converted value in mg m^{-3} is very high
N=number of assessments; AM=arithmetic mean; GM=geometric mean; GSD=geometric standard deviation

The mean inhalation exposure estimates for solids obtained by the tools range from 1.9 mg m^{-3} obtained with MEASE to 107 mg m^{-3} with the EMKG-EXPO-TOOL. It should be noted that these values are calculated across all situations, including those where the physical form was incorrectly assigned. Thus for example, the arithmetic mean value for the EMKG-EXPO-TOOL exceeds the maximum exposure prediction possible within the tool (10 mg m^{-3}). The EMKG-EXPO-TOOL includes a scale of use factor, i.e. the amount handled in the task, but does not take into account the percentage of the agent within a mixture, so some of the difference in estimates between this and the other tools can be explained by these parameters. The mean estimate for solids obtained with the STOFFENMANAGER is 34 mg m^{-3}. The same pattern can be seen for exposure to vapours, with lowest estimates of exposure obtained with ECETOC TRAv2, ECETOC TRAv3 and MEASE, highest estimates generated by the EMKG-EXPO-TOOL and intermediate levels using STOFFENMANAGER.

Variation between participants' responses was evaluated for each tool. Table 5.8 provides a summary of variance, on the natural log scale, associated with systematic differences between the levels of assessors' results ($Var_{assessor}$), the residual variance (Var_{res}), and the total variance (Var_{Total}), after taking into account the effect due to the difference in exposure level between exposure situations. The table combines assessments for exposure to volatiles and solids firstly for all situations, and then for only those situations which were applicable for a particular tool.

Table 5.8 shows that the variation between assessors can be extremely high. Systematic differences in level between assessors explain very little of this variation for any of the tools. In particular, for inhalation exposure, variance in the exposure estimates appears to be high for MEASE and the EMKG-EXPO-TOOL. For dermal exposure, the largest variance in estimated exposures was observed for RISKOFDERM, followed by MEASE.

When situations outside of the recognised scope of applicability of each tool were excluded, the total variance in most cases remained the same or reduced slightly, with the residual variance remaining high for all of the tools.

Table 5.8 Variance in exposure estimates after taking account of exposure situation (all situations/applicable situations only)

Tool Name	N	$Var_{assessor}$	Var_{res}	Var_{Total}	N	$Var_{assessor}$	Var_{res}	Var_{Total}
	All situations				**Applicable situations only**			
Inhalation exposure								
ECETOC TRAv3 (mg m^{-3})	350	0.09	2.5	2.6	326	<0.01	2.6	2.6
ECETOC TRAv2 (mg m^{-3})	405	0.28	1.9	2.2	365	0.30	2.0	2.3
MEASE (mg m^{-3})	398	0.35	6.1	6.4	151	0.80	3.6	4.4
EMKG-EXPO-TOOL (mg m^{-3})	397	0.28	3.7	4.0	313	0.14	3.1	3.2
STOFFENMANAGER (mg m^{-3}) (1)	309	0.61	1.6	2.2	280	0.52	1.2	1.8
Dermal exposure								
ECETOC TRAv3 (mg/ kg/ day)	350	0.47	1.6	2.1	326	0.30	1.6	1.9
ECETOC TRAv2 (mg/ kg/ day)	405	0.18	1.1	1.3	365	0.32	1.0	1.3
MEASE (mg/ day)	398	0.78	3.7	4.5	151	0.68	4.0	4.7
RISKOFDERM (hands) (mg) (1)	742	0.55	6.1	6.7	674	0.58	5.8	6.4
RISKOFDERM (body) (mg) (1)	311	0.10	5.2	5.3	288	0.16	5.2	5.4

(1) tool-predicted 90th percentile exposure estimate
N= number of assessments

Further analyses were carried out to determine whether the assessor's background characteristics, e.g. employment sector, could explain some of the remaining variance in the exposure estimates.

The variances were again expressed as GSDs, examination of which identified a number of minor differences between tools. For example, there was generally more variation related to situations involving solids compared with liquids-related scenarios for participants using MEASE. There appears to be least overall variation across the characteristics' groups for STOFFENMANAGER and the ECETOC TRAv2. Overall, it is felt that there are no evident significant effects of the various participant characteristics on the variation in estimates obtained, for example increased English language ability and increased years of experience did not always result in less variation.

The amount of contextual information provided in the situations could potentially affect the level of variation between users, with an expectation that more detailed descriptions might lead to less variation. The situations were therefore ranked in order of decreasing magnitude of GSD. The physical form of the substance, applicability of the tool, type and amount of descriptive information provided with each situation was then mapped to the rankings to allow visual comparison and identification of patterns. For each of the tools, the situations with most variation tended to contain high levels of detail (see Table 5.4), thus suggesting that additional contextual information did not appear to be linked to a decrease in variation between users.

The ranges of estimates generated by the participants are illustrated on a log scale as box and whisker plots by tool, exposure route and physical form in Figures 5.2-5.19 below.

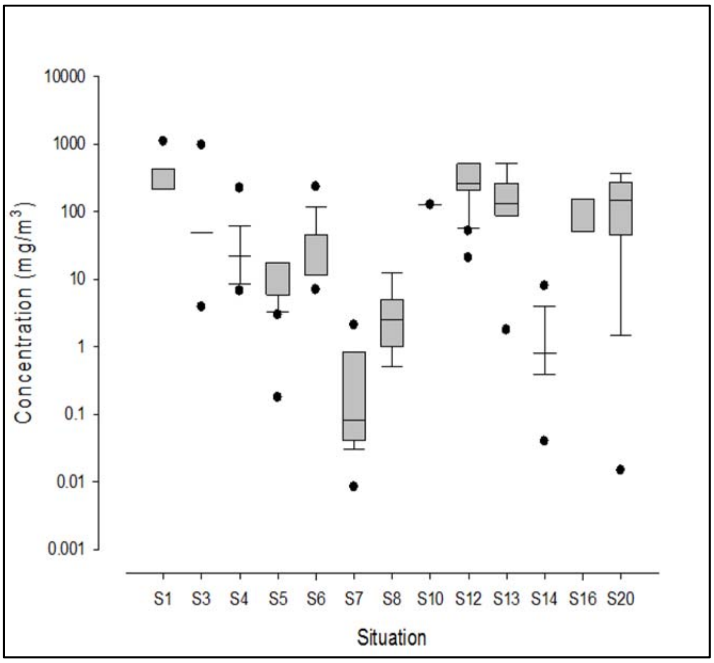


Figure 5.2 Inhalation estimates generated by participants using the ECETOC TRAv2 tool for situations involving exposure to liquids/ (mg m^{-3})

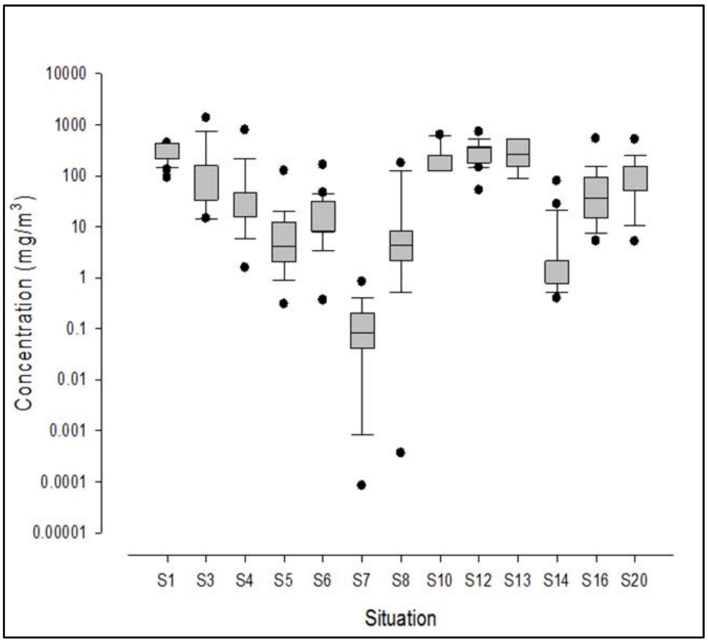


Figure 5.3 Inhalation estimates generated by participants using the ECETOC TRAv3 tool for situations involving exposure to liquids/(mg m^{-3})

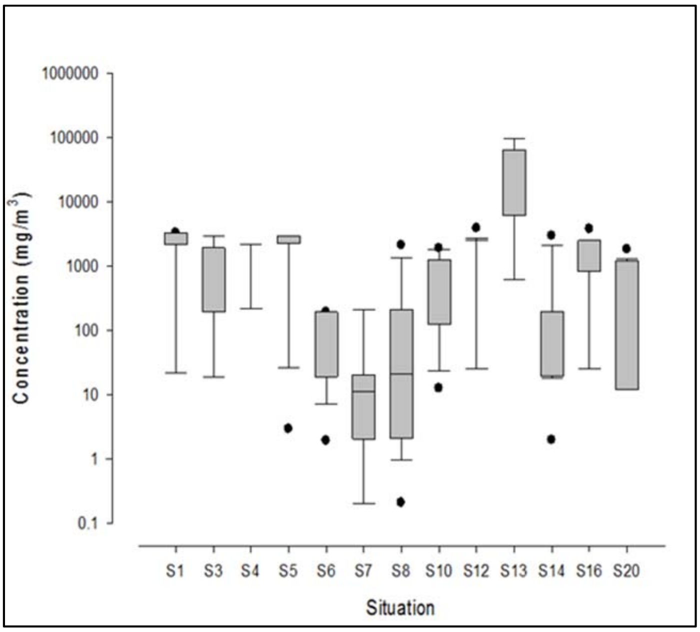


Figure 5.4 Inhalation estimates generated by participants using the EMKG-EXPO-TOOL for situations involving exposure to liquids/(mg m^{-3})

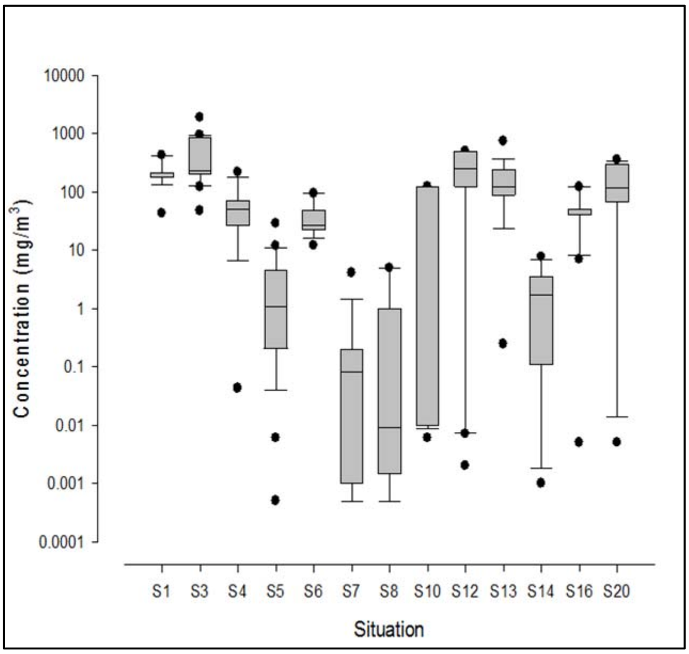


Figure 5.5 Inhalation estimates generated by participants using MEASE for situations involving exposure to liquids/ (mg m^{-3})

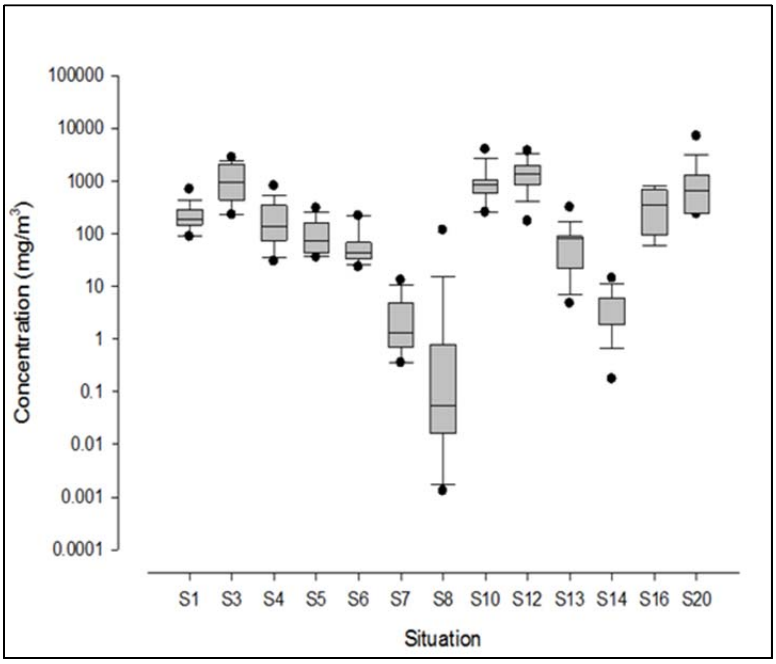


Figure 5.6 Inhalation estimates generated by participants using STOFFENMANAGER (90th percentile) for situations involving exposure to liquids/ (mg m-3)

