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

Substudy Report on External Validation Exercise

J. Lamb, B. G. Miller, L. MacCalman, S. Rashid, M. van Tongeren

baua:
Bundesanstalt für Arbeitsschutz
und Arbeitsmedizin

Research
Project F 2303

J. Lamb
B. G. Miller
L. MacCalman
S. Rashid
M. van Tongeren

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

Substudy Report on External Validation Exercise

Dortmund/Berlin/Dresden 2015

This publication is a substudy report resulting from the work package D16 of the project “Evaluation of the Tier 1 Exposure Assessment Models used under REACH (eteam) Project” on behalf of the Federal Institute for Occupational Safety and Health.
The responsibility for the contents of this publication lies with the authors.

Authors: Judith Lamb MSc
Dr. Brian G. Miller
Dr. Laura MacCalman
Shahzad Rashid
Dr. Martie van Tongeren
Centre for Human Exposure Science (CHES),
Institute of Occupational Medicine, Avenue North
Heriot Watt Research Park, Riccarton, Edinburgh,
United Kingdom, EH14 4AP

Cover figure: ritajaco/JanPietruszka/MoreISO/Mikefahl/mediaphotos/
ImageegamI/FotoSpeedy
(all) iStock

Cover design: Susanne Graul
Federal Institute for Occupational Safety and Health

Publisher: Federal Institute for Occupational Safety and Health
Friedrich-Henkel-Weg 1-25, D-44149 Dortmund
Postal address: P.O.Box 17 02 02, D-44061 Dortmund
Telephone +49 231 9071-2071
Fax +49 231 9071-2070
Email: info-zentrum@baua.bund.de
Internet: www.baua.de

Berlin:
Nöldnerstr. 40-42, D-10317 Berlin
Telephone +49 30 51548-0
Fax +49 30 51548-4170

Dresden:
Fabricestr. 8, D-01099 Dresden
Telephone +49 351 5639-50
Fax +49 351 5639-5210

www.baua.de/dok/6914122

ISBN 978-3-88261-157-1

Contents

Substudy Report on External Validation Exercise

Abstract

Tier 1 assessment tools are used frequently to provide exposure estimates as part of the substance registration process under Regulation (EC) No 1907/2006 (REACH). Using only a limited number of basic input parameters, these generic tools are designed to provide conservative exposure predictions for a wide range of exposure scenarios. This study aimed to validate tools recommended for use in REACH through comparison with inhalation and dermal exposure measurement data from a variety of sources. Restrictions on the type and sampling methods for the dermal data collected prevented their use in the validation, thus only inhalation exposure was addressed. Individual and summarised aggregated personal exposure measurements and associated contextual descriptions were obtained from several European providers and one US source. Exposure scientists from the Institute of Occupational Medicine coded the exposure scenario information using the parameter for each tool and exposure estimates were generated according to these inputs. A number of comparisons were carried out to examine the level of conservatism, including determination of the proportion of measurement values which exceeded the tool estimations and calculation of the ratio of the measurement value to the tool estimate. “High”, “medium” and “low” levels of conservatism were defined as where ≤10%; 11≤25% and >25% of the measurements exceeded the tool estimate, respectively. The impacts of various tool-implemented exposure determinants on the percentage of exceedances were investigated.

The Results suggested that across all of the physical forms and emission generation processes (collectively “exposure categories”), the tools appeared to be conservative, but with varying levels of conservatism observed. The tools appeared least conservative when estimating exposures during activities involving non-volatile liquids, which were evaluated only for the MEASE and STOFFENMANAGER tools and metal abrasion (ECETOC TRAv2 and v3 tools). The EMKG-EXPO-TOOL appeared to be sufficiently conservative for volatile liquids but less conservative for powders than the other tools. Differences in the level of conservatism for all of the tools were observed between data providers, PROC codes, domain, and the presence/ absence of local exhaust ventilation (LEV). 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 regarding the initial domain-specific estimates and the modifiers applied for LEV implementation should be re-evaluated. Correlations between the measurement results and tool predictions were generally stronger for powders and non-volatile liquids than for the other exposure categories. The comparator dataset was limited in some respects: relatively few comparator measurements were available for exposure to non-volatile liquids, metal dust and metal fume. The study results provide useful information both for tool developers and for users, particularly in terms of applications where the tools should perhaps be used with extra caution.

Key words:
exposure assessment; exposure modelling; validation; REACH; risk assessment

Teilbericht zur externen Validierung

Kurzreferat

Im Rahmen der Registrierung von Stoffen unter REACH werden Tier 1-Tools häufig zur Abschätzung der Exposition am Arbeitsplatz eingesetzt. Diese generischen Tools sollen mit einer begrenzten Anzahl an grundlegenden Eingabeparametern eine konservative Expositionsvorhersage für einen weiten Bereich an Expositionsszenarien ermöglichen. Die Studie zielte ursprünglich darauf ab, diese Tools, durch einen Vergleich mit inhalativen und dermalen Expositionsmessungen aus unabhängigen Datenquellen zu validieren. Auf Grund von Beschränkungen bezüglich Typ und Messtechnik der gesammelten dermalen Daten konnten diese in der Validierung nicht verwendet werden, daher wurde nur die inhalative Exposition adressiert. Individuelle und aggregierte personenbezogene Messdaten und entsprechende kontextuelle Situationsbeschreibungen wurden von verschiedenen europäischen Datenlieferanten und einer Quelle aus den USA gesammelt, in die Modellparameter kodiert und anschließend Modellberechnungen durchgeführt. Die Berechnungen wurden als in „hohem“, „mittlerem“ und „geringem“ Maße konservativ definiert, wenn Anteile von ≤10%; 11≤25% oder >25% der Messungen die Modellabschätzung überstiegen. Ziel war es, die Auswirkungen von verschiedenen in den Tools implementierten Expositionsparametern auf den Anteil der Überschreitungen zu untersuchen.
Die Ergebnisse zeigen, dass über alle Aggregatszustände und Prozesse (zusammenfassend „Expositionskategorien“) hinweg, der erreichte Grad an Konservatismus unterschiedlich ausgeprägt war. Am wenigsten konservativ erschienen die Tools bei Tätigkeiten mit nicht-flüchtigen Flüssigkeiten (nur für MEASE und STOFFENMANAGER evaluiert), sowie für Schleifprozesse mit Metallen (ECETOC TRA v.2 und v3). Das EMKG-EXPO-TOOL erschien ausreichend konservativ für flüchtige Flüssigkeiten, allerdings weniger konservativ für Stäube. In Bezug auf den ermittelten Grad an Konservatismus sind Unterschiede zwischen Datenlieferanten, PROCs, Arbeitsgebiet (industriell vs. professionell) und der An- oder Abwesenheit einer technischen Absaugung zu beobachten. Die Ergebnisse legen nahe, dass die Modellparameter „Arbeitsgebiet“ und „Lüftung“ einer Überarbeitung bedürfen. Dies gilt auch für arbeitsbereichs-spezifische Expositionsabschätzungen sowie die Modifikatoren zur technischen Absaugung. Die Korrelation zwischen den gemessenen Werten und Toolabschätzungen war für Stäube und nicht-flüchtige Flüssigkeiten generell stärker im Vergleich zu anderen Expositionskategorien.
Der Vergleichsdatensatz war in manchen Bereichen limitiert: Verhältnismäßig wenige Vergleichsmessungen waren für die Exposition zu nicht-flüchtigen Flüssigkeiten, Metallstäuben und Metallrauch verfügbar. Die Studie gibt sowohl Softwareentwicklern als auch für Anwendern nützliche Informationen, insbesondere in Bezug auf Aufgaben, bei denen die Tools nur mit Vorsicht verwendet werden sollten.

Schlagwörter:
Expositionsabschätzung; Expositionsmodellierung; Validierung; REACH; Risikoabschätzung

1 Introduction

The Institute of Occupational Medicine (IOM) and the Fraunhofer Institute for Toxicological and Experimental Medicine (ITEM) were contracted by the Bundesanstalt für Arbeitsschutz und Arbeitsmedizin (BAuA) to evaluate several generic Tier 1 exposure assessment tools recommended in the European Chemicals Agency (ECHA) document "*Guidance on information requirements and chemical safety assessment. Chapter R.14: Occupational exposure estimation*" as being suitable for chemical safety assessments (ECETOC TRAv2, ECETOC TRAv3, EMKG-EXPO-TOOL, MEASE v1.02.01, STOFFENMANAGER vs 4.5, and RISKOFDERM). This is known as the eteam project.

These 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.

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. Tischer et al proposed that a comprehensive validation exercise would also include an "operational analysis" to evaluate uncertainty arising from the application of the tool by different users, i.e. the tool's reliability.

A general paucity of model 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, which are summarised below.

The majority of these studies considered control banding tools, for example the UK Health and Safety Executive (HSE) COSHH Essentials toolkit, both in respect of its predictive ability and ease of use. The EMKG-EXPO-TOOL is based largely on COSHH Essentials, and is similarly supported by a set of Control Guidance Sheets for a range of processes. It is therefore appropriate and useful to consider these previous validations of the COSHH Essentials tool as also being relevant to the EMKG-EXPO-TOOL.

Lee et al (2009) evaluated COSHH Essentials for short-term and full-shift exposures in a printing plant. Measurements of isopropanol (n=188) and acetone (n=187) were collected and time-weighted average concentrations were evaluated for methylene chloride. Although overall the estimates were felt to be in accordance with the measured values, for some situations the probability of underestimation of exposure was >10%. Lee et al (2011) also carried out a comparison of the COSHH Essentials tool endpoints for exposure to a mixture of organic solvents whilst batch-making and bucket-washing in a paint manufacturing plant. The study used a variety of methods to compare the tool predictions with measured data from shift-long tasks. These included a comparison of a predicted probability distribution of the exposure with the ranges given in the tool for the task, under the various potential control approaches. The control recommendations from COSHH Essentials were also compared with controls recommended by experts on the basis of the measurement data collected and the relevant regulatory compliance standards. Lee et al (2009) found that the tool underestimated exposures to acetone, methyl ethyl ketone and xylene for bucket washing tasks where work was carried out in accordance with the relevant COSHH Essentials control guidance sheets.

In their evaluation of COSHH Essentials, Tischer et al (2003) compared the exposure ranges predicted by the tool with workplace measurement data from BAuA field studies, chemical industry risk assessments for existing substances and criteria documents used in the setting of occupational exposure limits. This evaluation included an assessment of the internal validation of the conceptual basis of the tool, i.e. the theoretical structure of the tool in terms of plausibility of the assumptions and agreement with established theories. In general, Tischer et al (2003) found that the predicted exposures were in accordance with the measurement data, or were conservative. However, for small scale handling of solvents, the estimates were in a number of cases lower than the relevant measurements, particularly where the task involved dispersion, e.g. spraying of glues or paints. The need for a comprehensive validation of exposure assessment tools using a larger and more comprehensive external dataset was identified.

Jones and Nicas (2006) compared the COSHH Essentials endpoints with measurement data for bag filling and vapour degreasing activities, and identified two types of errors. These were “over-controlled” errors, where the measured exposure was less than the upper value of the exposure band in the absence of the recommended control option, and “under-controlled” errors, where the measured exposure is greater than the upper limit of the predicted range, when the recommended controls were in place.

In an evaluation of the suitability of exposure assessment tools for use in Swiss workplaces, Kindler and Winteler (2010) found that the EMKG-EXPO-TOOL underestimated exposure during handling of powder and volatile liquids, where local exhaust ventilation (LEV) was used. The underestimation was attributed to the tool’s overestimation of the actual LEV efficiency, although the authors recognised the limited scope and size of the comparator data set. The study also considered the validity of the EASE tool (that is somewhat similar to the ECETOC TRA tools), which again was found to assume a higher efficiency for LEV than was achieved in practice.

Schinkel et al (2010) carried out a cross validation of the Stoffenmanager tool and used their results to refine the underlying model algorithms. The study found that the tool underestimated exposures where bulk transfers of material were being carried out and overestimated exposure in situations where small amounts of products were handled.

Koppisch et al (2011) carried out a validation of Stoffenmanager using exposure data for handling of powders/granules and machining of wood, stone and asphalt from the

German MEGA exposure database. The tool was found to underestimate exposure in a small number of scenarios relating to mixing activities ‘with LEV’ or ‘with full enclosure and LEV’ and the filling/ dumping of materials without the presence of LEV. The study found that over the whole data set, the measured values were higher than the 90th percentile of the Stoffenmanager estimates in 11% of powder/ granule handling cases and 7% of machining activity cases. The authors therefore considered the tool to be appropriately conservative for use in risk assessments under REACH.

A comparison of ECETOC TRAv2 estimates with workplace exposure data from solvent processes was carried out by Kupczewska-Dobecka et al (2011). The study compared the median of exposure measurements for acetone, ethyl acetate, toluene from a limited range of industrial sectors (shoe manufacture, refinery tasks and paint/ lacquer production) with the corresponding estimates generated by the ECETOC TRAv2. The study was ambiguous in its conclusions about the overall level of conservatism. The authors suggested that the estimates generated by the ECETOC TRAv2 would be suitable if an alternative PROC code (PROC 7 industrial spraying) was chosen in preference to the one used (PROC 10- application by roller or brush), and if the lower end of the predicted range assumed the presence of local exhaust ventilation (LEV), and the higher range that LEV was not used. They did not present any evidence that this substituted “better fit” PROC code was relevant to the gluing task described.

Hofstetter et al (2012) carried out a comparison of ECETOC TRAv2 estimates with measurement data from a limited number of simulated spray painting tasks. The study also compared mean 8-hour time weighted average measurement results and ECETOC TRAv2 predicted exposures with the estimates from the Advanced REACH Tool (ART) and another model. The authors found that, in comparison with the mean calculated 8-hour time weighted average exposures, all of the tools overestimated the exposure level, with the Tier 1 ECETOC TRAv2 tool being most conservative. The study was undertaken in a laboratory under controlled conditions, where environmental and operational conditions were regulated during a specific task, therefore application of its results to everyday exposure situations must be treated with caution.

The results from the above 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 REACH Tier 1 exposure assessment tools carried out across different agents and covering their ranges of applicability.

Work Package 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. The workplace data supplied included individual measurements (with one or more data points associated with a particular situation), and aggregated data which included statistical summaries of multiple measurements.

This report describes the methods used for generation of the relevant associated tool estimates for comparison with the workplace measurements and the external validation process. An evaluation of the comprehensive nature of the measurement data used for the external validation is presented, along with an assessment of the degree of conservatism achieved by the tools.

2 Methodology

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 v1.02.01 (referred to as MEASE in this report)
- STOFFENMANAGER® v4.5 (referred to as STOFFENMANAGER in this report)

To carry out the evaluation, a relational Microsoft Access database was developed, which included modules that contained information on:

i) contextual information on the exposure situations in which individual measurements were obtained or to which aggregated data were assigned;
ii) measurement results from related exposure situations;
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.

These exposure estimates obtained from the tools were subsequently compared with the corresponding measurement data for the specific situation. The development of the database, generation of tool estimates and comparison methods are described in detail below.

2.2 Formation of the database

2.2.1 Criteria for inclusion/exclusion of data

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 prepared (eteam Project Deliverable D7- evaluation of data sources (inhalation and dermal data)). 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.

General aspects of the data rationalisation/ consolidation process are described below, together with data provider-specific issues.

Providers were asked to submit their data using a Microsoft Excel-based data collection template this had been developed by the project team to allow the required inhalation or 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 (Appendix 1).

2.2.1.1 General Criteria for Data Selection

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

i) Common PROC codes/ handling categories

During the conceptual evaluation phase of the project, a number of PROC codes (PROCs 3, 4, 5, 7, 8a, 8b, 9, 10, 11, 13, 14 and 15) and equivalent 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 recognised that there were specific aspects of some tools which required evaluation outside of this list of common PROCs, for example estimation of exposure to fumes from hot metal processes, and dust from handling inorganic substances and the mechanical treatment of metals using MEASE (PROCs 22, 23, 24, 25, 26, 27a, 27b). Suitable data from several providers were therefore included accordingly.

ii) Physical form of substances

It was 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 recently 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.

iii) 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.
- 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. Data where mixture composition was not clearly stated were included at this stage pending subsequent collection of additional product information from manufacturers and other sources.

iv) Sample Type

The Tier 1 assessment tools provide estimates of personal exposure to substances. 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.

v) Purpose of Sampling

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

vi) 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.

2.2.1.2 Provider-specific Data Selection Criteria

i) Provider A

Prior to submission of the data to the eteam Project, initial selection of relevant exposure situations had been carried out by Provider A, whereby the majority of REACH-irrelevant substances and measurements of the respirable fraction of dusts were excluded. Within this dataset, further screening out of non-REACH relevant substances was then made by the eteam Project team, for example inhalable dust from wood, cement and polymer activities.

Situations with multiple measurements of organic solvents had also been pre-selected by the provider according to the same criteria described in Section 2.2.1.1.

Further selection of relevant situations (n=750) for the eteam Project was carried out by comparison with the list of common PROC codes. However, many of these exposure situations were not distinct as they covered the same activity, workplace and risk management measures. Hence, these were consolidated into a final set of discrete situations (n=158), with the associated measurement(s).

ii) Provider B

Contextual information and associated measurement data were submitted by Provider B using the Microsoft Excel inhalation data collection template. Some manual re-formatting of the spreadsheets was required to separate out different exposure situations and measurements prior to transfer into the database. Selection of the situations to be used for the external validation was then made using the process below.

A selection from an initial list of 853 records was made on the basis of REACH–relevance of the analyte; where a specific individual substance was not identified, the situation was excluded. Measurements of the respirable dust fraction were excluded as were measurements of sulphuric and hydrochloric acid mists as these were not covered by the tools being evaluated. Table 2.1 provides a list of substances that were excluded using the above criteria.

Initial PROC codes that were allocated by the provider were used to identify those situations with a PROC code that is common to all of the tools. Situations relating to the processing of metals were also included to allow evaluation of the MEASE tool. The remaining situations were then examined to identify where there were multiple analytes for the same sample, and a choice made from these as described previously.

The workplace data supplied included both individual measurements ($n \geq 1$) associated with a particular situation, and aggregated data for multiple workers within a situation (designated as Type 1 aggregated data). A total of 113 situations from this provider were included in the validation.

Table 2.1 List of substances excluded from the Provider B dataset

Substance	Basis for exclusion
Aromatic naphtha	individual substance not identifiable
Benzene solubles	individual substance not identifiable
Hydrocarbons	individual substance not identifiable
Inhalable dust	not REACH-relevant
Naphthas	individual substance not identifiable
Oil mist	mist- physical form not covered by tools
Total amines	individual substance not identifiable
Total dust (e.g. soy flake processing)	individual substance not identifiable/
Total fluorides	individual substance not identifiable
Total hexanes	individual substance not identifiable
Total hydrocarbons	individual substance not identifiable
Total isocyanates	individual substance not identifiable
Total nitrosamines (from rubber processing)	not REACH-relevant
Total paint mist	mist- physical form not covered by tools
Total particulates	individual substance not identifiable
Total VOCs	individual substance not identifiable
Respirable dust	respirable fraction not covered as a separate fraction by tools
Respirable particulates	respirable fraction not covered as a separate fraction by tools
Total Respirable dust	respirable fraction not covered as a separate fraction by tools
Sulphuric acid mist	mist- physical form not covered by tools
Hydrochloric acid mist	mist- physical form not covered by tools

iii) Provider C

Provider C supplied data as extracts from a database, in the form of coded contextual information (for example for risk management measures, product type, job title), and free text entries describing machine type and work area, which could be used as proxies for task descriptions. For reasons of confidentiality, the measurement data associated with the descriptions could not be provided contemporaneously.

An initial batch of Provider C data (around 350 data points) relating to exposure to process-generated and other dusts was supplied. The contextual information for these measurement data were translated by the project team into English.

Data relating to agents that were not REACH relevant were in the main excluded from this batch, for example those which related to exposure to soot during chimney cleaning tasks. A limited number of situations relating to “inhalable dust” which could be allocated easily to a particular substance were included. Further selection was then made on the basis of the named task being included in the list of common PROCs that are covered by all of the tools, resulting in a final subset that included 123 situations. The provider supplied product and activity/ risk management descriptions on separate Excel spreadsheets, which were merged prior to mapping of the Provider C variables to the eteam database variables and incorporation into the overall dataset.

A second batch of Provider C data (~ 11,000 data points) was supplied and required similar translation, sorting and formatting. Within these data, the process outlined above was initially carried out to select the situations for the external validation. Table 2.2 provides a list of substances that were excluded as the substance was a by-product of pyrolysis (e.g. polyaromatic hydrocarbons in soot) or the physical form was not covered by most of the tools (mists).

Table 2.2 Substances excluded from Provider C

Substance	Basis for exclusion
Acenaphthene	not REACH-relevant (pyrolysis product)
Acenaphthylene	not REACH-relevant (pyrolysis product)
Acetic acid	mist- physical form not covered by tools
Ammonia	gaseous- physical form not covered by all tools
Anthracene	not REACH-relevant (pyrolysis product)
Benz(e)acephenanthrylene	not REACH-relevant (pyrolysis product)
Benzo(a)anthracene	not REACH-relevant (pyrolysis product)
Benzo(a)pyrene	not REACH-relevant (pyrolysis product)
Benzo(e)pyrene	not REACH-relevant (pyrolysis product)
Benzo(g, h, i)perylene	not REACH-relevant (pyrolysis product)
Benzo(k)fluoranthene	not REACH-relevant (pyrolysis product)
Chrysene	not REACH-relevant (pyrolysis product)
Dibenzanthracene (a,h)	not REACH-relevant (pyrolysis product)
Fluoranthene	not REACH-relevant (pyrolysis product)
Fluorene	not REACH-relevant (pyrolysis product)
Fluoride / hydrofluoric acid	mist- physical form not covered by tools
Formic acid	mist- physical form not covered by tools
Hydrogen chloride / hydrochloric acid	mist- physical form not covered by tools
Indeno(1,2,3-c,d)pyrene	not REACH-relevant (pyrolysis product)
Nitric acid	mist- physical form not covered by tools
Orthophosphoric acid	mist- physical form not covered by tools
Phenanthrene	not REACH-relevant (pyrolysis product)
Pyrene	not REACH-relevant (pyrolysis product)
Sulphuric acid	mist- physical form not covered by tools

Within the Provider C dataset, there were situations which had multiple substances and products associated with a particular sample. All those situations where there were multiple products per situation/ sample/ substance were excluded. Next, samples with multiple associated substances were identified, for example, multiple metals or a number of organic solvents. As the measurement results were not available simultaneously with the situation data for reasons of confidentiality, the selection process described previously was modified as measurements below the limit of detection could not be identified.

Measurements noted as being below the limit of detection, may occur for a number of reasons, including situations where-

- the sample analysis generated results for a standard range of analytes, whether or not these were present (for example a standard analysis for a range of organic solvents), or
- the person was exposed to the substance during the activity described but at a very low level.

To avoid choosing those situations relating to a sample where analysis had been undertaken for substances which were not used in the activity of interest, situations where there was no detailed information given about the composition of the product were excluded. For the remaining situations with multiple analytes, one agent was selected taking into consideration both the compositional information available, i.e. was the amount of substance in the product included, and the frequency of use of the substance in industry.

The list of situations obtained using the exclusion process was then compared with the list of common PROC codes, with situations relating to hot processing and mechanical treatment of metals also included to allow an evaluation of the MEASE tool to be undertaken. To allow comparisons between datasets, the Provider C data were also matched with similar situations from other providers. A final total of 642 situations were added to the database.

As noted above, for data protection reasons, it was not possible to obtain the measurement data simultaneously with the exposure situation description outside of Provider C's premises. Transporting the other data to these premises was also unfeasible; a pragmatic solution was therefore required. The use of grouped data was considered as a suitable approach, which allowed inclusion of the data but preserved anonymity of source.

The situations were grouped by IOM according to agent, PROC code, physical form (powder, liquid) and emission potential (dustiness category; vapour pressure group) and presence or absence of LEV. Dustiness was assigned by IOM as high, medium or low, with the different STOFFENMANAGER and EMKG-EXPO-TOOL categories allocated into these common bands accordingly. Vapour pressure was designated as very low ($\leq$ 10Pa), low (10 Pa < vapour pressure < 500 Pa), medium (500 Pa < vapour pressure < 10 kPa) or high (vapour pressure > 10 kPa). A group required a minimum number of 3 measurements. If fewer than 3 measurements were available, then substances within the same dustiness or vapour pressure categories were grouped. This approach was possible in the majority of cases, resulting in a total number of 486 measurements included for this Provider in the external validation comparisons. The initial groupings were then checked by Provider C colleagues, and anomalies discussed and corrected. Statistical summaries (number of data points in each group, geometric mean, arithmetic mean, geometric standard deviation, median, maximum and the number of data points below the limit of detection) were provided by Provider C. These grouped data were designated as "Type 2 aggregated data".

Although the grouping process sacrificed some detail regarding the individual tool parameters, the level of differentiation was considered sufficient to allow comparison with tool estimates. The data were grouped using a similar level of detail to that provided under REACH to downstream users regarding the safe conditions of use for substances.

iv) Provider D

The data supplied by Provider D have been used previously by the data provider to evaluate STOFFENMANAGER and ART, but these data have not been used in the development or calibration of these tools. The exposure situations provided covered the following tasks: spray painting of locomotives and bogies, blending of paint, printing, cleaning of printing equipment, foundry core making and grinding of metal. One situation relating to the mechanical treatment of wood was also included for evaluation of the STOFFENMANAGER tool.

Data were provided in English on the Microsoft Excel eteam inhalation data collection template, and required only limited re-formatting prior to transfer into the database. A total of 11 situations from Provider D were used in the validation exercise.

v) Provider E

Provider E supplied situations relating to inhalation and dermal exposures during the following professional activities: spraying of anti-fouling paints, spraying of pesticides and insecticides in a variety of premises, spray application of wood preservative and spray disinsection of aircraft. Although pesticides are outwith the scope of REACH, in the absence of large numbers of measurements for low volatility substances and in particular dermal data, their inclusion was agreed with the Advisory Board.

The data from Provider E were well described in English using the Microsoft Excel eteam data collection template and could therefore be transferred in to the database automatically. Individual measurement results were provided for a total of 14 situations.

vi) Provider F

Provider F only supplied dermal data which related to exposure to heavy fuel oils during sampling, tanker loading and maintenance activities. Again, a small number of similar situations were identified (n=10) with 140 associated measurements, with sampling undertaken using a skinwipe technique. This method involved cleaning a specific area of skin with a fabric wipe, followed by solvent desorption of the contaminants and analysis using gas chromatography/ mass spectrometry. As for the other dermal data, the Provider F data were not used in the final comparison because of difficulty in combining results from different sampling methodologies.

vii) Provider G

The Project team made an initial selection of potential data from a database collated by Provider G. These data had not been previously used in tool development, and were selected on the basis of substance and activity type. In particular, several situations relating to exposure to metals were selected to provide an independent data source for validation of the MEASE tool.

The selected inhalation exposure situations were provided in the form of paper-based occupational hygiene reports, from which contextual information and measurement data were extracted manually by members of the eteam Project team. Non-eteam Project essential information was removed from the reports by Provider G colleagues prior to submission and all remaining company and personnel identifiers were redacted to preserve confidentiality.

During extraction of the data, it was evident that the nature of the survey visits was such that in some reports measurements from non-directly exposed employees were also included. To allow subsequent coding of the situations into the tools, relevant measurements were therefore selected on the basis of contextual information about tasks, for example samples from process operators were chosen rather than those taken on administrative staff.

The extracted information was either entered directly into the database from the report, or entered into the Microsoft Excel eteam Project inhalation data collection template, and then transferred into the database. A total of 74 situations were included in the database from Provider G.

viii) Provider H

The Provider H data related solely to metals industry situations and were supplied in English. For reasons of confidentiality, the data were provided in aggregated form: limited generic contextual information was thus supplied for each exposure situation title, with each set of measurement data relating to a range of physical forms and processes in a few instances. The exposure situations were supplied as combined tabulated descriptions of multiple parameters within a Microsoft Word document. The data set also included a number of references to large numbers of aggregated data from metal processing activities; however the detail provided in these sections was insufficient to allow coding into the tools.

It was necessary to identify and extract the relevant exposure determinant information for the various measurement data and then recombine these into a Microsoft Excel file, format the information into the agreed template and transfer it into the database. In some cases, the same summary data were linked to a number of different situation descriptions, thus the aggregated measurements were used multiple times. As for other similar datasets, random checks were done to verify that the transfers had been done correctly.