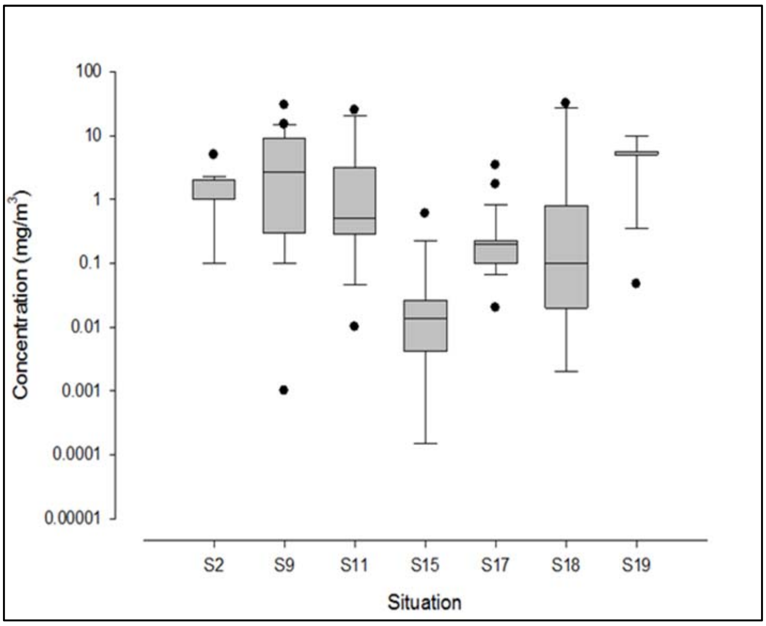


Figure 5.7 Inhalation estimates generated by participants using the ECETOC TRAv2 tool for situations involving exposure to solids/(mg m^{-3})

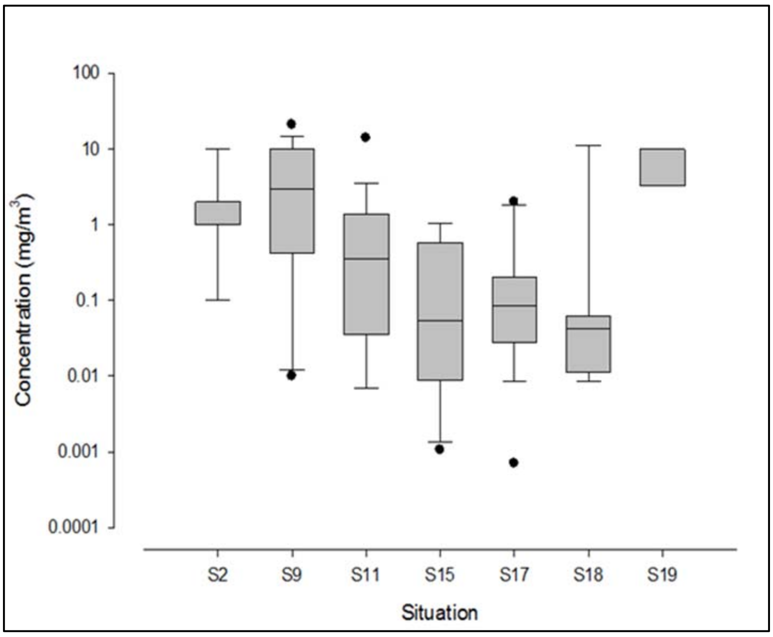


Figure 5.8 Inhalation estimates generated by participants using the ECETOC TRAv3 tool for situations involving exposure to solids/(mg m^{-3})

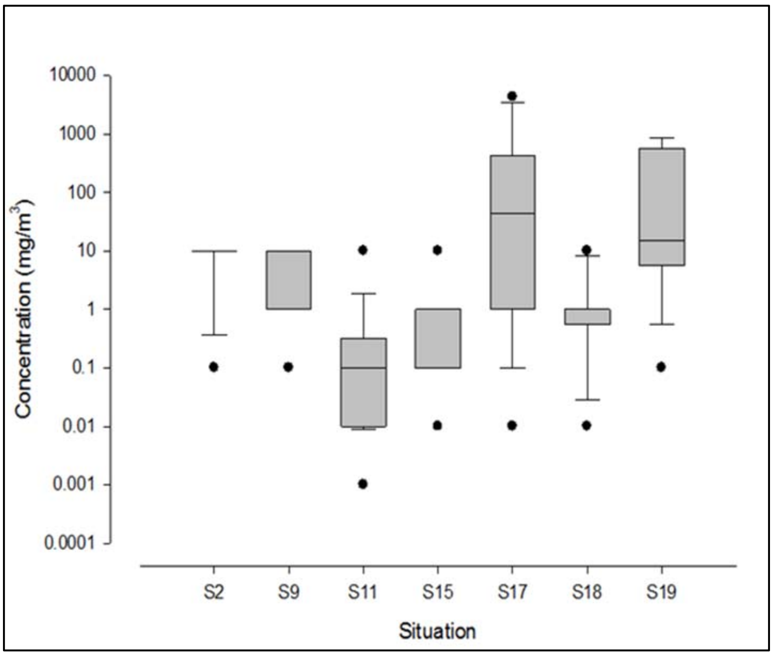


Figure 5.9 Inhalation estimates generated by participants using the EMKG-EXPO-TOOL for situations involving exposure to solids/(mg m^{-3})

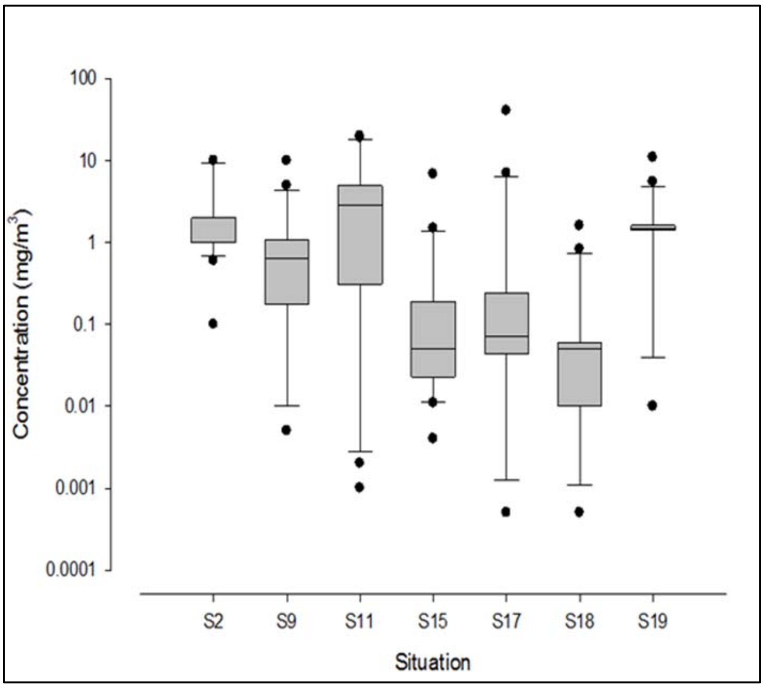


Figure 5.10 Inhalation estimates generated by participants using MEASE for situations involving exposure to solids/ (mg m^{-3})

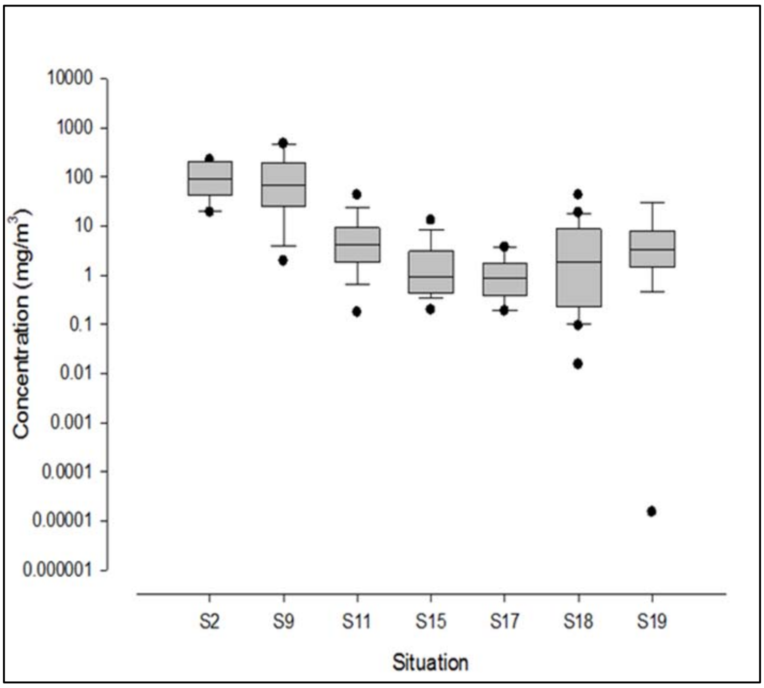


Figure 5.11 Inhalation estimates generated by participants using STOFFENMANAGER (90^{th} percentile) for situations involving exposure to solids/(mg m^{-3})

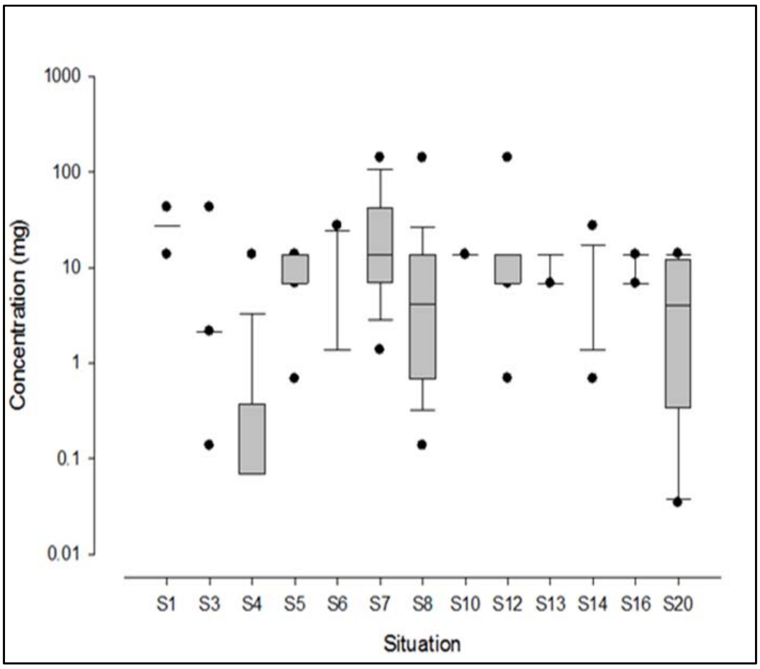


Figure 5.12 Dermal estimates generated by participants using the ECETOC TRAv2 tool for situations involving exposure to liquids/(mg)

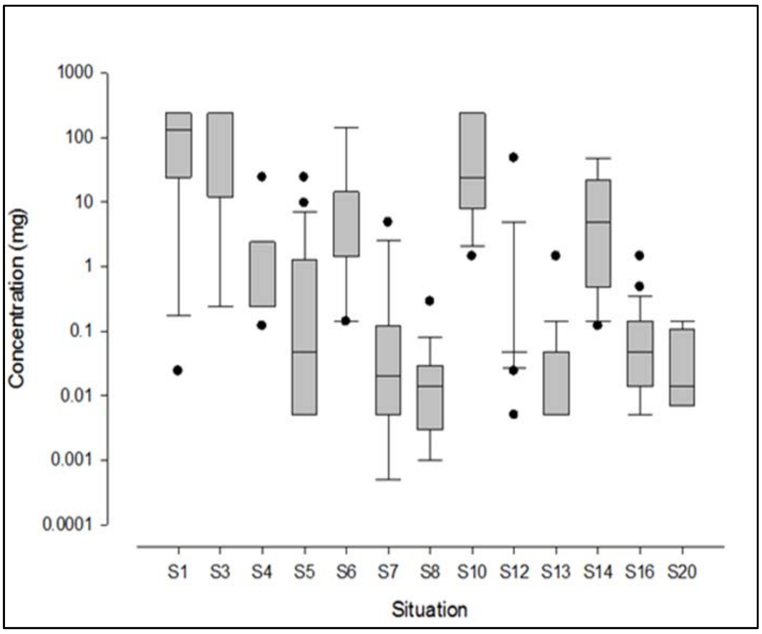


Figure 5.13 Dermal estimates generated by participants using the ECETOC TRAv3 tool for situations involving exposure to liquids/(mg)

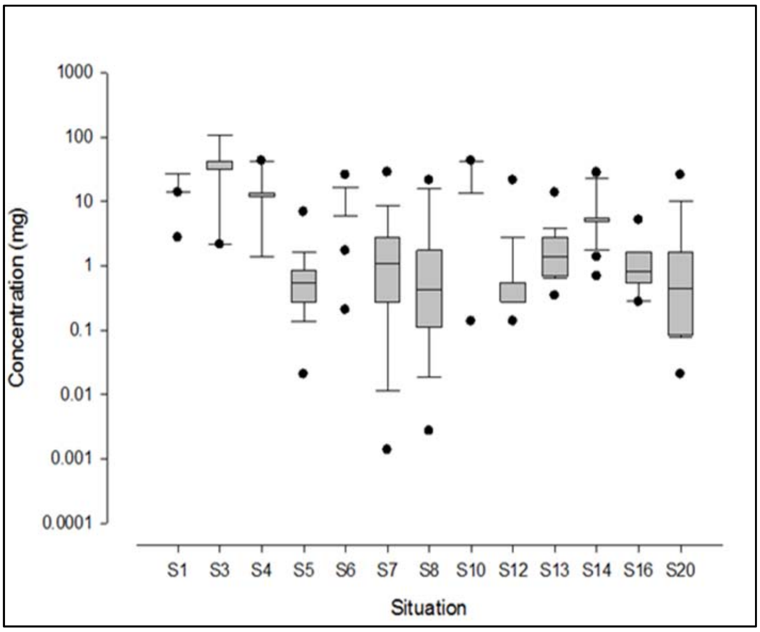


Figure 5.14 Dermal estimates generated by participants using MEASE for situations involving exposure to liquids/ (mg)

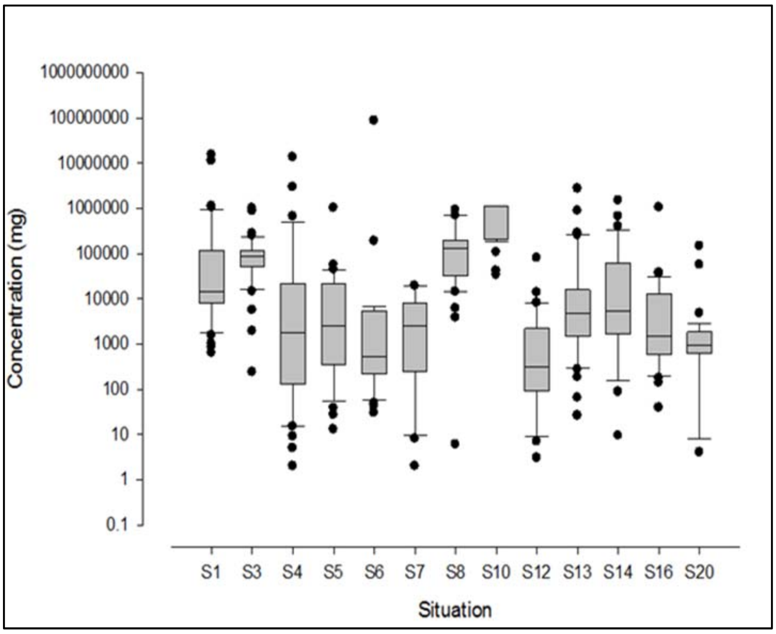


Figure 5.15 Dermal estimates (90th percentile for exposure to hands) generated by participants using RISKOFDERM for situations involving exposure to liquids/ (mg)

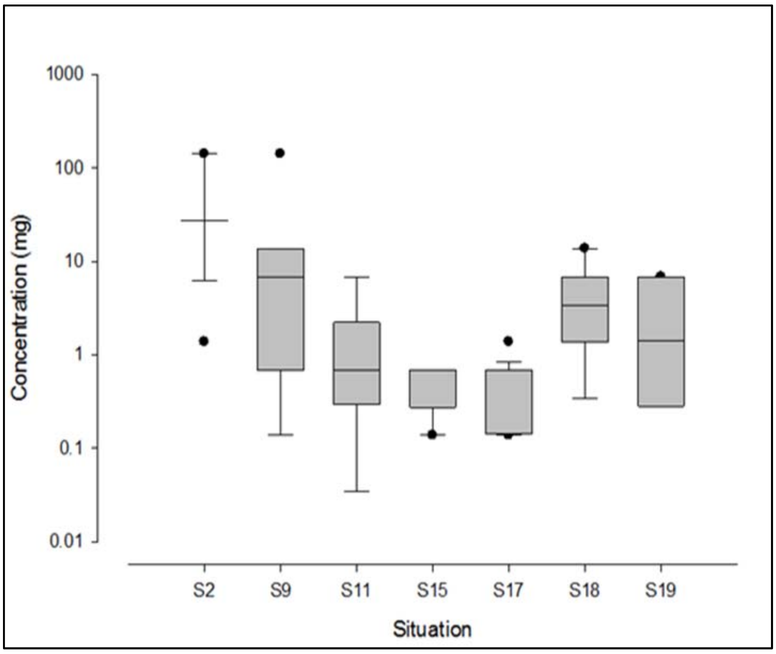


Figure 5.16 Dermal estimates generated by participants using the ECETOC TRAv2 tool for situations involving exposure to solids/(mg)

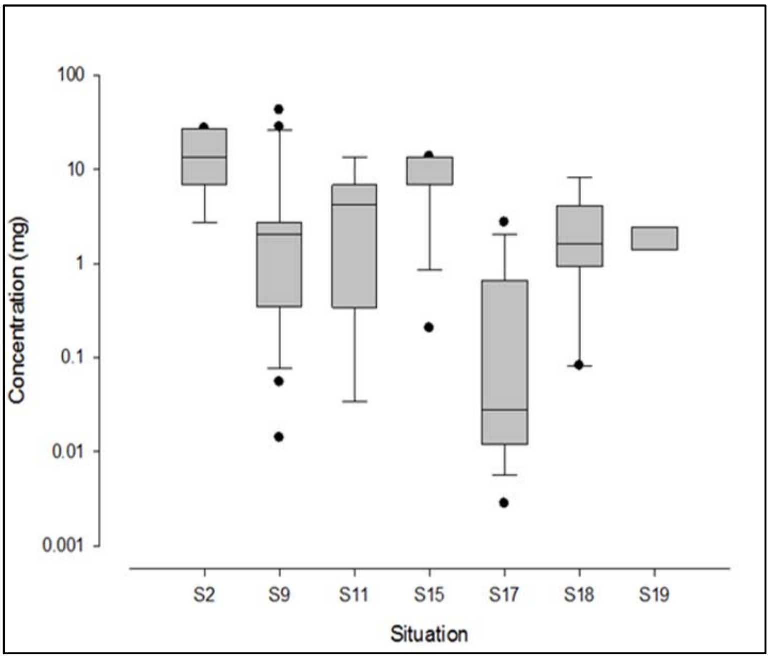


Figure 5.17 Dermal estimates generated by participants using the ECETOC TRAv3 tool for situations involving exposure to solids/ (mg)

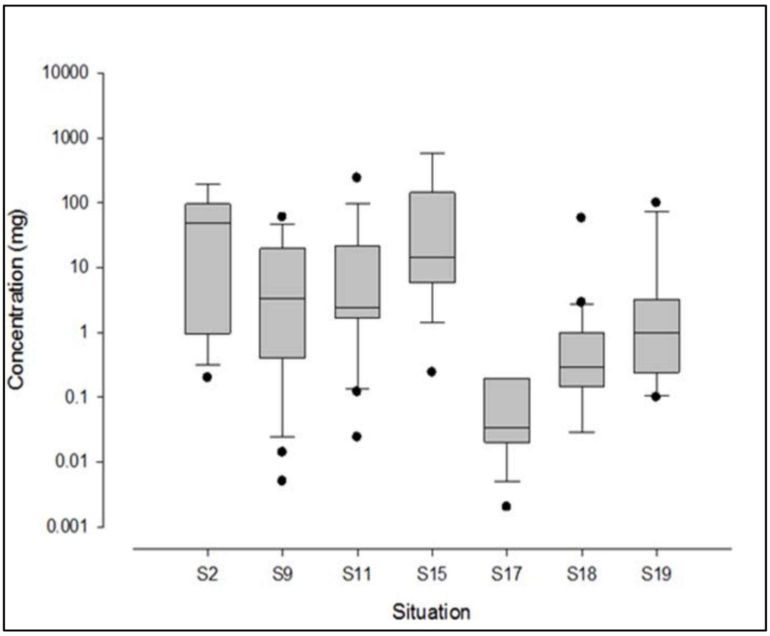


Figure 5.18 Dermal estimates generated by participants using MEASE for situations involving exposure to solids/ (mg)

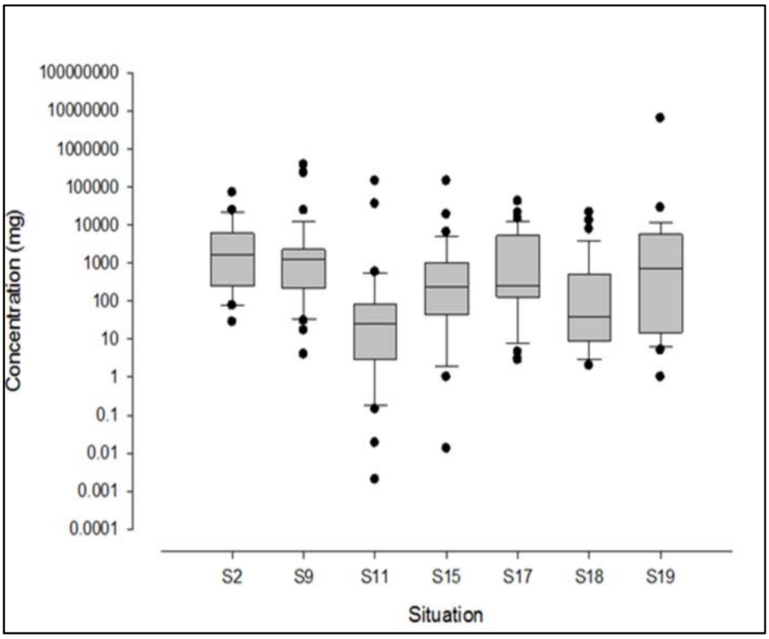
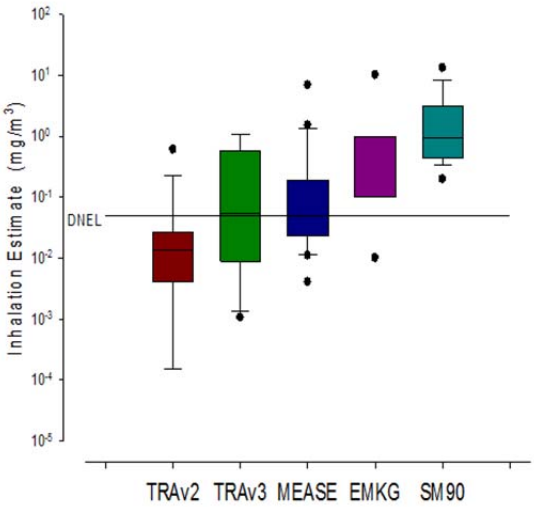


Figure 5.19 Dermal estimates (90th percentile for exposure to hands) generated by participants using RISKOFDERM for situations involving exposure to solids/ (mg)

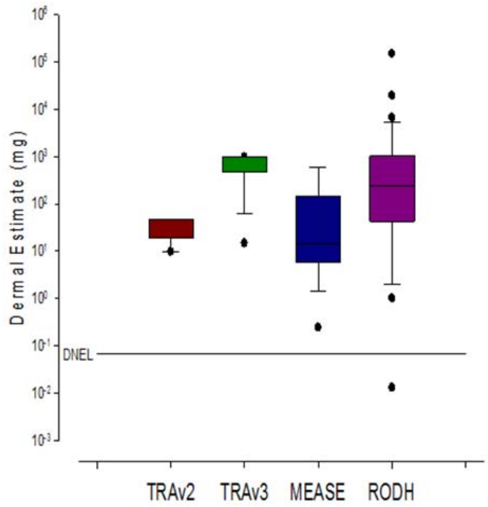
To illustrate this variation in more detail, examples of typical ranges of the estimates obtained from different participants are shown on a log scale by tool for Situation 15, which related to packing of nickel powder in Figure 5.20 (inhalation) and Figure 5.21 (dermal). The ranges of inhalation and dermal estimates generated by participants for Situation 7, covering changing of paint-contaminated filters in a spraybooth are shown in Figures 5.22 and 5.23 respectively. Dermal estimates for all tools are expressed as mass of contaminant (mg).

REACH requires the setting of Derived No Effect Levels (DNELs) for substances, which are exposure levels above which humans should not be exposed. DNELs are set with consideration given to the type of exposed person and the route, frequency and duration of exposure. For example, in Situation 15, a DNEL of 0.05 mg m^{-3} has been assigned to nickel powder for systemic effects from inhalation exposure. The range of estimates obtained from the BURE participants range widely around this value, suggesting that during a “real” assessment, the observed variation could lead to inappropriate and inconsistent conclusions about exposure being drawn.