The Provider H data were designated as “Type 1 aggregated data”, with a total of 76 situations incorporated into the database. Whilst the Type 1 data from Provider B were aggregated for multiple workers doing the same task in the same set of conditions, the provider H data represented a number of different PROC codes and physical forms. This initial aggregation method, across PROC codes, sites and physical forms, may have introduced additional uncertainty in these measurement data, as a direct link between the described conditions and specific workplaces was not available.

ix) Provider J

Provider J supplied exposure situations contained in a dermal exposure tool database. Many of these data had been used previously in the development of the

RISKOFDERM tool. The situations selected (n=20) related to exposures to pesticides and other low volatility substances, with the majority covering spray application followed by dipping and wiping tasks. The data were well described and included both solid and liquid substances. No detailed information was identified on the sampling method used to collect the specific measurements, which were from hands and forearms. The sampling methods noted included patch sampling of potential exposure as detailed above, and measurements of actual contamination inside gloves. As for the other dermal data collected, these measurements were not used in the final comparison because of difficulty in comparison between sampling methods.

x) Provider K

Provider K supplied two separate Microsoft Access databases, with task and other activity related information provided as coded entries and in non-English language free text. Both databases incorporated individual sample results for a range of activities covering several industry sectors. The databases were exported into Microsoft Excel spreadsheets for ease of use prior to language translation out of free text. Industry sectors where no measurements were available relating to REACH-specific substances were excluded as shown in Table 2.3.

Table 2.3 Inclusion and exclusion of industry sector data from Provider K (based on REACH relevance of the substances)

Provider K Database DB1		**Provider K Database DB2**	
Sectors included	**Sectors excluded**	**Sectors included**	**Sectors excluded**
Screen printing	Plastics recycling[a]	Printing/flexography	None
Furniture manufacturing	Car recycling	Car industry	
Exposure assessment Tool validation data	Textile recycling[b]	Optometrists	
Wood impregnation		Electroplating	

[a] One situation relating to compounding included
[b] One situation relating to gluing included

For both of the databases, within the remaining contextual information and measurement data, all situations relating to a single measurement were included. In total 423 situations were added to the database.

xi) Provider M

Data from Provider M were supplied in the form of an English language database of textual descriptions of exposure situations and related individual measurements. The situations were well described, and covered exposures to volatile organic substances and powders in a wide range of professional and industrial scenarios. A small number of these data may have been used in the development of the STOFFENMANAGER tool; however we could not identify these clearly. A number of situations were excluded using the same criteria as indicated previously: REACH-relevance, physical form, identifiable substance and allocation to common PROC codes. Table 2.4 provides a list of situations that were excluded using these criteria. A total of 67 situations were excluded using these criteria with 48 situations added to the database.

2.2.1.3 Summary of data by provider

A summary of the data provided for the external validation is given in Table 2.5. Additional detail regarding the numbers and types of situations used for the external validation exercise are given in eteam Project Deliverable D12: Description of Exposure Situations Used in the External Validation Exercise.

Table 2.4 Situations excluded from the Provider M database on the basis of REACH-relevance, physical form, non-specification and applicability of tools

Situation	Substance	Basis for exclusion
dumping of stones	inhalable stone dust	not REACH-relevant
milling asphalt	inhalable asphalt dust	task not covered by all tools
bagging fine powder	inhalable cement dust	non-specified substance
unloading ships	inhalable dust from sand/ calcinated petroleum coke	not REACH-relevant
unloading ships	bauxite and soy pellets	not REACH-relevant
sawing wood	inhalable wood dust	not REACH-relevant / task not covered by all tools
spraying of paint	total isocyanates	individual substance not identifiable
scooping of powder	inhalable dust	individual substance not identifiable
metal working/ turning	boron in metal working fluid mist	form/ task not covered by all tools
spreading of glue	total hydrocarbons	individual substance not identifiable
sandblasting of yachts	inhalable dust/ Cu(II)O	task not covered by all tools
cleaning of equipment	total hydrocarbons	individual substance not identifiable
mixing of paint	total hydrocarbons	individual substance not identifiable
rolling of paint	total hydrocarbons	individual substance not identifiable
handling of wood	inhalable wood dust	not REACH-relevant
broadband sanding	inhalable wood dust	not REACH-relevant
sawing	inhalable wood dust	not REACH-relevant
cleaning of premises	inhalable textile dust	not REACH-relevant / individual substance not identifiable
sorting of textiles	inhalable textile dust	not REACH-relevant / individual substance not identifiable
sweeping of premises	inhalable textile dust	not REACH-relevant / individual substance not identifiable
bagging plastic granules	inhalable plastic dust	not REACH-relevant
dumping plastic granules	inhalable plastic dust	not REACH-relevant
sorting plastics	inhalable plastic dust	not REACH-relevant
vacuuming plastic residue	inhalable plastic dust	not REACH-relevant
spreading glue	total hydrocarbons	individual substance not identifiable
dough making	inhalable flour dust	not REACH-relevant
spraying of insecticides	pesticide spray	individual substance not identifiable
wrapping bread	inhalable flour dust	not REACH-relevant
plastering	inhalable plaster dust	individual substance not identifiable
mixing plaster	inhalable plaster dust	individual substance not identifiable
dumping of powder in hopper	inhalable dust	individual substance not identifiable

Table 2.5 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 2 aggregated 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 2.5 Summary of data by provider (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 2.5 Summary of data by provider (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 Yes	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		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

2.2.2 Quality Control - data transferral

With the exception of the submissions from Providers F, G and M all of the data were transferred into the database from Microsoft Excel spreadsheets. With the exception of the data from Provider E, the datasets required significant re-formatting, cleaning, consolidation into discrete exposure situations and in some cases, language translation, prior to transfer. A random selection (5 - 50%) of the data for each provider was checked against the original submission following transfer to verify data were transferred appropriately.

2.3 Coding of Tool parameters

2.3.1 Translation of contextual information from exposure situations into tool input parameters

The external validation process required the generation of tool estimates from the collated exposure situations with which to compare the workplace measurement data. To do this, it was 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. Similar types of situations had been gathered from a number of different data providers, therefore this approach also assisted in the identification of systematic differences between coders for the same type of activity. Initial and follow up training sessions were provided to the coders, combined with regular discussions about the input process.

In general, 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 (see Appendix 2). The guidance and default values in the Quality Control Manual had been agreed with the Advisory Board in advance of the coding process, and a summary of the methods/ decision making processes followed is given below.

2.3.2 Choice and use of default parameters

During the coding process, a number of decisions were made regarding default tool input parameters. The decisions are outlined below.

2.3.2.1 <u>Fugacity: dustiness of solid materials</u>

As noted previously in this study and by others (Koppisch et al, 2012), there was very limited explicit information provided on the dustiness level of substances within the situation descriptions. Coders were instructed to seek information on the substance using appropriate web searches and to consider similar substances in making their decision about the best tool input option. In the absence of any available useful information on the substance or analogous materials, the coders were asked to choose the medium level of dustiness for the tool, and allocate a major uncertainty to the parameter. Absence of dustiness information generated a default level of medium dustiness in 89 situations.

2.3.2.2 Concentration

In the absence of specific substance concentration information within the contextual description for the situation, default concentrations as detailed in the Quality Control Manual and agreed with the Project Advisory Board were selected. Initially, for each tool a default value was chosen that reflected the median value or category. For the ECETOC TRAv2, ECETOC TRAv3 and MEASE, this meant that defaults of 5-25% were used for liquids, whilst for STOFFENMANAGER, a default of 50% was allocated. Hence for a given situation where the substance concentration was not clearly described, and where no external manufacturer's or other references were available, this difference in default values meant that the STOFFENMANAGER estimate was artificially higher than that from the ECETOC TRA and MEASE tools.
In the final comparison of the measurement data with tool estimates, a revised default concentration of 25% was used for the STOFFENMANAGER tool, as this was felt to both better reflect common substance concentrations in preparations and provide better parity with the other tools. The default concentration option was selected in 177 situations relating to liquids. There is no concentration adjustment within the EMKG-EXPO-TOOL for liquids, i.e. a concentration of 100% is assumed.

For solids, 5-25% was also used as a default for the ECETOC TRAv3 and MEASE tools and was selected in 8 situations. There is no concentration factor for solids incorporated into the ECETOC TRAv2, EMKG-EXPO-TOOL and STOFFENMANAGER tools.

2.3.2.3 Task duration

The ECETOC TRAv2, ECETOC TRAv3 and MEASE tools allow the user to adjust the exposure estimate to take account of task time within the worker's shift. For example, where an activity takes 2 hours out of an 8 hour shift, then the option of 1-4 hours can be chosen in the ECETOC TRA tools and MEASE. An exposure modifying factor of 0.6 is then applied to reduce the estimate accordingly.

Version 4.5 of STOFFENMANAGER estimates a task-based estimate rather than a time weighted average for a full 8 hour shift. Within the tool, no adjustment for duration of exposure was made when comparing these estimates with 8 hour shift long measurements which included time periods with no exposure. The EMKG-EXPO-TOOL allows the user to reduce the estimate in cases where the activity takes place for less than 15 minutes in the shift, however no other time-related modifiers are available.

The majority of the available measurement data were either task-based or 8-hr measurements where the task lasted for more than half of the full shift. As the tool estimates had to be compared with the measurement results, the coders were instructed to assign the highest duration of task/ exposure if the measurement was only related to one task, even if that task was less than 4 hours. For example, if the duration of a measurement was 2 hours, and the task monitored during this measurement lasting the full 2 hours (i.e. with no non-exposed time), then the coders entered >4hrs for ECETOC TRAv2 and v3 and MEASE. In total 93 out of 1131 situations included selection of the default duration.

2.3.2.4 Task description

The measurement data included variable amounts of information on the task carried out, ranging from very detailed task records to more limited descriptions of machine type. As such, it is possible that additional, unrecorded tasks may have taken place during the measurement period. The task described, and subsequently coded into the tools to generate estimates, may therefore have included additional non-modelled exposures.

2.3.2.5 Setting

As noted in eteam Project Work Package WI.6- Operational Analysis, assigning whether the particular situation should be industrial or public/professional with the ECETOC TRA and MEASE tools can be difficult. As there is no clear method outlined in the regulatory or tool guidance, the decision was made based on the guidance in the agreed Quality Control manual. Few of the situations were classed as professional compared to the large numbers which took place in industrial settings. In addition, those which took place in a professional setting related in the main to healthcare situations for example pathology work and dentistry and therefore represented a very narrow range of the overall dataset.

2.3.3 EMKG-EXPO-TOOL control approach

Users of the EMKG-EXPO-TOOL are directed to detailed control guidance sheets (CGS) for information on the control measures to be implemented to make the tool assessment valid. However, in the course of the exercise, it was not possible to verify that the exact control approach specified in any available CGS had in fact been implemented in the particular workplace situation being assessed. In addition, Control Approach 1 in the EMKG-EXPO-TOOL assumes a basic level of general ventilation, whilst the other tools allow an assessment to be made for situations where no control measures are present. Assuming parity of other inputs, this potentially reduces the EMKG-EXPO-TOOL estimate in such situations compared with the value generated by the other tools, decreasing its apparent relative conservatism.

2.3.4 Between-coder consistency

We have reported high levels of between user variation previously in eteam Project Deliverable D22: Between user reliability exercise. A variety of different quality control methods were therefore used to minimise inconsistency between the IOM coders when inputting exposure situation information into the tools to generate estimates for the external validation exercise. These methods are detailed below.

2.3.4.1 Blind re-coding of situations

A selection of the completed situations for each tool (10%) was randomly selected for re-coding by an exposure scientist who had not previously been involved in the initial coding of the situations. This exposure scientist did not have access to the original coding, thus the process was carried out blind. The outcome of these comparisons is summarised in Table A3.1 in Appendix 3, with examples given therein of identified discrepancies and the resultant actions taken.

Where differences were noted between the second coding and original entries, the situation description was checked, discussed and updates made as required. Similar situations were also checked to ensure consistency.

2.3.4.2 Cross checking of tool inputs by situation

Cross-checking of the inputs for all applicable tools was carried out by situation for the following parameters to ensure consistency of similar/ identical input parameters. Identified erroneous inputs were checked against the original coding for the relevant tools and situation description within the database, and where necessary corrected. The input parameters checked included:

- Molecular weight (2 typographical corrections made)
- Vapour pressure (2 missing entries and 5 typographical corrections made)
- Dustiness (36 corrections made)
- Concentration in preparation
- PROC code/ handling description (9 corrections made)
- Presence of LEV (29 corrections made)
- Duration of exposure (20 corrections made)
- CAS number (format standardised to allow easy importation into tools)
- Substance name (nomenclature standardised across providers)

2.3.4.3 Provider check of Type 2 aggregated data

As noted above, Provider C carried out additional checks on coding choices during the grouping process for the Type 2 aggregated data. To further ensure consistency, following this, cross checks were done between the Provider C data coding and the coding of similar situations from other sources. Any anomalies were checked against the original description and corrected as required before the final groupings were agreed.

Following completion of the various checks outlined above, the final set of tool estimates generated for the comparison exercise were considered to be consistent and appropriately verified in terms of the tool input parameters.

2.4 Generating Tool Estimates

To facilitate handling of the large numbers of exposure situations and reduce the risk of data entry errors during manual transfer of model input parameters from the database into the tool, 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). The regression coefficients provided by Schinkel et al (2010) were rounded to 2 decimal places and thus application of these parameters did not generate exactly the same results as those obtained using the online STOFFENMANAGER tool. Hence, the parameters used in the actual calculations within the STOFFENMANAGER tool were obtained from the model developers, which were rounded to 4 decimal places.

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 TRA v3 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.

2.4.1 Quality Control – Generation of exposure estimates

There are many safeguards built into the original tools to guide and assist the user to verify the “sense” of their inputs, for example logic checks between combinations of physical form and fugacity or process. To verify the results obtained for EMKG-EXPO-TOOL and STOFFENMANAGER, a number of test situations (10%) were run through the original tools for verification of the in-database tool method. These situations were randomly chosen to reflect a range of activities, substances and tool parameters, thus ensuring as far as reasonably practicable that the in-database versions of the tools had operated properly. Any differences were investigated, identified problems addressed and exposure estimates were recalculated. Following this additional checks were carried out to determine if any further issues remained. This process was continued until no further differences between the built-in approach and the real tool existed.

As the actual ECETOC TRAv2, ECETOC TRAv3 and MEASE tools were used, 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, as for STOFFENMANAGER and the EMKG-EXPO-TOOL, cross-checks of 10% of the situations were run through the original tools to confirm that the system was functioning correctly in terms of the export and import mechanisms. This process was also continued until the outputs of all of the simulated tools matched those from the original versions.

2.5 Descriptive analysis of measurement data

The first stage of the statistical analysis involved descriptive analysis of all the measured exposure data collected. The aim of this analysis 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.

The workplace exposure data were summarised 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 of $\leq$ 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)

The relevant limits of detection as supplied by the data providers for their respective situations were used for the calculations.

Descriptive statistics were generated using the Genstat statistical software package and SAS vs 9.3, with graphical representations of the data produced using Sigmaplot.

2.6 Comparison of Tier 1 tool output 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. All tool exposure estimates were expressed in mg m^{-3}, to facilitate inter-tool comparisons.

For the EMKG-EXPO-TOOL, which predicts an exposure range rather than a single value, the upper range value was used for the comparisons. This is in accordance with the REACH guidance which suggests using the upper limit of the band for exposure assessment. In case 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 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.

2.6.1 Comparison of individual measurement data with tool estimates of exposure

Where individual measurement points were available, these 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. Pearson correlation coefficients between the log-transformed measurement results and 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.

2.6.2 Comparison of aggregated measurement data with tool estimates of exposure

Similar comparisons were made between the two different types of 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 a number of situations the arithmetic mean was not provided. In this case we estimated the arithmetic mean as follows:

$$AM = \exp\left(\mathrm{m} + (0.5 \times s^2) \times \left((N-1) \times N^{-1}\right)\right)$$ **Equation 2.1**

Where m is log of the geometric mean, and s is the log of the geometric standard deviation.

The ratio of the measurement value over the tool-based estimate was calculated for the two aggregated data sets as described above and summarised by tool and exposure category.

For the Type 2 aggregated data, the arithmetic mean of the tool estimates for the group was compared with the arithmetic mean of the corresponding grouped data. 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 proportion of the aggregated measurements that are predicted to have exceeded the tool estimate, i.e. above the 1:1 line which would represent complete agreement, was estimated by assuming the measurement data followed a log-normal distribution, using the geometric mean and the geometric standard deviation of the measurements:

$$P(x_i > T) = 1 - \Phi\left\{Ln(T.GM^{-1}) \times \left(ln(GSD)\right)^{-1}\right\}$$ **Equation 2.2**

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.

For the Type 2 aggregated data, the geometric mean of the tool estimates was used as T.

2.7 Analysis of impact of exposure determinants on level of conservatism

The impact of different data-specific factors and exposure determinants on the comparison exercise results was investigated by tabulation and examination of the percentage of measurements exceeding the tool estimate 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 presence/ absence of local risk management controls/ LEV.

2.8 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 estimate 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 will be presented in this report.

3 Results

3.1 Description of workplace measurement data

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

3.1.1 Individual measurement data

3.1.1.1 Overview of individual measurement data

In total, the eteam database contained results from 2098 inhalation exposure measurements. The majority of the measurements were for volatile liquids. The overall number of individual measurements collected and used for the comparisons with the tool estimates of exposure are summarised in Table 3.1 by exposure category. It should be noted that Table 3.1 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 3.1 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 liquids[1)]	316	0.07	15	<0.001	36
Volatile liquids[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) $\leq$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.

3.1.1.2 Individual measurement data by provider

The individual measurement data provided for each organisation are summarised in Tables 3.2- 3.7 by exposure category.

i) Exposure to non-volatile liquids with vapour pressure $\leq$ 10 Pa

The majority of the non-volatile liquids originated from Provider M, and related to spray processes, for example aircraft disinsection, where the main exposure was to aerosols rather than vapours. As such, these data were not suitable for validation of the ECETOC TRAv2, ECETOC TRAv3 or EMKG-EXPO-TOOL. In addition, within this category, situations involving exposure to organic low volatility liquids were also considered to be outside of the scope of the MEASE tool. However, most of the data within this exposure category could be used to compare with the STOFFENMANAGER estimates.

Table 3.2 Individual measurement data for non-volatile liquids with vapour pressure ≤10 Pa by provider

Provider	N meas	GM (mg m^{-3})	GSD	Min (mg m^{-3})	Max (mg m^{-3})
A	9	0.3	2.1	0.20	1.5
B	49	0.3	3.8	0.001	2.1
E	33	0.5	17	0.003	36
G	14	0.004	7.0	<0.001	0.05
M	211	0.04	14	<0.001	16
TOTAL	**316**				

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.

ii) Exposure to volatile liquids with vapour pressure > 10 Pa

As could be expected, and in line with the main sampling reasons given by the providers, the majority of the exposure situations and associated measurements related to workplace exposures to volatile organic liquids (Table 3.3).

Table 3.3 Individual measurement data for volatile liquids with vapour pressure >10 Pa by provider

Provider	N meas	GM (mg m^{-3})	GSD	Min (mg m^{-3})	Max (mg m^{-3})
A	259	5.0	36	0.001	1508
B	592	51	9.0	0.017	1949
D	19	6.2	11	0.026	280
G	16	77	3.7	0.990	461
K	110	9.4	7.4	0.010	335
M	360	0.3	9.9	<0.001	213
TOTAL	**1356**				

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.

These data covered a broad range of common substances and activities. These common processes in turn represent a sample of the very large range of manufacturing and downstream uses for which assessments must be carried out under REACH.

In addition, the measurements were obtained using current sampling techniques which can be expected to be directly comparable to any measurement data collected for exposure assessment applied in REACH Chemical Safety Reports. We recognise that collection of multiple measurements for each situation would have reduced the uncertainty in the external validation process, compared with single measurement values. However; our data collection was constrained by the information available to us, and whilst multiple measurement data were collected in a number of cases, many of the situations in the overall data pool contained single measurement values.

Situations involving exposure to volatile organic substances were considered to be within the range of applicability of all of the tools, with the exception of MEASE. Although the non-applicability of MEASE to organic substances (in non-volatile, volatile or powdered form) is not clearly stated in the relevant ECHA and tool guidance documents, the developers of MEASE informed us that in their view the MEASE tool should not be used for assessment of exposure to such substances.

iii) Exposure during powder handling processes

In comparison with volatile liquids, fewer measurements were available for activities involving handling of powdered solids (Table 3.4). However; the dataset included a variety of common transfer, mixing and spraying processes.

Table 3.4 Individual measurement data for powder handling activities by provider

Provider	N meas	GM (mg m^{-3})	GSD	Min (mg m^{-3})	Max (mg m^{-3})
A	39	0.7	6	0.005	48
G	2	0.4	177	0.010	15
M	213	0.1	69	<0.001	446
TOTAL	**254**				

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.

iv) Exposure during metal abrasion processes

The data from abrasive metal processes covered a relatively small number of situations and concentrations, as shown in Table 3.5. These situations were included to allow validation of the predictions from MEASE, the ECETOC TRAv2 and the ECETOC TRAv3.

Table 3.5 Individual measurement data for metal abrasion by provider

Provider	N meas	GM (mg m^{-3})	GSD	Min (mg m^{-3})	Max (mg m^{-3})
A	37	0.4	4.6	0.01	5.4
B	43	0.1	6.2	0.001	8
D	2	3.5	2.7	1.7	7.0
G	2	0.04	5.8	0.01	0.1
TOTAL	**84**				

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.

v) Exposure during processing of metals

These data included exposures during a range of hot metal processes, for example welding, soldering and foundry work. As shown in Table 3.6, there were small numbers of measurements available for these processes in comparison with the other data categories.

Table 3.6 Individual measurement data for metal processing by provider

Provider	N meas	GM (mg m^{-3})	GSD	Min (mg m^{-3})	Max (mg m^{-3})
A	44	0.3	7.4	0.003	22.1
B	27	0.2	7.2	0.003	4.3
TOTAL	71				

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.

vi) Exposure during wood processing

A very small number of situations relating to woodworking activities had been submitted by providers A and D. Although unplanned, these were included for a very limited comparison with estimates from the STOFFENMANAGER tool.

Table 3.7 Individual measurement data for wood processing by provider

Provider	N meas	GM (mg m^{-3})	GSD	Min (mg m^{-3})	Max (mg m^{-3})
A	9	0.5	1.3	0.3	0.7
D	5	6.2	4.7	0.8	39
TOTAL	14				

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.

Summary

It can be seen from the summary tables that the individual measurements obtained covered a very wide range of exposure concentrations, from less than the relevant limit of detection to values which are comparatively high. The highest values have been examined and relate to processes which are considered to be at the lower end of the control spectrum, rather than instances of deliberate misuse. For example, hand spraying of high volatility liquids in the absence of LEV resulted in high levels in the workplace. As such, it is felt that the inclusion of these data is appropriate for the validation within the context of REACH, where the tools are expected to identify high potential exposures for more detailed assessment.

3.1.1.3 Individual measurement data by PROC code

The individual measurement data are shown by allocated PROC code in Table 3.8. The “common” PROC codes identified during the conceptual evaluation of the tools were used as a pre-selection criterion for all of the data providers. As such the majority of these PROC codes are adequately covered by at least one tool. The majority of the data supplied did not have a PROC code allocated, as it had been collected for non-REACH purposes. The PROC codes chosen therefore reflect the decisions made during the coding process used to translate the exposure situations into the required tool inputs. This decision making process is detailed elsewhere in this report and in the eteam Project Quality Control Manual (see Appendix 2).

The PROCs with the largest number of measurements across the categories were PROC 8b (Transfer of substance or preparation from/to vessels/large containers at dedicated facilities), PROC 11 (Non industrial spraying) and PROC 10 (Roller application or brushing). Individual measurements relating to exposures to non-volatile liquids were predominantly used in industrial or professional spraying activities.

Table 3.8 Individual measurement data by allocated PROC code

	PROC codes																	
Exposure category	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) ≤10 Pa.
[2)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa.

3.1.2 Type 1 aggregated measurement data

Table 3.9 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 for 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 3.9 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 liquids[1)]	2	42	0.01	1.5	0.01	0.01
Volatile liquids[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) ≤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.

Two providers (B and H) supplied Type 1 aggregated measurement data. These data are shown in Table 3.10 and Table 3.11 for the relevant provider 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 3.10 Type 1 aggregated data by PROC code and physical form (Provider B)

Physical form	**PROC Code**	**Number of exposure situations**	**Number of measurements[3)]**
Solids[1)]	5	1	2
	8b	3	13
	9	3	24
Liquids[2)]	5	11	100
	7	1	7
	8a	1	3
	8b	3	10
	9	23	142
	TOTAL	**46**	**301**

[(1)] powders
[(2)] includes non-volatile and volatile liquids
[(3)] number of individual measurements

Table 3.11 Type 1 aggregated data by PROC code and physical form (Provider H)

Physical form	**PROC Code**	**Number of exposure situations**	**Number of measurements[(3)]**
Solids[1)]	1	1	6
	3	2	102
	8a	3	36
	8b	14	550
	14	1	14
	21	3	41
	22	4	128
	23	2	92
	24	1	16
	27a	1	29
Non-volatile liquids[2)]	3	1	14
	4	1	28
	TOTAL	**34**	**1056**

[1)] includes powder handling, metal abrasion and metal processing [2)] non-volatile liquids are defined as liquids with a vapour pressure (at room temperature) $\leq$10 Pa. [3)] number of individual measurements

3.1.3 Type 2 aggregated data

Table 3.12 provides a summary of the measurement results available for the Type 2 aggregated measurement data. This table shows the number of measurements which were used in the validation. 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.

Table 3.12 Summary of Type 2 aggregated measurement data used for comparison with tool estimates (Provider C)

Exposure category	N grouped situations	N meas	GM (mg m^{-3})	GSD	Min AM (mg m^{-3})	Max AM (mg m^{-3})
Non-volatile liquids[1)]	4	23	<0.01	2.0	<0.01	0.01
Volatile liquids[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) $\leq$10 Pa. [2)] volatile liquids are defined as liquids with a vapour pressure (at room temperature) >10 Pa. N grouped situations: number of grouped exposure situations; N meas: number of measurements in the groups; 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.

The Type 2 aggregated data are shown by PROC code and physical form in Table 3.13. For these data, one measurement was available per exposure situation, with the situations grouped as described previously. These data cover the main types of processes and substances found in manufacturing and industrial/ professional end-use circumstances, and were thus considered to have sufficient coverage to allow their inclusion in a useful validation exercise.

Table 3.13 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

3.2 Comparison of individual measurement data with tool estimates

In the following section, the comparison between individual measurement results and the tool estimates is described.For each tool, the measurement data available for comparison for that particular tool are summarised, together with the tool estimates. The tool estimates were then compared with the measurement results by plotting the data. Finally, the ratios of the measurement result over the tool estimate were summarised and the percentage of the measurements exceeding the associated tool estimate provided.

3.2.1 ECETOC TRAv2

Table 3.14 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 3.14 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	107	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 3.15 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 3.15 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 3.1 to 3.3 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.