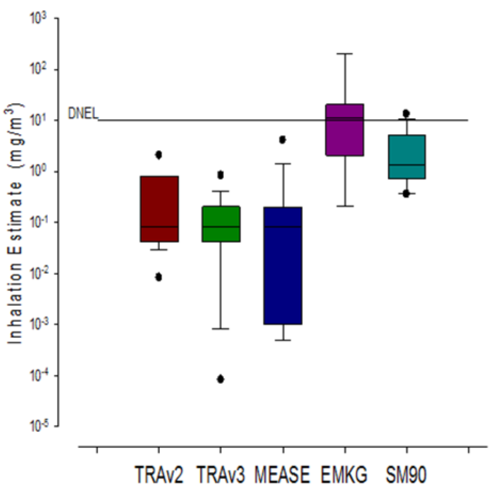
SM90= 90th percentile estimate from STOFFENMANAGER

Figure 5.20 Range of inhalation exposure estimates from Situation 15: Packing of nickel powder



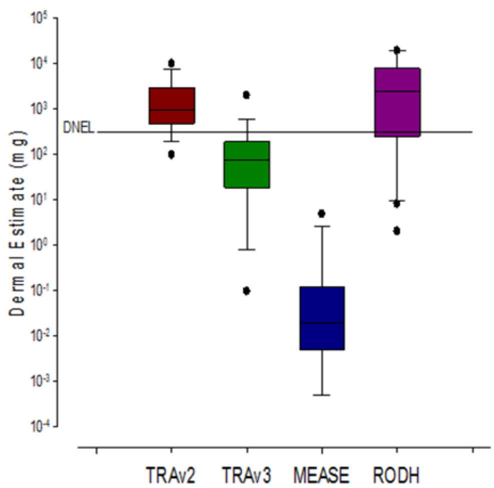
RODH = RISKOFDERM estimate for hand exposure

Figure 5.21 Range of dermal exposure estimates from Situation 15: Packing of nickel powder



SM90= 90th percentile estimate from STOFFENMANAGER

Figure 5.22 Range of inhalation exposure estimates from Situation 7: Changing of filters in a paint spraybooth with exposure to N-methyl pyrrolidone



RODH = RISKOFDERM estimate for hand exposure

Figure 5.23 Range of dermal exposure estimates from Situation 7: Changing of filters in a paint spraybooth with exposure to N-methyl pyrrolidone

From Figures 5.20 – 5.23 the highest and lowest inhalation and dermal estimates from each of the tools generally varied by factors of between 10 and 10000. Ranges of estimates covering similar orders of magnitude were evident in all of the BURE situations, for both dermal and inhalation exposures. These differences in estimates were driven in the main by variation in choice of activity-related parameters, such as the PROC code for ECETOC TRAv2, ECETOC TRAv3 and MEASE, the task characterisation input in STOFFENMANAGER and the DEOs (Dermal Exposure Operations) in RISKOFDERM. Other input parameters also contributed significantly to the observed variation in results, e.g. substance characteristics (dustiness and % in preparation) and ventilation. For the ECETOC TRAv2, ECETOC TRAv3 and MEASE tools, the choice of activity setting, i.e. professional or industrial, also led to significant observable variation between participant estimates. Within the RISKOFDERM tool, there were substantial differences in the free text numerical inputs for the application rate and cumulative duration of exposure parameters, which are multiplicative and so contributed to very large variation between the users' final estimates.

5.3.4 Discussion

Between the start of the REACH Registration period in 2008 and September 2014, around 40,000 substance dossiers had been submitted to ECHA (ECHA, 2014), of which approximately 6,000 originated with Small and Medium Enterprises (SMEs), the remainder being presented by large organisations. The scale of the Registration process has thus necessitated the assessment of exposure by a range of different actors, with varying levels of experience, competence and professional support. The effectiveness of the REACH process relies on consistency between registrants to ensure that hazards are identified and risks assessed in the same manner across different sectors and countries. The information generated in the assessments, often summarised in the form of tool input parameter descriptions, must then be disseminated to, and interpreted by a very large and varied downstream user population.

In modelling exposure for a particular work activity, an assessor must interpret and translate the situation into the required tool parameters. To describe the exposure effectively, the same range of determinants has to be considered. This can be done explicitly within a tool by the inclusion of more parameters and/ or more options within each of these parameters from which to choose. Alternatively, where only limited numbers of input choices are available, the assessor must use their knowledge and experience to provide supplementary information on missing determinants. A degree of subjectivity will always therefore be present in any assessment process. The BURE results suggest that when presented with brief, identical descriptions of exposure situations, such subjectivity can lead to very different results being generated by different users of the Tier 1 assessment tools.

The study population is considered to be representative of a normal range of tool users in terms of frequency and purpose of tool use, familiarity with tools, English language ability, REACH familiarity and level of experience of exposure assessment. There were minor systematic differences between users as individuals, and no consistent observed impact of their personal characteristics on the amount of variation in estimates. Exposure situations with higher levels of between-user variation were in general well described, with information on the majority of parameters provided. Additional contextual information about the exposure situation itself does not therefore appear to improve consistency between assessors. This is consistent with other related research, where the provision of additional contextual information increased the validity of exposure estimates compared with a measured or identified concentration, but did not increase the reliability of assessments (Friesen et al., 2011; Stewart et al., 2000). De Cock et al. (1996) found that the phased provision of additional detail, including written background information on tasks, had little effect on the level of agreement between assessors of pesticide exposure. De Cock et al. postulated that additional information may have simply reinforced the assessors' initial decision to some degree. It could also be postulated that more information requires more subjective interpretation, thus increasing the likelihood of differing decisions between assessors.

Whilst there was observed variation between choices made for the majority of parameters in the BURE, in the context of REACH, it appears that the greatest impact on the resultant estimates arises from differences in choice of PROC code/ activity descriptor and of the dustiness level. Additional situation-related information may not assist in reducing variation, however BURE participant feedback suggested that the provision of clearer, sector-specific examples of activity/ PROC code within the relevant REACH documentation and tools would be very useful.

The erroneous attribution of local and secondary control measures because of errors in interpretation of workplace situation information was also noted by Schinkel et al. (2014). The study, looking at the reliability of the ART tool, found extreme deviations from a "gold standard estimate" could be caused by assessors failing to include relevant exposure controls accurately. Errors in allocation of the LEV and local control parameters have a significant effect on the estimate obtained, and were a source of considerable variation in the BURE. In a REACH context, it can be assumed that assessors will know if risk controls were present, as they are in fact specifying the RMM options needed to describe a safe scenario. Erroneous choice of RMMs is therefore considered less likely.

Non-tool-related causes of between-user variation were also observed. Erroneous choices of physical form contributed to significant between-user variation in a number of situations, in particular the designation of metal fume as a liquid. To avoid artificial reduction in the observed between-user variation, all of these values were included in the analyses, as representing valid, albeit incorrect, participant input choices. In a real-life context, careful reading of the available tool guidance would reduce such errors.

The evaluation of the usability and user-friendliness of the tools described earlier in this Chapter showed that participants were positive about these aspects of the tools and the guidance/ help functions provided. All of the tools were reported to be easy to learn, particularly the MEASE and EMKG-EXPO-TOOL. Many of the BURE participants were recruited via their involvement in the user-friendliness evaluation, therefore there was an overlap between the two populations. The results of the BURE suggest a mis-match between the participants' perceptions of learning and using the tools and the consistency of the estimates generated. Tool guidance did not seem to be consistently applied by users, and more reliable estimates were not generated by those tools which were perceived to be simpler to learn and use.

Generating valid and consistent estimates of exposure thus relies not only on the tools themselves, but also on the manner in which they are used. REACH document Chapter R12 (ECHA, 2010) notes that a sufficient level of occupational hygiene expertise is required for the identification of the most suitable PROC for a particular application. There is therefore a responsibility on tool users to make sure that they are competent and able for this task. Great emphasis is placed on the training and competence of occupational hygienists carrying out workplace exposure measurements; however, there is no similar requirement for users when generating and interpreting results from exposure assessment tools. As these modelled estimates are then used in place of workplace measurements, this approach seems somewhat contradictory.

The tools are Microsoft Excel or web-based and freely available, however it has been shown that ability to operate the software is not enough to ensure consistency between users. Variation was common amongst participants of all backgrounds, including those with extensive experience of exposure assessment, and our results did not suggest that previous knowledge of the substance or exposure situation itself increased consistency. However, the current approach to tool dissemination is particularly difficult for inexperienced or professionally-isolated assessors, who may have no mental or peer-generated benchmark against which to gauge the competence and validity of their assessments. Participation in online or in-person training covering the basics of tool applicability and operation may increase consistency for all assessors. If provided in conjunction with a comprehensive guide to tool use, this approach could reduce variation caused by unfamiliarity with the tools and their full range of capabilities.

Previous studies have noted that the use of more than one assessor can increase the validity of subjective assessments compared with an identified standard. As noted previously (Semple et al., 2001; Kunac et al., 2006; Schinkel et al., 2014), the implementation of a consensus/ team approach could also be helpful in identifying discrepancies or errors in interpretation of determinants.
Modelled tool estimates are used for exposure assessment, often in the absence of comparable or corroborating measurement data. Whereas calibrated sampling equipment and laboratory accreditation for chemical analyses are considered essential in ensuring the quality and reliability of measurement data, no analogous methods of quality control are applied to exposure assessment tools. The processes for collecting and using the required information are common to many of the Tier 1 and higher Tier tools. Whilst there is guidance in Chapter R14 regarding the exposure assessment process under REACH, there is no generalised procedure for carrying out assessments using tools for REACH or other purposes. The development of a standard operating method for tool operation would be of benefit in reducing between and within user variation. This document could cover the essential steps of carrying out an exposure assessment using tools, as is currently done for the use of sampling equipment. The combination of a standard method, tool guidance and where available, sector-specific information would form a comprehensive user support framework, which could in turn be the basis of a quality control scheme. In this scheme, tool users could participate in regular assessments

of different types of exposure situations, akin to the existing “round-robin” exchange schemes for fibre counting and chemical analyses. Over time, the feedback that users received would allow them to improve and standardise their assessment performance, thus minimising between-user variation.

The tools evaluated within BURE are commonly used both within REACH and in other contexts, for example to manage chemical risks in SMEs. The level of between-user variation observed thus has a number of implications. Within REACH, registrants’ use of the tools to iterate a set of descriptive safe use conditions within a sector-based support framework may reduce variation, although it is not clear how widespread these networks are. However, downstream users receiving and implementing these descriptions in the workplace may experience the same difficulty in interpreting the information as the BURE participants, leading to inconsistent implementation of risk controls.

For non-REACH-related tool use, the assessor support networks may be more limited still, thus there is significant potential for under- or overestimation of exposure, and associated risks to worker health or business finances respectively. All of the BURE participants reported some level of experience in tool use and exposure assessment: for SMEs, where non-expert use of the tools is normal and indeed, encouraged, even higher levels of between-user variation may exist.

In conclusion, the BURE results suggest significant potential for inconsistency in the exposure estimates obtained by different Tier 1 tool users, which could impact on the effectiveness of the REACH processes for identifying and, ultimately controlling, health risks from hazardous substances. Implementation of additional support and quality control systems for all tool users could help to reduce between-assessor variation, thus ensuring the protection of worker health and avoidance of unnecessary business risk management expenditure.

6 Uncertainty of the Tier 1 exposure assessment tools

6.1 Introduction

In this part of the project the uncertainty of Tier 1 tools was assessed qualitatively on the basis of the corresponding World Health Organisation (WHO) guidance document Uncertainty and data quality in exposure assessment (WHO, (2008) and the official ECHA guidance document Chapter R.19: Uncertainty analysis (ECHA, 2008). According to the WHO guidance document, uncertainty is a “lack of or imperfect knowledge concerning the present or future state of an organism, system, or (sub)population under consideration, which may affect its accuracy or relevance. Uncertainty can be reduced, at least in principle, by improving the quality and/or amount of information.”

In relation to exposure tools this means that the resulting estimated exposure may deviate from reality, e.g. due to imperfect knowledge about exposure and its influencing factors and/ or a lack of data that can be used for the tool development.

There are sources of estimate uncertainty at every stage of the risk assessment process, starting with the exposure situation and its documentation (i.e. scenario uncertainty- not tool related; for example omitted exposure pathways or unreported RMMs). Other sources of uncertainty can be related to parameters (parameter uncertainty – can also be a part of the tool uncertainty, e.g. input parameter definition, sampling errors) or the algorithm that connects the different input parameters (tool uncertainty; e.g. ideal gas law, dependencies) (see Figure 6.1).

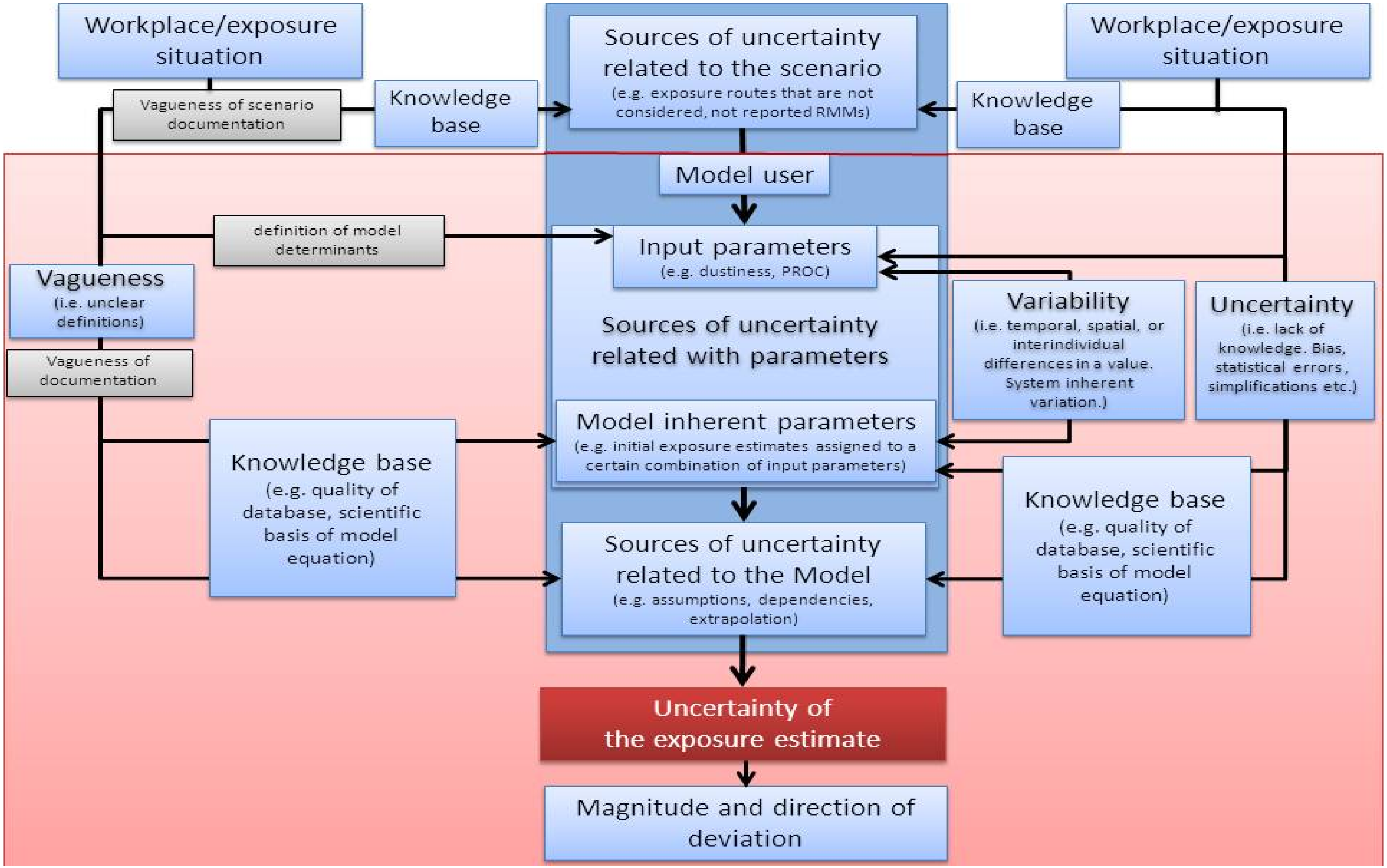


Figure 6.1 Aspects of uncertainty- Concepts outside of the light red area are beyond the scope of WPII.1