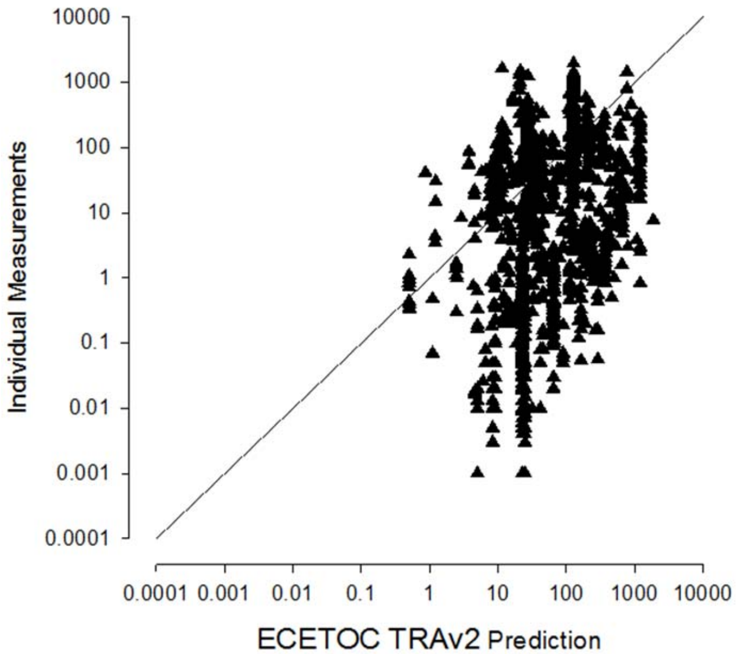

Figure 3.1 Measured data vs ECETOC TRAv2 estimates of exposure to volatile liquids (vapour pressure >10 Pa) (mg m^{-3})

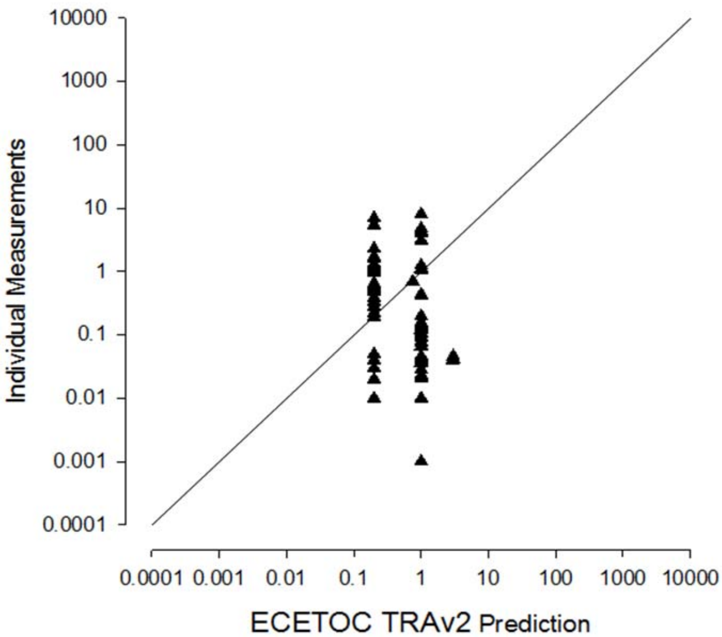

Figure 3.2 Measured data vs ECETOC TRAv2 estimates of exposure during metal abrasion (mg m^{-3})

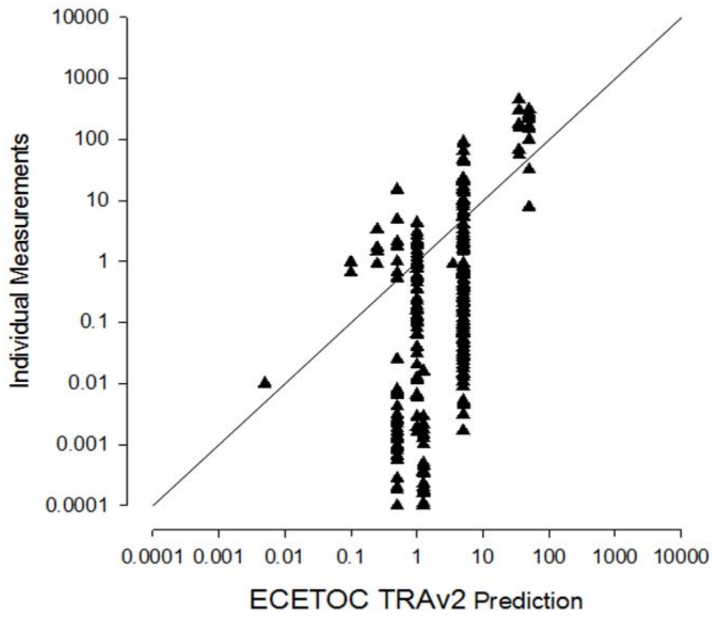

Figure 3.3 Measured data vs ECETOC TRAv2 estimates of exposure during powder handling processes (mg m^{-3})

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 3.16 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 3.16 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%

[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.

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, in comparison with this dataset, the tool appears to underestimate exposure compared with the assumed prediction level for each of the categories.

3.2.2 ECETOC TRAv3

The same measurement data were available for comparison with the ECETOC TRAv3 as for ECETOC TRAv2, hence Table 3.17 is identical to Table 3.14.

Table 3.17 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 3.18). 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 3.15).

Table 3.18 Summary of the ECETOC TRA v3 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 3.4 - 3.6 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 $r=0.69$, $p<0.001$).

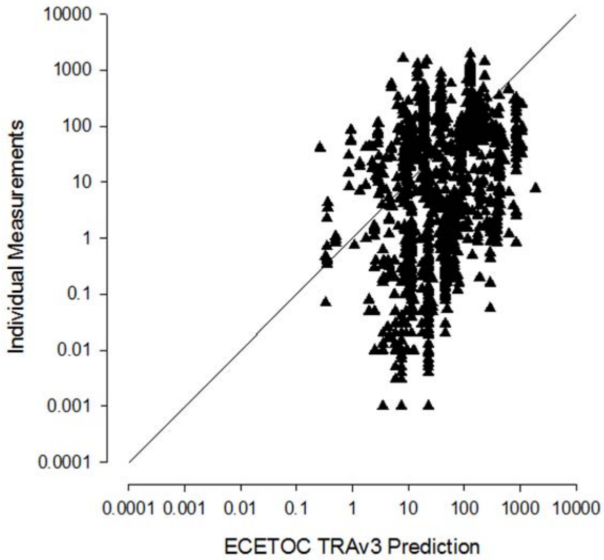

Figure 3.4 Measured data vs ECETOC TRAv3 estimates of exposure to liquids with vapour pressure >10 Pa (mg m^{-3})

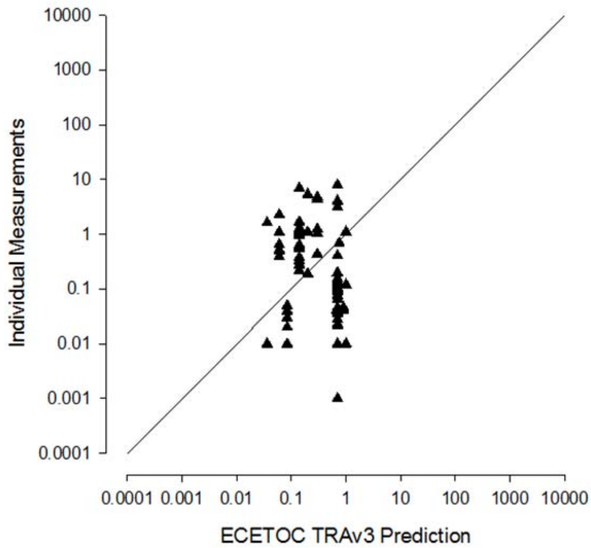

Figure 3.5 Measured data vs ECETOC TRAv3 estimates of exposure during metal abrasion (mg m^{-3})

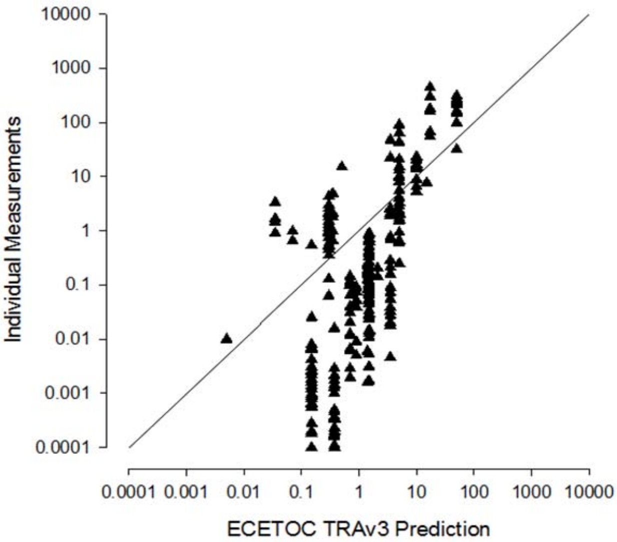

Figure 3.6 Measured data vs ECETOC TRAv3 estimates of exposure during powder handling processes (mg m^{-3})

However, the ratios of the measurement values over the relevant ECETOC TRAv3 estimates (Table 3.19) are higher than for ECETOC TRAv2 (Table 3.16). 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 3.19 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.

3.2.3 MEASE

For MEASE comparisons were carried out of 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 3.20).

Table 3.20 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 again 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 3.21).

Table 3.21 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	0.3	96

[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 tool estimates; GM: geometric mean of tool estimates; GSD: geometric standard deviation of tool estimates; Min: lowest tool estimate; Max: highest tool estimate.

Figures 3.7 to 3.10 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.

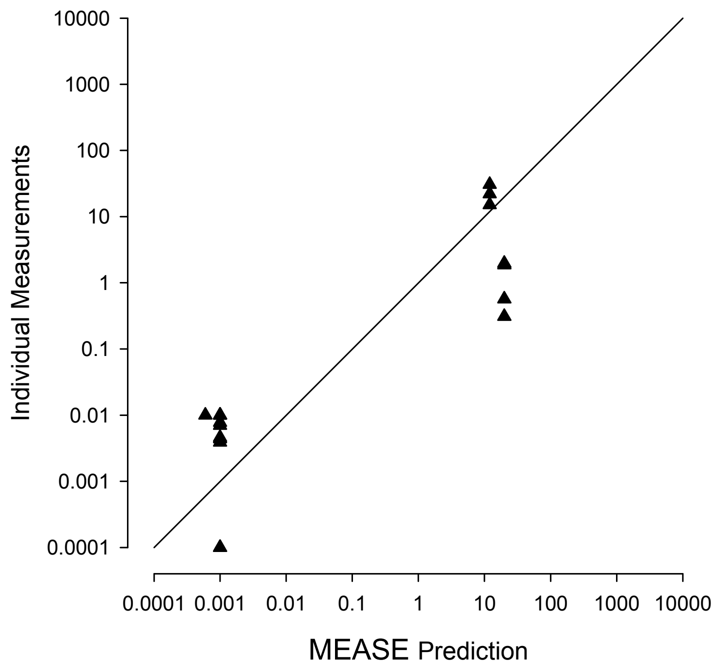

Figure 3.7 Measured data vs MEASE estimate of exposure to liquids with vapour pressure ≤10 Pa (mg m^{-3})

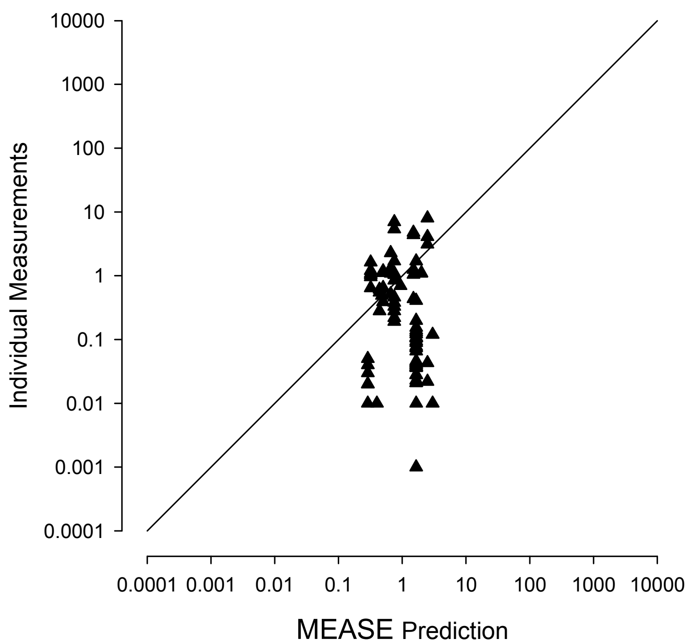

Figure 3.8 Measured data vs MEASE estimate of exposure during metal abrasion (mg m^{-3})

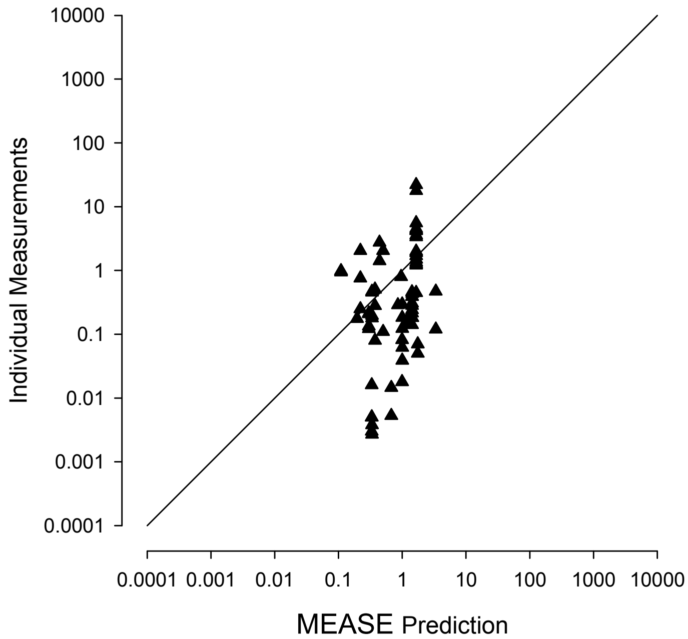

Figure 3.9 Measured data vs MEASE estimate of exposure during metal processing (mg m^{-3})

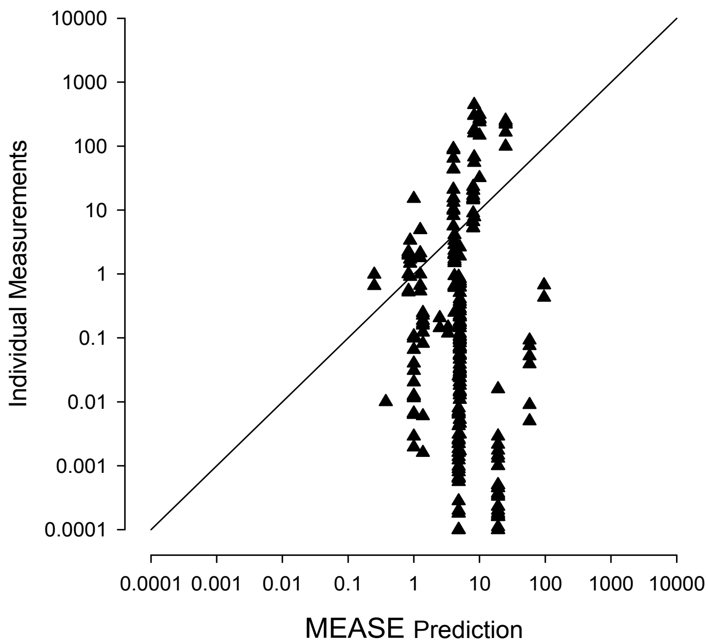

Figure 3.10 Measured data vs MEASE estimates of exposure during powder handling processes (mg m^{-3})

The ratios of the measurement data over the MEASE estimates are shown in Table 3.22, together with the percentage of cases in which the measurement was greater than the tool prediction.

Table 3.22 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	79	< 0.001	54	23%

[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 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.

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 3.23 and 3.24).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 3.23 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 3.24 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 3.11 and 3.12 again provide the scatterplots for volatile liquids and powder handling, respectively.

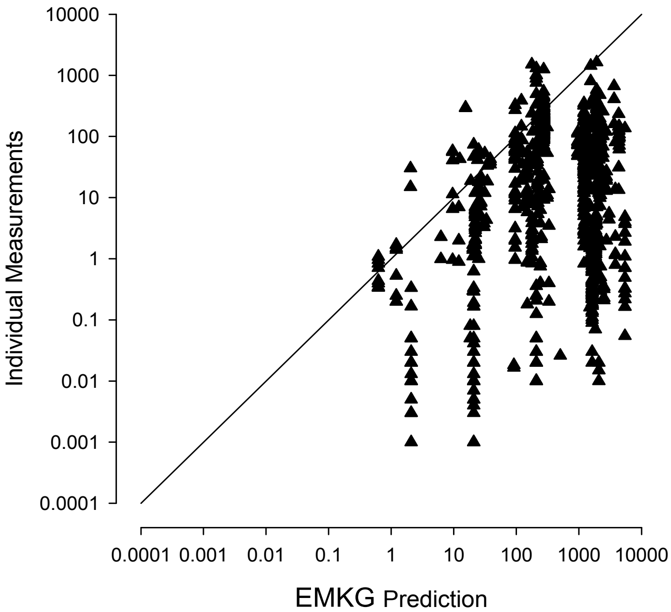

Figure 3.11 Measured data vs EMKG-EXPO-TOOL estimates of exposure to liquids with vapour pressure >10 Pa (mg m^{-3})

From Figure 3.11, 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 3.25). The Pearson correlation coefficient between the log-transformed tool estimates and log-transformed measurement results was 0.28 (p<0.001).

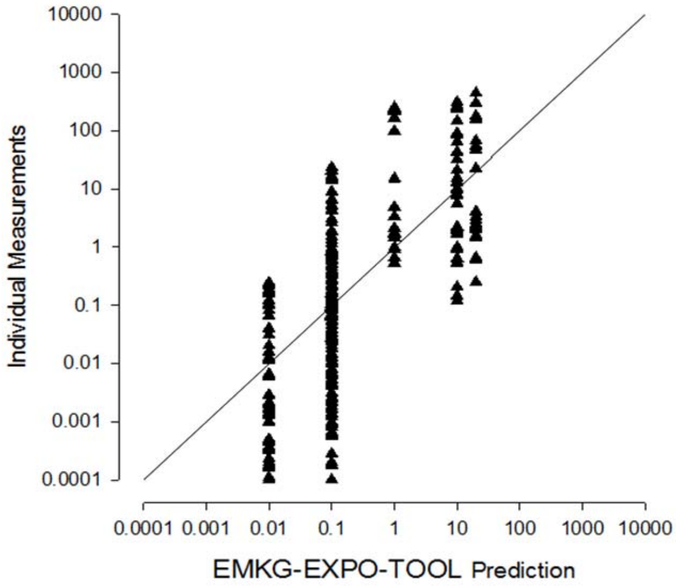

Figure 3.12 Measured data vs EMKG-EXPO-TOOL estimates of exposure during powder handling processes (mg m^{-3})

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 3.12, a large number of points lay above the 1:1 line.

The ratios of the measurement values over the relevant EMKG-EXPO-TOOL estimates are presented in Table 3.25, together with the percentage of measurement results which exceed the corresponding tool prediction.

Table 3.25 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 3.25 confirm that for volatile liquids, the EMKG-EXPO-TOOL was sufficiently conservative in comparison with this data set, as the AM and GM of the ratio of the measurements over the tool estimates are both less than 1 and only 7% of the measurements exceed the tool estimates. The 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 3.25, 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 3.26.

Table 3.26 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 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.

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 3.27 below.

Table 3.27 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 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 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; $p < 0.0001$).

3.2.5 STOFFENMANAGER

STOFFENMANAGER generates estimates of different percentiles of the exposure distribution, e.g. the 50th, 75^{th,} 90th and 95th percentiles of the exposure distribution. Following discussions 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, 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 3.28).

Table 3.29 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, with the exceptions of powders, where the AM of the 75th percentile tool estimate is lower than that for the measured data, although the GM of the 75th percentile is higher than the GM of the measurement results.

Table 3.28 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 3.29 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 3.13 to 3.16 give the scatterplots between STOFFENMANAGER estimates and measurement results for both the 75th and the 90th percentiles. When the 75th and 90th percentile plots are compared, the cloud of data points for the 90th percentile moved to the right compared to the 75th percentiles, as the 90th percentile estimates are higher. The number of measurements that are above the 1:1 line will therefore be reduced. 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 3.30). 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.

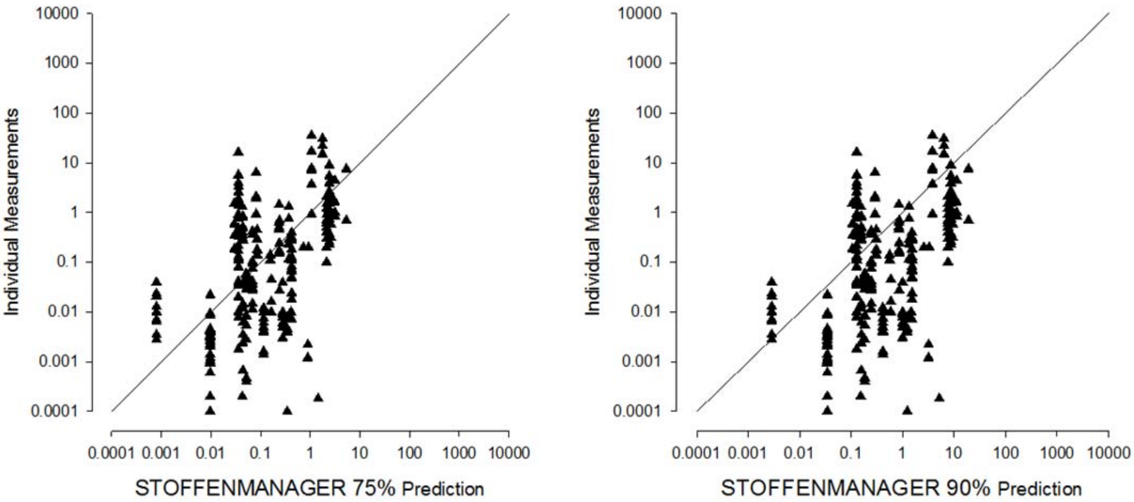

Figure 3.13 Measured data vs STOFFENMANAGER estimate of the 75th and 90th percentile of the exposure distribution- non-volatile liquids with vapour pressure ≤10 Pa (mg m^{-3})

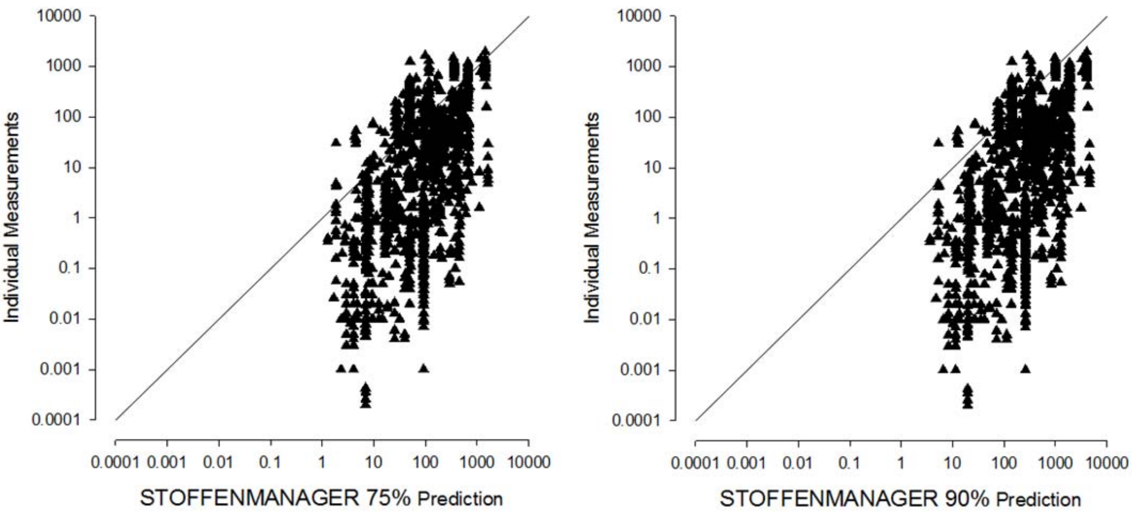

Figure 3.14 Measured data vs STOFFENMANAGER estimate of 75th and 90th percentile of the exposure distribution – volatile liquids with vapour pressure >10 Pa (mg m^{-3})

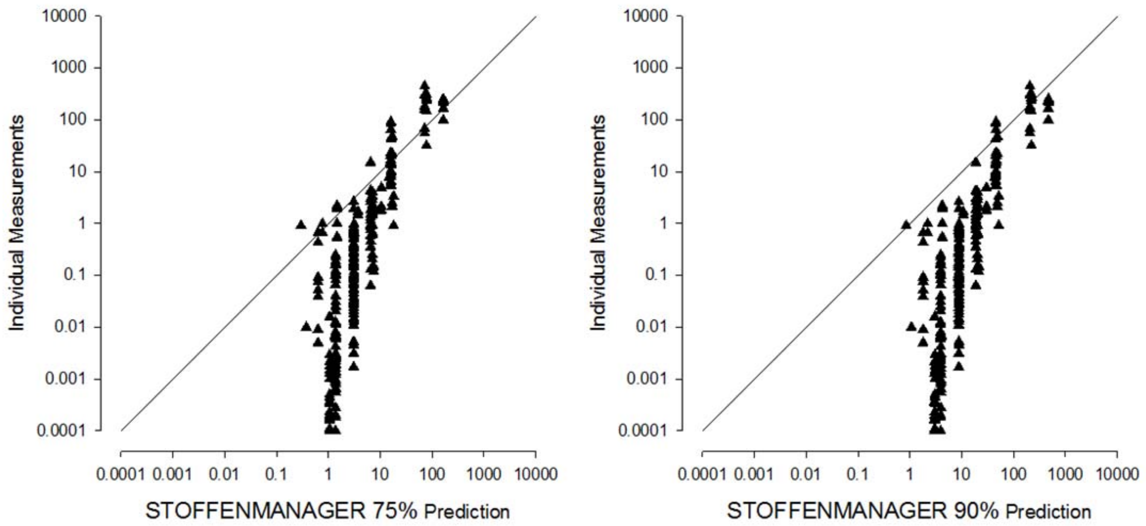

Figure 3.15 Measured data vs STOFFENMANAGER estimate of 75th and 90th percentile of exposure distribution during powder handling processes (mg m^{-3})

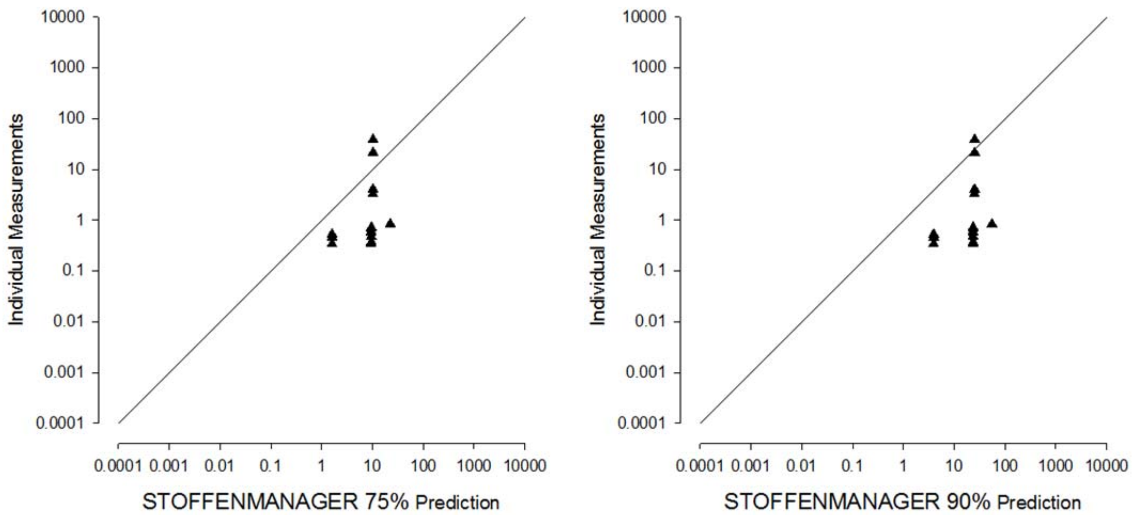

Figure 3.16 Measured data vs STOFFENMANAGER estimate of 75th and 90th percentile of exposure distribution during wood processing (mg m^{-3})

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 statistically significant correlation was observed between the tool estimates and measurement results.

Table 3.30 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 underestimate the exposure compared to the measurements.

When using the 75th percentile, the AM of the ratios is greater than 1 (2.6), whilst the GM of the ratios is below but relatively close to 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, during 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 3.30 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.

3.2.6 Level of conservatism by data provider

Table 3.31 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 measurement levels for the different providers reported in Tables 3.2 to 3.7 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 3.31 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

	Data Provider																				
Exposure category	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

3.2.7 Level of conservatism by PROC codes

Table 3.32 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 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 3.32 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

3.3 Comparison of aggregated measurement data with tool estimates

Within this section, the results of comparisons of tool estimates with those exposure situations for which aggregated data were provided are described. 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.

3.3.1 ECETOC TRAv2

Table 3.33 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 3.34 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 3.33 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	<0.01	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.

[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.

Table 3.34 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 TRA v2 estimates for the exposure situations; Min TRAv2: lowest ECETOC TRAv2 estimate; Max TRAv2: highest ECETOC TRAv3 estimate.

Figures 3.17- 3.19 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 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.