In order to evaluate tool uncertainty, possible sources of uncertainty such as input parameters or assumptions were for each tool and categorised according to transparency (i.e. available background information), knowledge base (i.e. quality of underlying information) and quality of the input parameter definition (level of detail, vagueness) as far as possible. If possible, a rough indication of the direction and magnitude of the estimate's deviation was also given. In this context it should also be noted that Tier 1 estimates are meant to be conservative, i.e. a certain tendency to overestimate exposure is not considered to be a disadvantage. As a consequence, in some cases where the Tier 1 assessment predicts a risk, refinements with higher Tier tools are possible and recommended.

Common results for the uncertainty evaluation and a selection of example situations for each tool have been summarised in evaluation matrices which are detailed fully in eteam Project Deliverable D24: Uncertainty of Tier 1 models- final report) (Hesse et al., 2014). In the following subsections, a short summary and discussion of some general issues will be given.

6.2 Comparison and discussion

6.2.1 Knowledge base

6.2.1.1 <u>Datasets</u>

An exposure tool can be based on a set of measured data or pure "expert judgement". However, these two extreme cases are rarely found in reality, while a combination of both approaches is usually more feasible. Depending on the available data, some parts of a tool may be based on a set of measured exposure data, whilst the basis of other parts may be scientific judgement or unpublished information. In addition, a certain amount of scientific judgement is always needed to construct the tool around its measured basis of datasets, for example in the selection of relevant parameters or the assignment of scores for a statistical model fitting procedure.

Although all these approaches are in general able to generate accurate results the usage of experimental data increases knowledge and transparency of the tool and thus, decreases uncertainty. Moreover, a higher number of datasets decreases the statistical error. The published data for the evaluated Tier 1 tools are summarised in Table 6.1, from which it is clear that there are great differences both between, and within, each tool.

The number of datasets per use category ranges from 0 (MEASE) up to more than 2000 (MEASE, ECETOC TRA) for the inhalation tools and from 0 (MEASE, ECETOC TRA) up to more than 300 (RISKOFDERM) for the dermal tools. The dermal tools are generally based on fewer data then the inhalation tools. There are also some tools for which none or only a part of the used datasets is published (datasets per use category for STOFFENMANAGER; EMKG-EXPO-TOOL; ECETOC TRA and MEASE for non-metal specific processes).

Table 6.1 Approximate numbers of measured datasets used for tool development [(1)]

Number of datasets	MEASE	ECETOC TRAv2 and v3	EMKG-EXPO-TOOL	STOFFEN-MANAGER	RISK-OFDERM
Inhalation					
Number of datasets for inhalation exposure	> ~6500[(2)]	> 4000	not published	> 1000 (+146 respirable stone dust) (520 solids and 432 liquids)	n.a. / outside scope
Number of datasets for inhalation exposure, per use category[(3)]	0-2544[(2)]	146-2544	not published	not published	n.a. / outside scope
Reflected tool parts	Datasets represent PROCs 21-27b. Only solids included.	Datasets represent PROCs 21-25	not published	Datasets represent all implemented process descriptions (26 handling categories including wood/stone categories). Solids and liquids.	n.a. / outside scope
Years covered by datasets	Risk Assessment Reports (RARs) from 2003-2008[(2)]	Risk Assessment Reports (RARs) from 2003-2008	not published	1994-? (not all years published)	n.a. / outside scope
Dermal					
Number of datasets for dermal exposure / Hands	> 500	>250	n.a. / outside scope	n.a. / outside scope	> 500
Number of datasets for dermal exposure / Hands, per use category	0-285	0-125	n.a. / outside scope	n.a. / outside scope	13-195 (no separation into solid and liquid published)
Reflected tool parts(hands)	Datasets represent three of four exposure ranges assigned to the EASE use description. Only solids.	Datasets represent PROCs 21-25. Only solids	n.a. / outside scope	n.a. / outside scope	Datasets represent DEO units 1-5 (DEO unit 1 and 4 solids, DEO units 1-5 liquids)

Table 6.1 Approximate numbers of measured datasets used for tool development [(1)] (continued)

Number of datasets	**MEASE**	**ECETOC TRAv2 and v3**	**EMKG-EXPO-TOOL**	**STOFFENMANAGER**	**RISKOFDERM**
Years covered by datasets	1999-2005	1999-2005	n.a. / outside scope	n.a. / outside scope	1996-2004
Dermal exposure / Body	n.a. / outside scope	n.a. / outside scope	n.a. / outside scope	n.a. / outside scope	> 650
Dermal exposure / Body, per use category	n.a. / outside scope	n.a. / outside scope	n.a. / outside scope	n.a. / outside scope	57-331 (no separation into solid and liquid published)
Reflected tool parts (body)	n.a. / outside scope	n.a. / outside scope	n.a. / outside scope	n.a. / outside scope	Datasets represent DEO units 2-6 (DEO unit 4 and 6 solids, DEO units 2-6 liquids)
Years covered by datasets	n.a. / outside scope	n.a. / outside scope	n.a. / outside scope	n.a. / outside scope	1996-2005
RMM efficiencies					
Datasets for RMM efficiencies	> 400	> 4000 (inhalation) > 250 (dermal)	not published	> 1000 (+146 respirable stone dust) (520 solids and 432 liquids) RMM efficiencies are a result of the fitting procedure using all datasets available for inhalation exposure (including scenarios with and without RMMs)	> 500 (hands) > 650 (body) RMM efficiencies are a result of the fitting procedure using all datasets available for dermal exposure (including scenarios with and without RMMs)

Table 6.1 Approximate numbers of measured datasets used for tool development [(1)] (continued)

Number of datasets	MEASE	ECETOC TRAv2 and v3	EMKG-EXPO-TOOL	STOFFENMANAGER	RISKOFDERM
Datasets for RMM efficiencies per control measure	12-280	146-2544 (inhalation) 0-125 (dermal)	not published	not published	Hands: 13-195 (no separation into solid and liquid published) Body: 68 per RMM and 331 per 2 RMMs (no separation into solid and liquid published)
Reflected tool parts	Physical state for underlying datasets is not known.	LEV efficiencies for PROCs 21-25. For other PROCs and further RMMs /PPE no sets of measured data are published, however rationales for efficiencies are given in ECETOC TRA documentations TR 93, 107, 114 .	not published	Datasets represent all implemented RMMs (6 RPE types, 3 different worker situations, 7 categories describing the application of LEV, ventilation and containment). Solids and liquids.	All implemented RMMs: DEO unit 1: Ventilation DEO unit 4: Directed airflow and segregation DEO unit 5: LEV
Years covered by datasets	2000-2007	2003-2008 (inhalation) 1999-2005 (dermal)	not published	1994-? (not all years published)	1996-2005

[1] One dataset refers to one datapoint as published in the available references: MEASE: number of values (inhalation data); number of counts (HERAG, 2007); efficacy values (Fransman et al., 2008); ECETOC TRA: number of values (inhalation + dermal data); Stoffenmanager®: number of samples, RISKOFDERM: number of data. [2] Approximate number. Number of underlying datasets has been increased since development of draft report EBRC, 2008. There is a certain overlap with the ECETOC datasets for metal processes.[3] use category = one process/task/use description within the tool. For ECETOC TRA and the inhalation part of MEASE this categorisation is the PROC system, for the dermal MEASE part it is the categorisation into EASE use patterns, for RISKOFDERM it is the DEO unit categorisation, for Stoffenmanager® it is the differentiation into tasks.

6.2.2 Validation studies

Similar differences can be observed for available validation studies with measured exposure data. Although those studies do not change the tool estimate itself, they are able to inform potential users about reliability and scope of the different models and thus, may decrease the general uncertainty of a risk assessment.

The number of published validation studies prior to the eteam project is limited for all of the tools. No validation studies have been published for MEASE and RISKOFDERM, whereas for RISKOFDERM one comparison with other exposure tools and biological monitoring exists (Boogaard et al., 2008; Vink et al., 2010), which suggests conservative results of the tool. For ECETOC TRA, three publications exist which show varying results but mainly show overestimations of exposure. For STOFFENMANAGER four publications are available (Koppisch et al., 2012; Schinkel et al., 2010; Vink et al., 2010; Arnone et al., 2013), which again show varying results including both over- and underestimations. However, it is discussed that the results are at least partly within the fraction of underestimations which would be expected considering the estimated percentile. For the EMKG-EXPO-TOOL, one validation study has been published and so far (Kindler et al., 2010*)*, no underestimations have been reported. However, more publications exist about COSHH Essentials, which forms the basis of the EMKG-EXPO-TOOL (see Chapter 2).

6.2.3 General tool approach

The approach that has been used to construct the underlying model algorithm for the tools is one of the most difficult aspects of uncertainty to evaluate. In general, there are tools mainly based on a set of logic criteria, those which refer to initial exposure estimates which are then modified by operational conditions or risk mitigation measures via reduction efficiencies, and ones that refer to statistical modelling procedures (e.g. linear mixed effects models) fitting measured exposure data to a given algorithm. Combinations of these approaches are also often used (e.g. first choice of DEO unit (→ logic tree), then linear mixed effects modelling for RISKOFDERM).

The influence of the choice of tool approach on its uncertainty can be large, as the reflection of parameters and dependencies between these are obviously different. However, although some publications discussing the general advantages of certain tool approaches exist, their specific influence on the accuracy of the exposure estimate cannot be quantified.

6.2.4 Parameters

6.2.4.1 Quality of input parameter definition

Input parameters can be based on quantitative definitions (e.g. vapour pressure) or on qualitative descriptions with varying levels of detail. While the former allows for a categorisation with clear boundaries, the latter may be vague, i.e. the boundaries between categories may be unclear and lead to wrong assignment of parameters which results in wrong exposure estimates. This type of uncertainty source is strongly related to the BURE exercise, in which the reproducibility of exposure estimations by different users was evaluated.

Input parameters which are defined often, or indeed only, in a qualitative way are dustiness (e.g. “like flour”), the use description (e.g. PROCs, DEO units) and the type of setting (professional vs. industrial). All these examples have also been shown to result in a high number of different assignments in the course of the BURE. In case of the use categorisation this seems to refer to all categorisation approaches, although the level of detail used for the different use categories as well as the general basis (task based / process based) differs greatly between the tools.

Overall the quality of the definition of input parameters is considered to be a crucial aspect in relation to the overall uncertainty of a tool estimate, as the assignment of a wrong parameter may easily lead to high deviations up to more than three orders of magnitude including over- and underestimations of exposure and can even influence the options for other input parameters.

6.2.4.2 Tool-inherent reflection of input parameters

The tool-inherent reflection of an input parameter can be a modifier assigned to operational conditions such as concentration or duration, an initial estimate assigned to a use description or an exposure reduction efficiency caused by the application of a risk mitigation measure.

An example is the exposure reduction caused by the application of local exhaust ventilation systems. The efficiencies assigned to this measure may differ not only between tools but also between situations or exposure routes and overall range from ~50% for STOFFENMANAGER up to 95% for the ECETOC TRA and MEASE. The reasons for these different defaults are rarely given, as construction details for the relevant control measures are not usually given within the tool or accompanying publications. An exception is the EMKG-EXPO-TOOL, for which detailed control guidance sheets exist which include information about the expected design of implemented measures.

Similar differences exist for other tool inherent parameters, thus, the level of conservativeness of the estimates may vary accordingly.