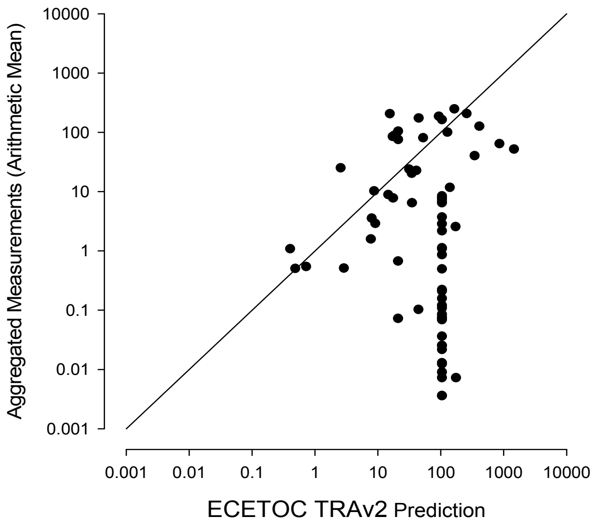

Figure 3.17 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv2 predictions (volatile liquids) (mg m^{-3})

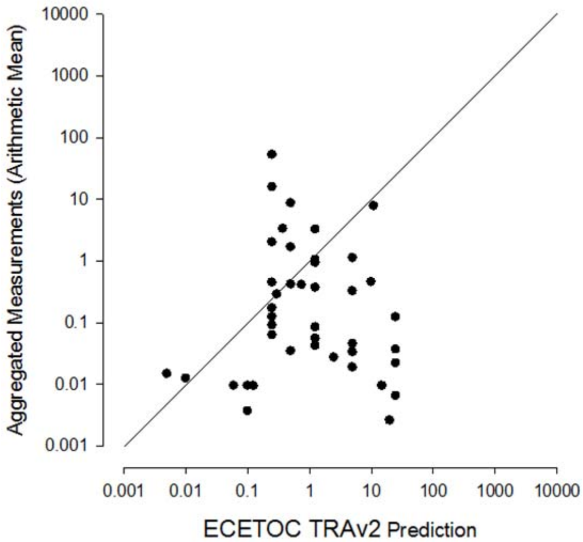

Figure 3.18 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv2 predictions (powders) (mg m^{-3})

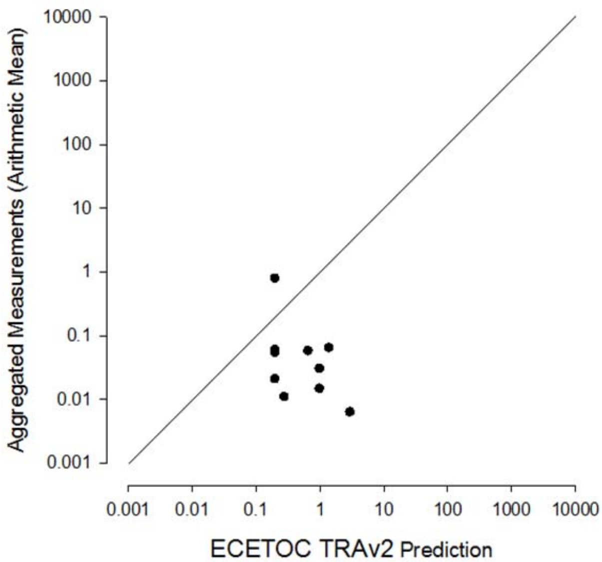

Figure 3.19 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv2 predictions (metal abrasion) (mg m^{-3})

Table 3.35 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 3.35 Summary of the ratios of the arithmetic mean of the aggregated measurement results over the arithmetic 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.

3.3.2 ECETOC TRAv3

The available aggregated measurement results for comparison with ECETOC TRAv3 (Table 3.36) were the same as for the ECETOC TRAv2 (Table 3.33). Table 3.37 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 3.34).

Table 3.36 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 3.37 Summary of the ECETOC TRAv3 estimates by exposure category available for comparison with (aggregated) measurement data (mg m^{-3})

Exposure category	N Sit	Mean TRAv3	Min TRAv3	Max TRAv3
Volatile liquids[1)]	69	82.54	0.38	1051.60
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 TRA v3 estimates for the exposure situations; Min TRAv3: lowest ECETOC TRAv3 estimate; Max TRAv3: highest ECETOC TRAv3 estimate.

Figures 3.20- 3.22 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.

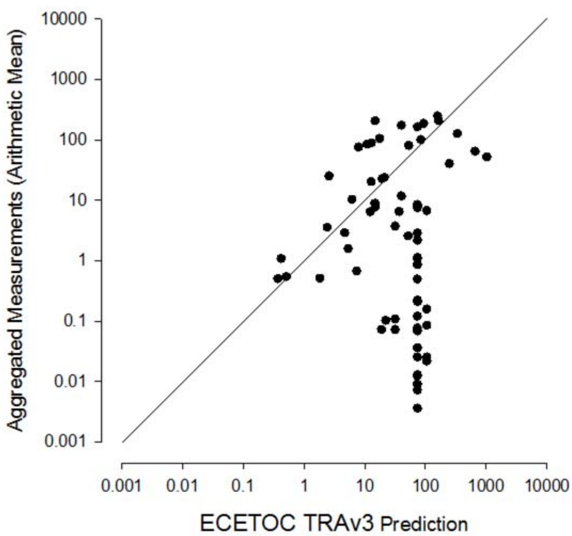

Figure 3.20 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv3 predictions (volatile liquids)(mg m^{-3})

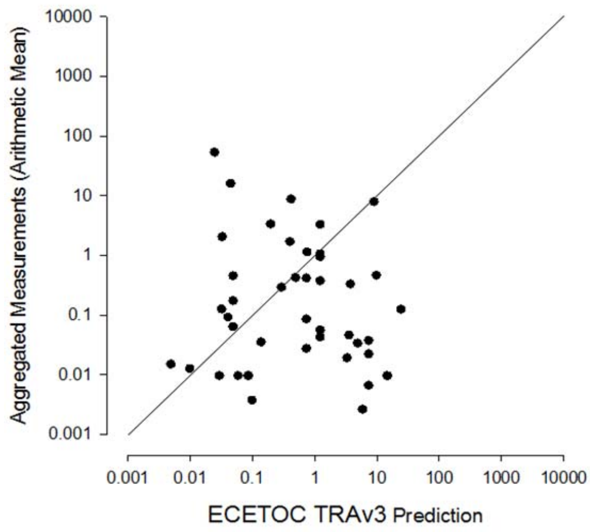

Figure 3.21 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv3 predictions (powders) (mg m^{-3})

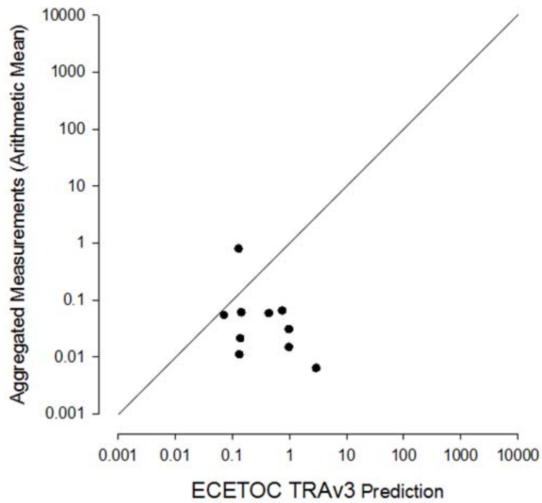

Figure 3.22 Comparison of the AM of the aggregated measurement data compared with the AM of the ECETOC TRAv3 predictions (metal abrasion) (mg m^{-3})

The AM and GM of the ratios of the measured values over the tool-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 3.38).

Table 3.38 Summary of the ratios of the arithmetic mean of the aggregated measurement results over the arithmetic mean of the ECETOC TRAv3 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	1.17	0.05	<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.

3.3.3 MEASE

Tables 3.39 and 3.40 and Figures 3.23- 3.26 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 measurements over the MEASE estimates are higher than 1. The estimated percentage of measurements that have exceeded the MEASE estimates was 54% (Table 3.41). 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 ($r=0.45$, $p=0.1963$). However, for metal processing and powder handling there was no evidence of a correlation between measurement results and tool estimates.

Table 3.39 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 3.40 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	1.11	0.04	5.50
Metal processing	25	0.74	0.08	6.72
Powder handling	45	4.00	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.

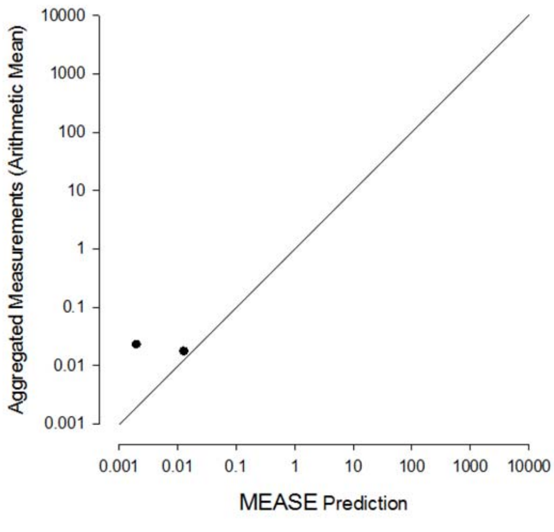

Figure 3.23 Comparison of the AM of the aggregated measurement data compared with the AM of the MEASE predictions (non-volatile liquids) (mg m^{-3})

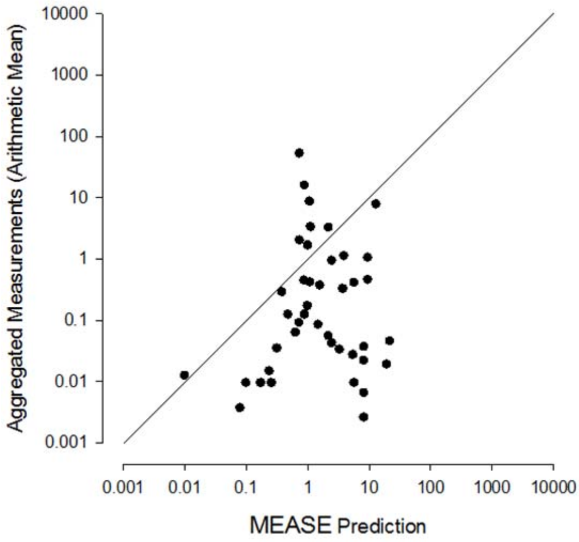

Figure 3.24 Comparison of the AM of the aggregated measurement data compared with the AM of the MEASE predictions (powders) (mg m^{-3})

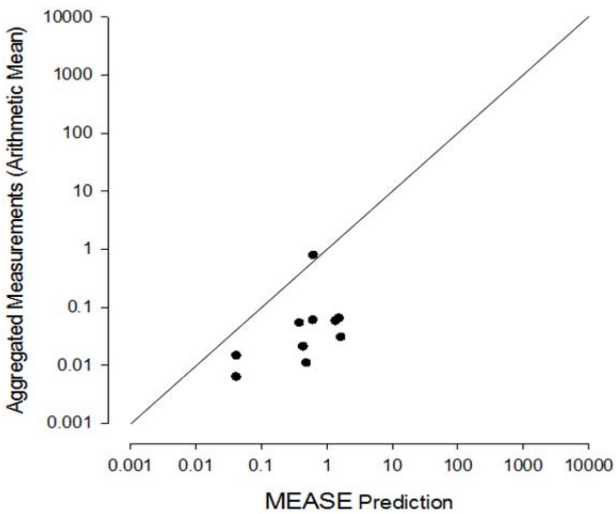

Figure 3.25 Comparison of the AM of the aggregated measurement data compared with the AM of the MEASE predictions (metal abrasion) (mg m^{-3})

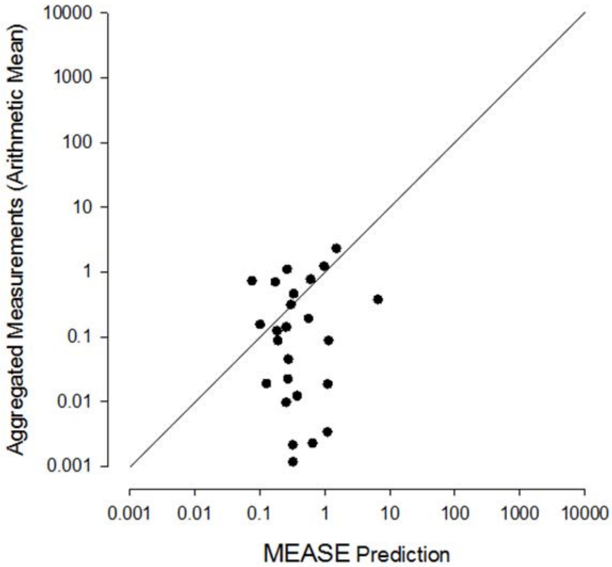

Figure 3.26 Comparison of the AM of the aggregated measurement data compared with the AM of the MEASE predictions (metal processing) (mg m^{-3})

Table 3.41 Summary of the ratios of the arithmetic mean of the measurement results over the arithmetic mean of the MEASE 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
Non-volatile liquids[1)]	2	42	6.32	3.88	1.33	11.31	54
Metal abrasion	10	98	0.21	0.08	0.01	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.

3.3.4 EMKG-EXPO-TOOL

The aggregated measurements used for comparison with estimates from the EMKG-EXPO-TOOL are summarised in Table 3.42. The corresponding tool estimates are shown in Table 3.43. 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 3.42 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 3.43 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	4.86	0.01	15.00

[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 3.27 and 3.28.

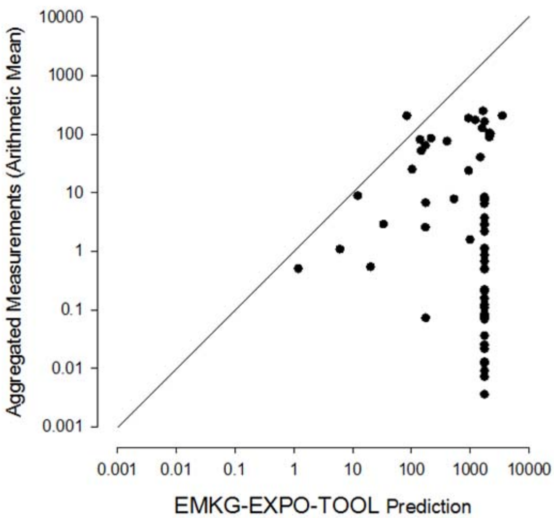

Figure 3.27 Comparison of the AM of the aggregated measurement data compared with the AM of the EMKG-EXPO-TOOL predictions (volatile liquids) (mg m^{-3})

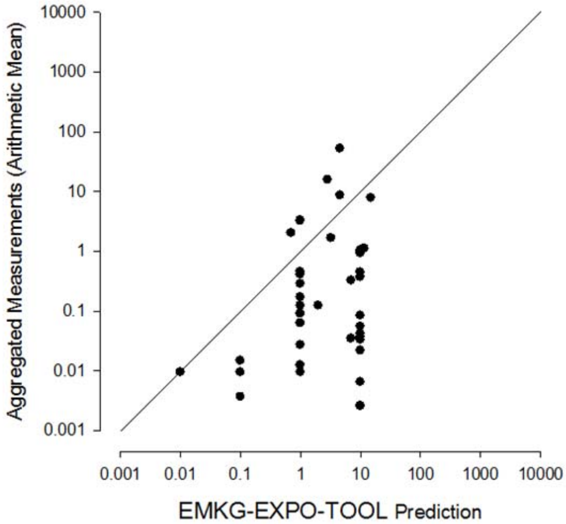

Figure 3.28 Comparison of the AM of the aggregated measurement data compared with the AM of the EMKG-EXPO-TOOL predictions (powders) (mg m^{-3})

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

Table 3.44 Summary of the ratios of the arithmetic mean of the measurement results over the arithmetic mean of the EMKG-EXPO-TOOL 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 liquid[1)]	62	476	0.11	<0.01	<0.01	2.36	2
Powder handling	42	817	0.78	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.