6.2.4.3 Resolution and level of detail

Almost all of the parameters implemented in the various Tier 1 tools are categorised to varying levels of extent. Thus, while in reality there is usually a smooth increase of exposure when, for example, the concentration of the substance in question is increased, within the tools there is only a limited number of possible categories corresponding to a limited number of exposure estimates.
As these categorisation approaches are not identical for all tools, one situation may lead to different categorisations for different tools. As an example, one scenario calculated for two substances with vapour pressures of 490 Pa and 510 Pa would lead to different results for MEASE, ECETOC TRA, STOFFENMANAGER and the EMKG-EXPO-TOOL, but would lead to identical results in RISKOFDERM. Two substances with vapour pressures of 510 Pa and 6000 Pa would however lead to identical results for all of the tools except STOFFENMANAGER and RISKOFDERM.

As the Tier 1 tools are intended to be conservative, these categories must reflect the worst case of all scenarios summarised within each of them. Obviously, this leads to overestimations for scenarios which do not represent this worst case.

The level of detail is represented by the number of input parameters each tool offers. In general for the dermal tools, the number of parameters is mostly comparable. The number of parameters is highest for STOFFENMANAGER amongst the inhalation tools, which is consistent with its claim to be a Tier 1.5 rather than a Tier 1 tool.

Overall, the dermal models are often less complex, i.e. they offer a lower resolution and fewer input parameters, than the inhalation models. However, the overall level of detail and resolution and therefore also the resulting uncertainty always depend on the situation assessed.

In principle, some of the uncertainty may be reduced by adding additional parameters to the tools and increasing the resolution (i.e. going from a lower to a higher tier model. However, increasing the number of parameters or categories within a parameter may also increase uncertainty if these are not well defined or if the information available from the scenarios is not sufficiently detailed.

6.2.4.4 Omission of parameters of potential relevance for exposure estimation

It is clear that the omission of possibly relevant parameters may lead to uncertainties of the exposure estimate. However, there is no simple approach to define what may be missing and how this factor may affect the exposure estimate.

One possibility is the Tier 1 approach as defined in ECHA guidance document Chapter R14, as it gives information about the minimum level of information which should be available in order to perform a Tier 1 exposure assessment. These parameters are the physical state, information about fugacity (dustiness/ vapour pressure), concentration, level of containment, presence and efficiency of LEV, duration and a description of the process or task to be assessed. In comparing the tools with this list, there is always at least one tool which does not take into account one of the corresponding parameters.

A number of studies have evaluated the relevance of higher Tier parameters, e.g. personnel training, weather, moistness of skin or other, branch-specific details. Again, it should be noted that these parameters are not Tier 1 compatible. Their implementation may even decrease tool user-friendliness and consequently increase the probability of wrong parameter assignment.

The effect of omission depends heavily on the situation and the omitted parameter itself. Ideally, any omission of important parameters should be addressed by added level of conservatism, e.g. if the concentration of a substance in mixture is neglected or if risk mitigation measures and personal protective equipment are not taken into account. However, there are many cases were no prediction is possible (e.g. physical state) and the influence on the exposure estimate may be different for each situation.

It should also be noted that the Tier 1 approach as defined in guidance document R14 may itself bear some uncertainty, i.e. it is not completely certain if the parameters listed are actually appropriate to perform a sufficiently accurate and conservative exposure estimation.

6.2.5 Assumptions

Often the assumptions used in tool development are unique to the tool. However, there are some that are more commonly used, e.g. the ideal gas law (only used for conversion of units in some tools) or assumptions related to use of good occupational hygiene practice.

According to the British Occupational Hygiene Society (BOHS), good occupational hygiene practice involves the recognition, assessment and control of risks from workplace hazards such as chemicals, dusts, fumes, noise, vibration and extreme temperatures.

The evaluated tools follow different approaches concerning its implementation. While the ECETOC TRA (v2 and v3), the EMKG-EXPO-TOOL and parts of MEASE are based on the assumption that good occupational hygiene practice is followed. Good practice can be also be described via the choice of parameters in STOFFENMANAGER and partly MEASE and RISKOFDERM (e.g. via the choice of percentile or through description of cleaning and maintenance procedures).

This is primarily related to the tool’s scope, i.e. as long as the user is informed about the tool and its underlying assumptions and acts accordingly, the assumption that good occupational hygiene is practiced is not a source of uncertainty per se.

However, as for the definition of input parameters, there is only limited information about the definition of good occupational hygiene practice that has been used for tool development. Detailed descriptions of expected risk management measures are only laid down in the external control guidance sheets of the EMKG-EXPO-TOOL with reference to external guidance documents required for the other tools.

6.2.6 General considerations under REACH

Under REACH, downstream users are obliged to follow the scenario(s) provided in the course of the registration process. Errors or vagueness during the documentation of a situation or mistakes during tool input are therefore to a certain extent compensated: if the safe use description does not fit the actual workplace, the workplace has to be adapted or the downstream user has to create and register a new scenario.

However, it is still necessary for the downstream user to interpret the provided scenario in a correct way (e.g. assignment of PROC code, assessment of LEV design), i.e. there is more than one point in the risk assessment process where uncertainty due to parameter definitions and assignment may appear.

6.3 Conclusions and recommendations

In conclusion and summary, there is always some uncertainty in any exposure assessment. Although this uncertainty does not arise solely from the tool and its application, tool-related uncertainty should evidently not be neglected. Moreover, the type and level of uncertainty is always situation dependent. Each individual situation requires an assessment of whether the correct parameters have been assigned, the tool was used within its scope and the outputs have been interpreted appropriately.

To some extent, uncertainties may be compensated by error compensation within the tools. However, the degree of such compensation cannot be predicted without detailed information about the situation being assessed.

Further tool developments and improvements should consider user friendliness implications, the ability of users to choose the correct input parameters and the level of detail and resolution that the tool provides. Although not always the case (as demonstrated in the BURE), higher tool complexity has the potential to lead to higher between-user variability and thus, may increase uncertainty. Therefore proposed changes in the complexity of the tool structure should be carefully evaluated before they are implemented.

Where possible, any new tool parameters should be defined quantitatively. However, this will only lead to less uncertainty if the corresponding quantitative reference data are available to the user. If a certain test or study is not required under REACH, for example skin moisture readings, results may not be available. In addition, exposure and other measurements are also uncertain to some extent. It should be carefully considered which type of information is appropriate to be included in an exposure model and how sampling procedures or measurements should be performed to avoid further uncertainty.

The BURE has shown that there are some parameters which are prone to induce a high level of variability due to their vague or insufficiently-detailed definition. In particular these are: the use categorisation for all tools, the intrinsic dustiness which is defined qualitatively for all tools except MEASE, the type of setting (professional/ industrial) and the definition of risk management measures.

The resulting variability can potentially be decreased in different ways. Obviously, the definition of the corresponding parameters should be as precise as possible to reduce the need for subjective interpretation. However, the knowledge of the user about their tool is also of high relevance, therefore to decrease the total level of uncertainty, it is crucial that they are well informed about both the models and the situations that will be assessed.

7 Overall project conclusions

In considering the project findings as a whole, a number of conclusions can be reached, which are summarised below.

7.1 Conceptual evaluation of tools

The large differences in the underlying concepts, strengths and limitations of the various tools within this project inhibit a straight forward comparison for many of their features. Identification of the best or most appropriate tool for a particular exposure scenario is therefore often difficult.

As all of the evaluated tools are classified screening tools (at Tier 1 or Tier 1.5 level), it cannot be expected that all details of an exposure situation are incorporated in a realistic way.

When selecting the most appropriate tool for a particular exposure scenario, users must consult the available background information to determine the scope and range of applicability of possible candidate tools, must ensure that they fully understand the operation and limitations of the tools, for example via the tool guidance, and ensure that they have the relevant contextual information to input the required parameters.

7.2 Evaluation of data sources, Data gathering protocol and Development of the database

The collection of a comprehensive set of measured data with which to compare the tool estimates was a primary aim of the eteam project. It was desirable that comparator data were collected across the range of applicability of the maximum number of tools. Data collection therefore concentrated on situations that were applicable under the majority of the tools. This by default meant that situations described by a number of PROC codes as used under REACH were not included in the validation process.

It has been observed previously that the sourcing and collation of detailed contextual information on workplace situations is difficult, and in the context of tool validation, with its requirement to ensure that the relevant input parameters are addressed, this difficulty is magnified. Whilst much of the data supplied was usable, limited contextual information required allocation of agreed default parameters during input of a number of exposure situation into the tools, for example in relation to concentration or dustiness.

From the initial returns by the providers, the data identified covered a variety of industries and categories of use, including upstream and downstream processes across the chemical and other manufacturing and service sectors. The submissions received were predominantly from EU countries, in particular Germany, the Netherlands and the United Kingdom with additional data from the United States of America also used.

The majority of the available data related to measurements of personal inhalation exposures, with comparatively few dermal measurements identified for a limited range of substance categories. Comparison of the limited number of dermal estimates of exposure was further complicated, and ultimately precluded, by the range of measurement techniques used for sample collection and the absence of conversion factors between results from different methods.

The potential inhalation dataset was comprised predominantly of exposures to vapours and, to a slightly lesser extent, dusts. Of these vapour exposures, the vast majority related to the use of organic solvents, with smaller numbers of exposures to other non-solvent substances identified. Within the dust exposures (including powders; granules; fumes and droplets), many were to a range of non-ferrous metals, with the remainder comprising agent-specific or generic inhalable dusts. Detailed information on dustiness was not generally provided. The dataset included measurements of long-term (> 4 hour) shift average, short-term and task-based exposures. A wide range of exposures, from very low to relatively high (and in a number of cases above recommended occupational exposure limit values) was collected.

Despite a large effort to develop a comprehensive exposure measurement database for the comparison exercise, there remained important gaps. Relatively few measurement results could be used for non-volatile liquids, aqueous solutions and exposure to metals during abrasive and hot processes. In addition, as noted above data were not available for the full range of possible PROC codes mentioned in the REACH guidance. The results and observations made within this report should therefore be considered in the light of the above limitations.

7.3 Dataset evaluation and comparison with tool estimates

Comparisons of the Tier 1 exposure assessment tool estimates with individual and aggregated inhalation measurements obtained from a variety of data sources were carried out. The comparisons focussed on the level of conservatism of the tool estimates (i.e. their tendency to overestimate exposure) when compared to the measurement results and the correlations between the measurement results and tool estimates.

The level of conservatism was expressed in two ways. Firstly, the percentage of measurements that were higher than the corresponding tool estimate was examined, with the level of conservatism defined in this case as follows:

- High – where ≤10% of measurements exceeded the tool estimate
- Medium- where 11≤25% of measurements exceeded the tool estimate
- Low- where >25% of the measurements exceeded the tool estimate

The limited number of input parameters required for first tier exposure assessment using the tools being evaluated can give rise to considerable levels of inherent uncertainty. We therefore considered the tools to be sufficiently conservative if the estimates of these tools were comparable with the 90^{th} percentile of an exposure distribution. We also considered the ratio of the measurement results to the tool estimate, where a geometric mean of the ratios below 1 was taken as an additional indicator that the tool was conservative to some degree for that situation.

Of the exposure categories, most comparator data were available for volatile liquids, followed by powder handling. Fewer data from the other exposure categories could be included in the external validation. This arose from a necessity to maximise the applicability of the measurements to the maximum number of tools possible, whilst still covering specific categories of interest, for example metal processing.

Based on the combined individual and aggregated results available in this study, the EMKG-EXPO-TOOL was the only tool that appears to be highly conservative for volatile liquids, when using the criterion of <10% measurements above the tool estimate. This is most likely to have arisen because the concentration of the substance in the mixture is not taken into account within the EMKG-EXPO-TOOL. If the estimates were to be adjusted for the mixture content, the observed level of conservatism will clearly be reduced. There was only a moderate correlation between individual measurement results and tool estimates for the EMKG-EXPO-TOOL for this exposure category, but not for the aggregated data. The degree of correlation may however increase if concentration is taken into account.

STOFFENMANAGER is also conservative for this category, with 11% of measurements for exposure to volatile liquid vapours exceeding the 90th percentile tool estimate. The ECETOC TRAv2 and ECETOC TRAv3 were observed to be less conservative in comparison with the overall dataset for volatile liquids, with 26% and 32% of the measurements exceeding the tool estimate.

A relatively high overall number of data points were collected for powder handling, with differences again noted between the tools in terms of both level of conservatism and the degree of correlation with the measured values. For powder handling, STOFFENMANAGER appears to provide very conservative estimates when using both the 75th and 90th percentiles. Furthermore, MEASE could also be considered conservative, with around 11% of measurements exceeding the tool estimates. However, ECETOC TRAv2 and v3 are judged to have only a medium level of conservatism for this category, with 16% and 21% of the estimates exceeded by the measurement value. A similar finding was observed for the EMKG-EXPO-TOOL.

In relation to exposures during abrasion of metals, the ECETOC TRAv2 (24% of the measurements exceeding the tool estimate) and MEASE (18% of measurements in exceedance) were of medium conservatism, with the ECETOC TRAv3 judged to be of a low level of conservatism (exceedance in 26% of cases). It should be noted that there were very few data points for certain of the metal abrasion and metal processing process codes. For example, no individual measurements were available for PROC 21, only aggregated data. Similarly, the metal processing data available were primarily from welding/ brazing and cutting tasks, rather than basic metal production activities such as furnace operation.

Metal processing activities were assessed only using MEASE, as, in agreement with the relevant developers, none of the other tools were considered applicable. In relation to this dataset, the tool was observed to be of a medium level of conservatism (14% of measurements > tool estimates).

In comparison with this dataset, limited evidence of conservatism was found for STOFFENMANAGER and MEASE in relation to prediction of exposures to non-volatile liquids. For STOFFENMANAGER, 15% of the measurements exceeded the tool 90th percentile estimate, whilst for MEASE the tool exposure prediction was exceeded in 58% of cases.

Whilst acknowledging the limitations in the data set and methodologies as described before, it is felt that these results provide a good basis for identifying areas where tool performance may need to be improved. Consideration of the following areas may be of assistance in future tool development.

Although not incorporated as inputs for all of the evaluated tools, PROC codes were used to describe the tasks/ activities for the workplace situations used for comparison with the tool estimates. Differences were noted between the PROC codes for all of the tools, with variation also observed between exposure categories. The following PROC codes and exposure categories were associated with lower levels of conservatism, and so are worthy of further investigation.

- Exposures to volatile liquids for PROC 14 were generally underestimated by all of the tools. The ECETOC TRAv3 also produced less conservative estimates for industrial spray processes (PROC 7) for this exposure category, with the ECETOC TRAv2 more conservative but the percentage of measurements exceeding the corresponding estimates also relatively high.

- For handling of powders, some differences between PROC codes were observed for MEASE and STOFFENMANAGER, but not for ECETOC TRAv2, ECETOC TRAv3 and EMKG-EXPO-TOOL. All of the tools appeared less conservative for PROC 8a, which relates to less well controlled transfer processes, and with the exception of STOFFENMANAGER, PROC 14-associated powder handling exposures were also underestimated to a certain degree by the other tools.

- For non-volatile liquids, differences between PROC codes were observed for STOFFENMANAGER, with higher percentages of measurements exceeding the tool estimate for PROC 11 (non-industrial spraying). For MEASE, the tool appeared less conservative for PROC 13, although only a few comparator data (n=10) were available.

- There were also some differences observed between the numbers of measurements exceeding the tool estimates for the various PROC codes for metal processing (evaluated for MEASE only). Whilst around 30-40% of the measurements exceeded the tool estimate for PROCs 22 and 25, for PROC 23 the tool appeared to be very conservative with only 7% of the measured data greater than the corresponding prediction.

The numbers of data points available generally precluded further stratification of the analyses by PROC code in combination with other factors such as LEV, domain or dustiness. Some combinations did however include enough data to allow more detailed assessment of the impact of these factors together with PROC on the percentages of measurements exceeding the tool estimates, thus further clarifying those areas where the tools may be less conservative than expected.

The results from the stratification exercise were generally in accordance with those from the overall comparison. In general, for volatile liquids the tools were less conservative where LEV was present. Consideration should therefore be given to the assumptions made about control efficiencies within the tools- the results suggest that these may be overestimated in comparison with the actual effectiveness in the workplaces from which the measurement data originated.

The level of conservatism varied by PROC for powder handling with LEV: for example PROC 5 generated less conservative estimates where LEV was present compared with where it was absent, whilst for PROC 8b the converse was observed.

The observed impact of domain and LEV on the level of conservatism suggests that these two aspects of tool operation require review. In particular, the assumptions made in relation to domain regarding the initial base exposure estimates and the modifiers applied subsequently for LEV implementation should be re-evaluated.

Due to the limited availability of varied data types for non-volatile liquids and metal dusts or fumes, we cannot make any firm conclusions on the performance of the tools and further studies are required. However, the results suggest that the level of conservatism for these exposure categories may need to be improved.

In the second part of the comparison process, correlations between the estimates of exposure and the measured values for the different exposure categories and for the data types were determined. Differences in the level of correlation of the measurement data with the tool estimates were noted both between exposure categories and comparator data type.

The correlation between the tool estimates and measurement data was better for powders and non-volatile liquids, followed by volatile liquids then the other exposure categories. This suggests that the tools are better at predicting potential exposure in these categories compared with the metals-related situations. The predictive power of the tools could thus be further enhanced, for example by the inclusion and/ or revision of certain input parameters (e.g. concentration of the mixture for EMKG-EXPO-TOOL and effectiveness of control measures, all tools).

The above findings provide suggestions for areas which could be addressed by model developers to improve the tools so that they are appropriately conservative for all or the most important exposure situation types.

7.4 Operational Analysis: Evaluation of tool usability and reliability

To evaluate the user-friendliness of the tools, interviews and an online survey of tool users with a representative range of experience and backgrounds were carried out. It is clear from this evaluation that users perceive the tools to be easy to source, download and use in a satisfactory manner for the intended purpose. Survey respondents were positive about the help and guidance documentation available, and in general felt that the tools were appropriately conservative.

The findings of the Between User Reliability Exercise suggest that in practice, achieving consistency in tool inputs is more challenging than these reported user perceptions suggest. Significant variation in user inputs for a number of parameters was observed, in particular in relation to activity/ task; dustiness and risk management measures.

The BURE results suggest significant potential for inconsistency in the exposure estimates obtained by different Tier 1 tool users, which could impact on the effectiveness of the REACH processes for identifying and, ultimately controlling, health risks from hazardous substances. Implementation of additional support and quality control systems for all tool users could help to reduce between-assessor variation, thus ensuring the protection of worker health and avoidance of unnecessary business risk management expenditure.

7.5 Uncertainty of the Tier 1 exposure assessment tools

There is always some uncertainty in any exposure assessment. Although this uncertainty does not arise solely from the tool and its application, tool-related uncertainty should evidently not be neglected. Moreover, the type and level of uncertainty is always situation dependent. Each individual situation requires an assessment of whether the correct parameters have been assigned, the tool was used within its scope and the outputs have been interpreted appropriately. Maximising user knowledge of both the tool and the exposure situation being assessed will also reduce uncertainty.

Further tool developments and improvements should consider user friendliness implications, the ability of users to choose the correct input parameters and the level of detail and resolution that the tool provides. Proposed changes in the complexity of the tool structure should be carefully evaluated before they are implemented.

Where possible, any new tool parameters should be defined quantitatively, and the relevant quantitative reference data provided to the user. The uncertainty associated with the reference data, for example exposure measurements, should also be considered.

The definition of input parameters which have been shown by the BURE to be prone between user variability should be as precise as possible. These include the use categorisation for all tools, the intrinsic dustiness, the type of setting (i.e. professional vs industrial) and the definition of risk management measures.

8 Overall project recommendations

8.1 Introduction

The swift development and distribution of simple and conservative screening tools was necessary to facilitate the timely processing of the large numbers of exposure assessments required under REACH. In common with the REACH process itself, it has been recognised that the tools will require further and ongoing development and validation in the light of the experience gained during the initial registration processes.

From consideration of the results of all of the work packages, a number of very positive features of the exposure assessment tools have emerged. The tools are perceived to be easy to access, install, use and understand, and although the tools appear to underestimate exposure in some cases, they are generally conservative in their estimation of exposure.

No clear picture emerges regarding a “best” tool for a particular purpose, as all have a complex mix of scope, strengths and limitations. The results from the eteam Project evaluation exercises do however suggest a number of potential development areas which could maximise the efficiency, reliability and validity of use of all of the tools. In this section, we therefore look at the use of exposure assessment tools as a whole, rather on an individual tool basis.

These areas of potential improvement can be split into those which relate to

- the background information and guidance documents available to users,
- tool performance and degree of conservatism,
- user competency and associated support networks and
- quality control of exposure modelling processes

Suggestions for further development in relation to these topics are given below.

8.2 Provision of Background information and guidance documentation for tools

To use the tools most effectively for exposure assessment under REACH, or within a chemical risk management system, the user must identify, navigate and understand the relevant supporting information. It is clear that identification and operation of the correct tool or tools for the desired purpose will be made easier, more consistent and more representative of the exposure being assessed if this essential information is presented in a suitable, coherent and accessible format.

Within the context of REACH, a wide range of information is available to registrants regarding the registration process in general, and exposure assessment in particular. The REACH document “Guidance on information requirements and chemical safety assessment Chapter R.14: Occupational exposure (2012)” (ECHA, 2012) gives an overview of the methods that can be used for exposure assessment, for example the use of measurement data or exposure modelling. Guidance is also given on describing uses of substances, with reference to the use of PROC codes within ECHA document “Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system (2010)” (ECHA, 2010).

8.2.1 Guidance on applicability of tools

The evaluation of the conceptual basis of the tools, the between user reliability exercise and the external validation exercise have highlighted the importance of tools being used for their designed purpose, i.e. within their range of applicability. The initial stage of any exposure modelling task should be the identification of the appropriate tools; clarity and consistency about the domain of applicability of the tools within the REACH documentation is therefore essential.

Such clarity was not always observed: for example within Chapter R14, the non-applicability of the ECETOC TRAv2 to molten non-mineral solids is highlighted in one section, whilst in another the fugacity categories (taken from the tool) for PROCs 23-25 are given for metals. Also, Chapter R12 states that “with two exceptions only, all process categories listed in Appendix R.12-3 can be used as an input parameter to the ECETOC TRA tool to derive a Tier 1 exposure estimation for workers”, suggesting that the tool can be used for any of the non-excepted activity types. The exceptions are assumed to be PROC 26 and 27a/b, which are noted within Chapter R12 to have no corresponding entry in the ECETOC TRA. Within the ECETOC TRAv2 and v3 tools, the fugacity tables suggest that metal processes with temperature greater than the substance’s melting point may be assessed, however from direct communications with its developers, the non-applicability of the tool to hot metal fume-generating processes has been confirmed.

A similar issue was identified for the MEASE tool. The tool developers have confirmed that the tool should not be used for assessing exposure to volatile organic liquids or powdered organic materials, for example pharmaceuticals. The tool is described in Chapter R14 in the context of assessment of exposure to metals and inorganic substances; however there is nothing to indicate that it is unsuitable for organic vapour exposure estimation. Within the tool itself, it is possible to select parameters and generate exposure estimates for volatiles without triggering an error message, and the initial estimate look-up table provided in the MEASE documentation gives values for vapour exposure taken from the original ECETOC TRA tool (EBRC, 2014). The possibility of combining volatile organic materials with range of PROC codes is also given in the MEASE documentation, again perhaps suggesting to the user that this is an appropriate use of the tool. Similarly, the use of MEASE for powdered organic materials was also contraindicated by its developers, however no REACH guidance regarding this exclusion was identified.

Input parameters which are not within the applicability range of the tool should be removed, disabled or in some way flagged up as inappropriate.

The EMKG-EXPO-TOOL is available via a link from Chapter R14, and the tool homepage includes information on its applicability domain, for example non-applicability to open spray processes. Chapter R14 also directs the reader to a table of Control Guidance Sheets from the UK Health and Safety Executive (HSE) COSHH Essentials tool for further information on the work activities and risk management measures. The table includes, for example, spray processes, which have been confirmed by the EMKG-EXPO-TOOL developer to be outside of the tool's scope. Following the link in Chapter R14 to the German language version of the control guidance sheets takes the user to a list of available information, which does not include spray processes. It is therefore possible that the tool could be used for a non-applicable process and that users in different countries are operating the tool differently for the same activity. Both of these will increase variation between users and decrease consistency within REACH.

Using these three tools as examples, it is felt that a consistency review of the relevant REACH, and related tool, guidance to remove contradictory information and improve clarity about the ranges of applicability would help prevent accidental misuse of the tools outside of their correct scope and reduce associated between user variation. Within this project, an applicability matrix was developed and presented in the Appendix of Deliverable D4 (Gathering of background information and conceptual evaluation). This matrix could be used to quickly identify the tools that can be used for a specific scenario.

8.2.2 Accessibility of background information

It would also be helpful for users if all of the relevant documentation were available either within the tool itself or via accessible links within the tool to supplementary references. In addition, information should be clearly signposted and provided in a summarised and user-friendly manner, for example essential information should be collated within one document, rather than split between several sources. This is particularly important for information relating to the applicability of the tool to the process and/ or physical form.

With the exception of the User Guide for the ECETOC TRAv3, which covers installation and inputting of parameters, we did not identify any readily accessible comparable step-by-step guides for carrying out assessments using the tools within the tool guidance. It is felt that the preparation of simple guides to tool use, which could be based on the existing and helpful pop-ups, comments and information boxes within the input screens, would assist users to operate tools effectively. These could incorporate information on applicability and parameter choice guidance together with information on the basic software operation of the tool. At present, the requirement for users to intentionally click on an information tag or comment box within the tools or to access separate external reports to get essential guidance increases the likelihood that important material might be missed.

Presentation of all of the relevant essential information in a clear format would facilitate user comparison of all of the different input options available and so their potential impact on the estimate. The inclusion of example assessments for a representative number of process/ activity types would also be of benefit in clarifying the process and reinforcing the range of applicability of the tools.

8.2.3 Guidance on input parameters

We recognise that the tools are by nature generic and thus must cover a wide range of potential exposure situations. However, the provision of additional detail on the tool-specific input options for more subjective parameters would be of great assistance. For example, the inclusion of sufficient exemplar tasks to illustrate the meaning of a PROC code, or providing a suitable range of comparator substances to help users to assign dustiness.

From the between user reliability exercise, it was clear that some specific inputs were more challenging for participant to interpret than others, for example PROC code, setting/ domain and dustiness. Feedback from focus group and BURE participants indicated that they did not find the existing guidance regarding the choice of the most appropriate PROC to be adequate, for example in relation to describing ancillary activities such as maintenance, sampling and cleaning.

From observation of the guidance in Chapter R12, there is more detail supplied on non-occupational exposure use descriptors, for example Environmental Release Categories. Whilst it is appreciated that the provision of such specific examples might be challenging in terms of describing occupational exposures in a relevant manner across all industry sectors, the supply of more detail in the REACH guidance documents on common processes may be very beneficial to exposure assessors whether using tools and/ or measurement data in the registration process.

The results from the BURE suggest that tool users may find differentiation between similar PROCs challenging, for example between PROCs 8a, 8b and 9. In addition, a user’s requirements in relation to tool use for a particular situation may vary, for example a very conservative estimate may be required in some instances. In such situations, it would be of benefit to users to be able to know with more certainty how the tool estimates are potentially impacted by the chosen options. Anecdotally, and from feedback obtained in WP I.6, this kind of informal sensitivity analysis is common practice, and indeed is the basis of the iteration process used to produce the REACH exposure assessment.
Although there is some information available to users within the tool descriptions, and for example in the tables of look- up values within some tools, the grouping of similar PROC codes or handling descriptions would assist users in identifying more or less conservative options to suit their purpose. Such grouping and clear description of possible alternatives would allow users to try the various options with more certainty about their impact, i.e. to carry out a more informed sensitivity analysis. It would also therefore help significantly with the scaling process carried out by downstream users when comparing their use with the supplier’s exposure scenario.

At present there is a basic list of PROCs provided, which are roughly grouped into activity types, for example manufacture/ formulation type processes, transfer processes and spraying processes. Providing a more defined hierarchy of PROC codes may assist tool users in selecting a more or less conservative option to suit their purpose, and also help reduce between user variation.

The allocation of a professional or industrial domain to a situation was also problematic for some participants in the BURE and focus group. We could not find detailed systematic information on how the domain should be allocated. However; the guidance suggests that where there is uncertainty about the domain, a conservative approach is to assume a professional, and therefore less well controlled, setting. Additional REACH guidance on a systematic method of allocating domain would perhaps be helpful in avoiding both overly conservative and under-estimation of exposure.

Users reported that they were generally satisfied about the layout of the tool entry screens; however some participants identified that input masks could be made clearer, through the use of a simpler and less complex design. To maximise the effectiveness of all of the above suggestions regarding in-tool information provision, any tool updates should adhere to current best practice in terms of user-software interfaces, in particular in relation to simplicity, clarity and accessibility issues such as font size, colour and contrast.

8.3 Tool performance and degree of conservatism

From comparison with the eteam Project dataset, variation was noted between and within tools in relation to the degree of conservatism. There were a number of aspects of the tools which were associated with less conservative estimates and some suggestions are made below regarding the following main areas of development: risk management measure assumptions; domain and PROC code/ activity descriptor.

8.3.1 Risk management measures

The tools make varying assumptions relating to the effectiveness of risk management measures, and in particular controls at source such as LEV. From our results, it appears that the actual effectiveness may be less than that assumed by the tools. The tools are being used to specify risk management measures in the context of REACH exposure assessments, thus the assumptions made by the tools regarding LEV effectiveness may be theoretically possible. To achieve these levels of control, additional information on the design and specification of control measures is necessary. With the exception of the EMKG-EXPO-TOOL, which refers the user to control guidance sheets giving detail on system type and design, none of the other tools provide explanations of possible control options. Many of the simple descriptions given, for example “LEV”, are likely to be difficult to implement, particularly for downstream users of the substances, who are perhaps less knowledgeable about the pros and cons of different designs. The inclusion of additional information, akin to that provided by the EMKG-EXPO-TOOL may assist users in identifying best practice for the design and implementation of new systems and allow comparison with existing risk management measures that may require upgrades. Although covered by chemical risk management legislation, it may also be helpful for the tools to include a reminder that control measures must be maintained and tested to ensure their continued effectiveness.

When using the tools for chemical risk management exposure assessments, users should take into account the underlying assumptions about control effectiveness when interpreting the tool outputs in relation to their own workplaces. The inclusion of additional detail mentioned above regarding design and specifications may be of assistance.

For some exposure categories, for example powders, many of the tools were less conservative in exposure situations where LEV/ localised controls were not present. This suggests that in some cases the initial estimates may not be representative of the full range of workplace exposures. Additional calibration or similar refinement of the tool estimates in these circumstances followed by re-validation could therefore be carried out to align the predictions more closely with actual exposures. Differences in the level of conservatism was also noted for dustiness, however the dataset did not include large numbers of substances of high or low dustiness. As such, further calibrations and revalidations should include as wide a range of intrinsic dustiness as possible.

8.3.2 Domain

For those tools which categorise uses as professional/ public or industrial, our results suggest that tools provide less and in some cases insufficiently conservative exposure estimates in industrial settings. The tool-inherent assumptions regarding higher general levels of risk management and their effectiveness for these settings may be overestimated. The differences in domain-specific base exposure estimates, and indeed in relation to control effectiveness, should therefore be revisited. Further calibration and validation activities should thus include both setting types.

8.3.3 PROC code/ activity

Differences were noted for the tools in relation to the level of conservatism for particular process/ activity types. These were summarised for all of the tools using PROC code: PROC 14, PROC 11 and PROC 8a, relating to tabletting/ compression/ extrusion/ pelletisation processes (volatile liquids and powders), non-industrial spraying activities (non-volatile liquids) and transfer of materials at non-dedicated facilities (powders). In addition to the general calibration and re-validation processes mentioned above, there may also be some potential benefit from review of these process types.

When implementing further tool developments, it should also be borne in mind that whilst exposures in EU countries have been decreasing for many substances over time, this pattern may not continue when new countries join the EU. As the exposures may be higher in such circumstances, the estimation processes and level of conservatism associated with the tools may require future review.

8.4 Reliability of tool estimates/ quality assurance

Generating valid and consistent estimates of exposure evidently relies not only on the tools themselves, but also on the manner in which they are used. REACH document Chapter R12 notes that a sufficient level of occupational hygiene expertise is required for the identification of the most suitable PROC for a particular application. There is therefore a responsibility on tool users to make sure that they are competent and able for this task.

Contrastingly, and interestingly, in ECHA document “Guidance for downstream users Version 2.0 (December 2013)”, the use of Tier 1 and higher tier exposure assessment tools for scaling by downstream users is suggested, but with the caveat that the tools should be reliable for non-expert use. We have shown that reliability of the tools when used by a range of expert and non-expert users is limited, thus between-user variation for the proposed tool-based scaling method is likely to be similar in magnitude, even with support from suppliers.

In modelling exposure for a particular work activity, an assessor has to interpret and translate what they know about the situation into the required tool parameters. To describe the exposure effectively, the same range of determinants has to be considered, whether this done explicitly within a tool by the inclusion of more parameters and/ or more options within each of these parameters, or less obviously by the user supplementing any gaps using their prior knowledge or experience. A degree of subjectivity will always therefore be present in any assessment process, thus the identification of potential methods of minimising the impact of this subjectivity on the validity and reliability of the resultant exposure estimates are of interest and importance.

When carrying out measurements of exposure in workplaces, great emphasis is placed on the competence of the person doing the task, with basic training in occupational hygiene generally being highly desirable. At present there is no similar requirement for users to undertake formal training in the operation of the assessment tools or interpretation of the resultant estimates. As these modelled estimates are then used in place of workplace measurements, this approach seems somewhat contradictory.

With the exception of STOFFENMANAGER which requires user registration, the tools are freely available to download as Microsoft Excel files either directly, or in the case of the ECETOC TRAv2 and ECETOC TRAv3, by following a link sent by the tool developer.

The tools are then ready to operate, without any formal online or in person training being provided. We have shown that large between user differences can occur. For inexperienced exposure assessors in particular, who may have no mental benchmark about the veracity of their estimate, the current approach makes it difficult to gauge how competent their assessments are.

Regardless of experience and prior knowledge of the tools, it is felt that all users could benefit from a more structured approach to the use of exposure assessment modelling tools. This approach should be described within a Good Exposure Modelling Practice guidance document.

The processes for collecting and using the required information are common to many of the Tier 1 and higher Tier tools. Whilst there is guidance in Chapter R14 regarding the exposure assessment process under REACH, there is no generalised procedure for carrying out assessments using tools for REACH or other purposes. The development of a good exposure modelling practice document would be of benefit in improving estimate validity and reducing between and within user variation.

This best practice document could cover in general terms the essential steps of carrying out an exposure assessment using tools, i.e. scope, required essential contextual information, level of detail, interpretation of results, reporting of outputs and quality control. This would be similar to current documentation relating to the use of occupational hygiene sampling equipment.

Furthermore, the following recommendations should also be considered.

8.4.1 Certification of tool users

Where the outputs of exposure assessments are being used in a regulatory context, for example under REACH or the Chemical Agents Directive, the restriction of tool use to trained and certified assessors should be considered. Suggested topics for accredited training courses could include:

- the good exposure modelling practice document for tool users
- the guidance from Chapter R14 on the basic information needed to carry out a suitable assessment, (for example a description of the activity, substance characteristics, risk management measures and general environment)
- background information on the tools, limitations and between tool differences
- the exact procedure for operating specific tools
- generation and interpretation of tool outputs in REACH and other contexts
- requirements for maintenance of assessor performance.

8.4.2 User support networks

Within the context of REACH, communications from Advisory Board colleagues have indicated that within industry, the tools are used in a support framework including Use Maps and generic exposure scenarios. These management systems allow an assessor to contextualise, synchronise and standardise their estimate within their industry sector and so should reduce between user variation. However, we do not have information on how widespread this approach is amongst REACH actors within smaller industry sectors and in particular amongst downstream users.

For all of the tools, it would seem prudent to replicate and extend this approach, for example by developing sector specific guidance to support accredited tool users in carrying out assessments. This would be of particular benefit to smaller organisations where assessments may be less frequently carried out, by less experienced personnel and in isolation from other exposure assessors with which to compare their estimates. It would also benefit consultancy organisations working on behalf of smaller enterprises, who may be working in unfamiliar sectors.

Two of the tools, STOFFENMANAGER and EMKG-EXPO-TOOL were developed from control banding systems, designed to help small and medium enterprises to assess and manage risks from hazardous substances. Discussions with the Advisory Board suggest that these tools may still be more commonly used for this purpose rather than for REACH. Some of this user-support network may already be in place via other chemical risk management initiatives, however the further development of additional sector-specific guidance and support for tool users may help to minimise between user variation and improve estimate validity.

8.4.3 Parallel use of tools and measurement data

In the absence of a completed validation process for the existing exposure assessment tools, REACH document Chapter 14 recommends that users compare the results of modelled estimates from one tool with other applicable tools and/ or measurement data. The document notes that this will reduce the uncertainty in the risk assessment process. It could be beneficial to apply several tools as it will often not be feasible to establish the most appropriate or best model for a certain exposure situation. To facilitate the use of different tools and to ensure that this is done consistently, a Use Map was developed as part of the project. This Use Map suggests for a certain set of scenario descriptors the most appropriate model parameters for the various tools.

It is not known how often measurement data have been used in preference or conjunction with modelled estimates for previous REACH exposure assessments. The use of even limited amounts of data as a comparator, i.e. where numbers are not sufficient to utilise on a standalone basis, may help users to determine the legitimacy of their modelled assessments.

8.4.4 Team assessment

During the BURE, subjective assessment of situations was required, with each participant using their own knowledge of exposure and skill level in operating the tool to generate an estimate. For some of the parameters, there may be more than one viable option, and it has been shown that the participants varied significantly in their opinion as to which was the best fit.

Previous studies have noted that the use of more than one assessor can increase the validity of subjective assessments compared with an identified standard. As noted by others (Schinkel et al., 2013; Semple et al. 2001; Kunac et al., 2006), it is felt that the use of a consensus/ team approach may be helpful. Tool input parameters could be generated separately by a small team of accredited assessors and any discrepancies discussed. This process need not take place for every assessment, however might be done as a regular in-house or sector-driven quality control check on assessor performance and development.

In addition to genuine variation caused by differences between users in their choice parameters for particular exposure determinants, a proportion of the variability observed related to simple errors in interpretation of the descriptive information supplied, for example the inclusion of LEV when none was present. Errors of this type would also be minimised by the use of a team approach.

8.4.5 Quality control

Successful completion of the above training would demonstrate an initial level of competence in tool operation. Once accreditation was achieved, on-going maintenance of competence and skills would be required. Other assessment methods require participation in quality control schemes, for example the round-robin exchange schemes for fibre counting and chemical analyses. Exposure assessors could participate in regular assessments of different types of situations, which would be compared with a gold standard assessment and between participants. Over time, the feedback that participants receive would allow them to improve and standardise their assessment performance, thus minimising between user variation.

Once submitted to ECHA under REACH, there is a legal requirement for at least 5% of substance dossiers to be checked either on a random or targeted basis (ECHA, 2014). This check may result in no action being taken; follow up with a quality observation letter or a request for further information. The choice of approach will depend on the issues identified. This stage of the REACH process would seem to provide a convenient additional opportunity to assess consistency of the application and outputs of the exposure assessment tools used for estimation within the CSR.

In the light of the results of the eteam project, there are a number of opportunities to improve the existing tools in terms of the guidance, presentation, operation and quality assurance of user outputs. Implementation of the suggested improvements could help to increase the validity of tool exposure predictions and reduce inappropriate and inconsistent application of the tools, thus ensuring the protection of worker health and avoidance of unnecessary business risk management expenditure.

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