3.3.5 STOFFENMANAGER

The aggregated measurement data available for comparison with the STOFFENMANAGER estimates (75th and 90th percentiles) are summarised in Table 3.45.

Table 3.45 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 3.46).

Table 3.46 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 3.29 – 3.31).

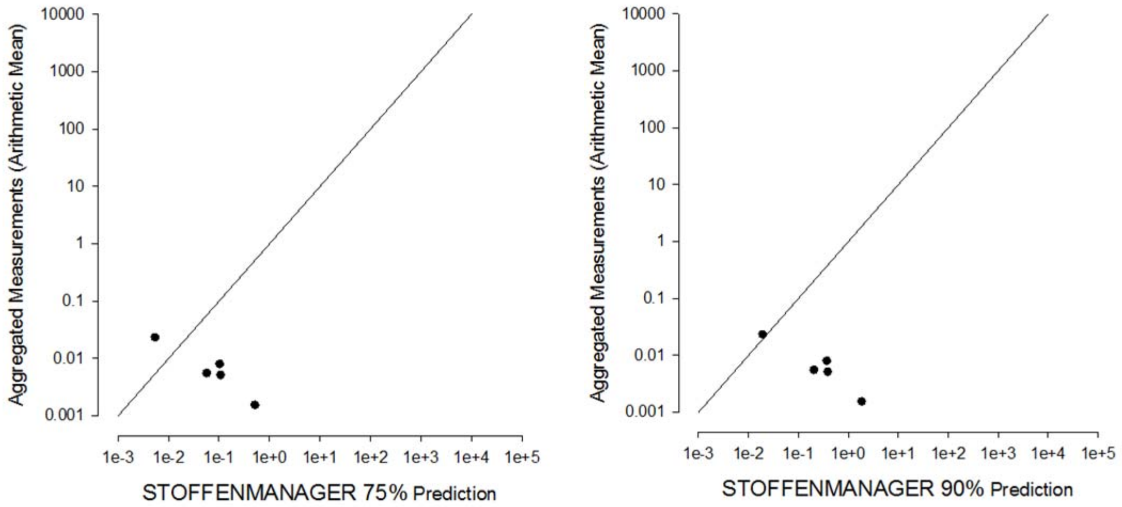

Figure 3.29 Comparison of the AM of the aggregated measurement data compared with the AM of the STOFFENMANAGER predictions (75th and 90th percentiles) – non-volatile liquids (mg m^{-3})

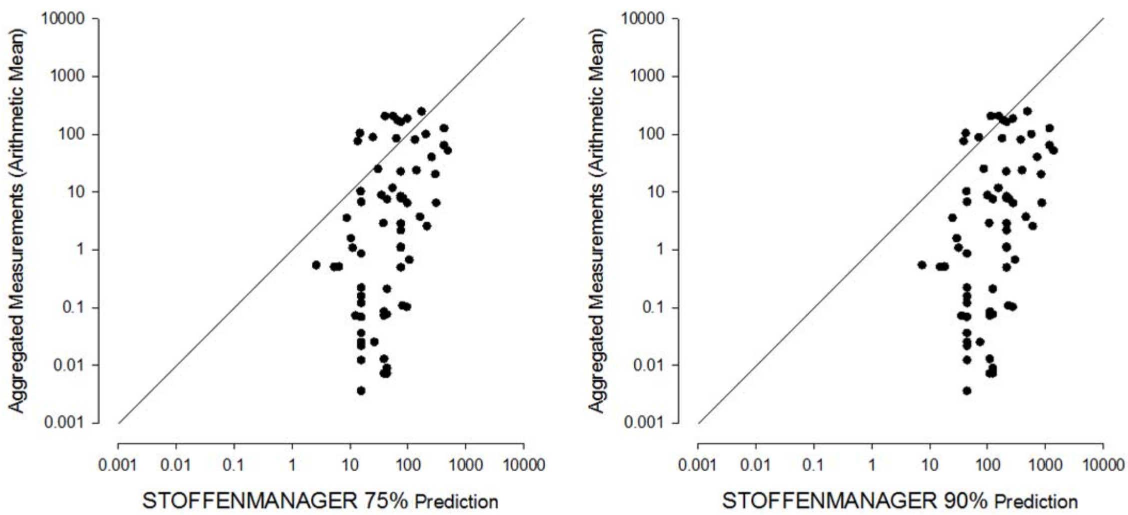

Figure 3.30 Comparison of the AM of the aggregated measurement data compared with the AM of the STOFFENMANAGER predictions (75th and 90th percentiles) –volatile liquids (mg m^{-3})

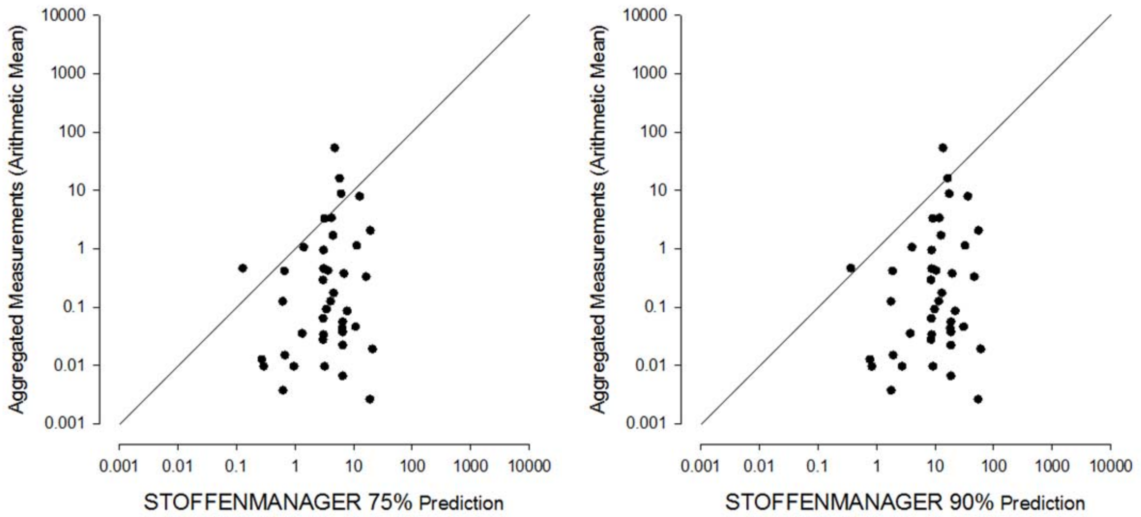

Figure 3.31 Comparison of the AM of the aggregated measurement data compared with the AM of the STOFFENMANAGER predictions (75th and 90th percentiles) –powder handling (mg m^{-3})

Table 3.47 summarises 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 3.47 Summary of the ratios of the arithmetic mean of the measurement results over the arithmetic 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.

3.4 Impact of tool parameters on level of conservatism

Table 3.48 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 3.48 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.

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.

Table 3.48 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

3.5 Impact of use of default parameters

As noted in Section 2.3, 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 investigated. Table 3.49 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 3.49 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 Discussion

4.1 Overview

This report 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 measurements exceeded the tool estimate

As reported elsewhere in the eteam Project (Work Package II.1: Uncertainty of Tier 1 models), 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 90th percentile of an exposure distribution. For STOFFENMANAGER, which generates and exposure distribution, the estimates for the 75th and 90th percentiles. STOFFENMANAGER estimates were considered to be sufficiently conservative if the percentage of the 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 case the EMKG-EXPO-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.

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.

4.2 Overall level of conservatism

The overall level of conservatism was evaluated using the percentage of measurements exceeding the tool estimates.

Table 4.1 provides an overview of the proportions of measurement that exceeded the tool estimates for the combined individual and aggregated datasets.

Table 4.1 Proportion of measurements exceeding the tool estimate, by exposure category (individual and aggregated measurements combined)

	Non-volatile liquids			Volatile liquids			Metal abrasion			Metal processing			Powder handling		
Tool	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	24	-	-	-	1101	180	16
ECETOC TRAv3	0	-	-	1842	586	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

The largest number of measurement results available for comparison with tool estimates was for volatile liquids. Based on the combined individual and aggregated results available in this study (Table 4.1), 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 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 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 90th 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.

$$\%S > T = \frac{\sum_{i=1}^{N} \frac{\sum_{j=1}^{n_i} P_{ij}}{n_i}}{N} \quad \textbf{Equation 4.1}$$

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 4.2 together with %M>T as reported previously.

Table 4.2 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.

4.3 Differences in level of conservatism between data types and providers

Table 4.1 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, whilst there are some differences between exposure categories, on examining the data from each of the providers, the sets with outlying mean levels of exposure are generally 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 and percentage of exceedances 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 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 related to 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.

4.5 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.

4.5.1 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.

4.5.2 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.

4.5.3 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 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.

4.5.4 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.

4.6 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, with the results of the stratification exercise given in Appendix 4, Tables A4.1 – A4.4. In the following sections, only those combinations of PROC and input parameter which gave rise to observable differences in level of conservatism are discussed.

4.6.1 Powders

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

4.6.1.1 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.

4.6.1.2 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.

4.6.1.3 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.

4.6.1.4 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.

4.6.2 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.

4.6.2.1 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.

4.6.2.2 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.

4.6.2.3 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

4.6.2.4 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.

4.6.3 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.

4.6.3.1 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.

4.6.3.2 Concentration in mixture

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

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.

4.6.4.1 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.

4.6.4.2 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.

4.6.4.3 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.

4.6.4.4 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.

4.6.5 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.

4.7 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 4.3 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. Differences in the level of correlation of the measurement data with the tool estimates were noted both between exposure categories and comparator data type.

Table 4.3 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	0.31	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)

Based on individual measurement results, strong (r=0.9) and moderate (r=0.6) correlations were observed for non-volatile liquids for MEASE and STOFFENMANAGER, respectively. This suggests that, whilst the tools may not be sufficiently conservative 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 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 and suggested 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 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.

4.8 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.

4.8.1 Dataset

4.8.1.1 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 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 and resources 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 model 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 could be used 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.

4.8.1.2 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 measurement 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.

4.8.2 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.

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, and these generally covered a narrower range of process/ activity types. 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 4.1, 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 75^{th} and 90^{th} 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 available 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 regarding the initial base exposure estimates in relation to domain 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 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.

6 Acknowledgements

We would like to thank the members of the eteam Project Advisory Board and the other data providers for their assistance with data collection, the external validation process and in the preparation of this and other Deliverable reports throughout the course of the project.

We would also greatly appreciate the assistance of the following IOM colleagues; Dr Andrew Apsley, Dr Karen Galea, Dr Melanie Gorman Ng, Dr Anne Sleeuwenhoek and Professor John Cherrie for their help during the external validation exercise and in the preparation of this report.

References

Crawford JO, Cowie H, Lamb J, van Tongeren M, Galea KS. (2012). eteam Project Deliverable D18: Report on the User-Friendliness of Tier 1 Exposure Assessment Tools used under REACH.

EBRC Consulting GmbH, MEASE documentation: http://www.ebrc.de/industrial-chemicals-reach/projects-and-references/mease.php. Accessed 12 May 2014.

European Chemicals Agency (2010). Guidance on information requirements and chemical safety assessment. Chapter R.12: Use descriptor system. Helsinki: ECHA.

European Chemicals Agency (2012). Guidance on information requirements and chemical safety assessment. Chapter R.14: Occupational exposure estimation. Helsinki: ECHA.

European Chemicals Agency Compliance checks
http://echa.europa.eu/regulations/reach/evaluation/compliance-checks Accessed 12 May 2014

Gorman Ng M, de Poot S, Schmid K, Cowie H, Semple S, van Tongeren M (2014) A preliminary comparison of three dermal exposure sampling methods: rinses, wipes and cotton gloves. Environmental Science: Processes & Impacts. DOI: 10.10139/c3em00511a.

Helsel DR. (2012). Statistics for censored environmental data using Minitab® and R. Hoboken, NJ: John Wiley and Sons.

Hesse S, Hahn S, Schroeder K, Mangelsdorf I, Lamb J, van Tongeren M (2012). eteam Project Deliverable D5: Gathering of background information and conceptual evaluation. (Final report)

Hesse S, Hahn S, Schroeder K, Mangelsdorf I, Lamb J, van Tongeren M.(2014). eteam Project Deliverable D24: Uncertainty of Tier 1 models. (Final report).

Hofstetter E, Spencer JW, Hiteshew K, Coutu M, Nealley M (2012) 'Evaluation of Recommended REACH Exposure Modelling Tools and Near-Field, Far-Field Model in Assessing Occupational Exposure to Toluene from Spray Paint' Ann. Occup. Hyg., 2013 57(2), pp. 210-20

Jones RM, Nicas M, (2006) 'Evaluation of COSHH Essentials for vapour degreasing and bag filling operations' Ann. Occup. Hyg., 2006 50 (2), pp. 137-47

Kindler and Winteler R (2010) Anwendbarkeit von Expositionsmodellen für Chemikalien auf Schweizer Verhältnisse Teilprojekt 1: Überprüfung der Modelle "EASE" und "EMKG-Expo-Tool" Staatssekretariat für Wirtschaft SECO 2010. Accessed on 11th August 2014, http://www.seco.admin.ch/suchen/index.html

Koppisch D, Schinkel J, Gabriel S, Fransman W and Tielemans E. ‘Use of the MEGA Database for the validation of the Stoffenmanager Model’ Ann. Occup. Hyg., 2012 56 (4), pp. 426- 439

Kromhout H (2002) ‘Design of measurement strategies for workplace exposures’ Occup Environ Med (59), pp. 349-354

Kromhout H, Symanski E and Rappaport SM (1993) ’A Comprehensive Evaluation of Within- And Between-Worker Components of Occupational Exposure to Chemical Agents’ Ann. Occup. Hyg., 1993 37 (3), pp. 253-270

Kromhout H, Fransman W, Vermeulen R, Roff M, van Hemmen JJ (2004) ‘Variability of Task-based Dermal Exposure Measurements from a Variety of Workplaces Ann. Occup. Hyg., 2004 48 (3), pp. 187-196

Kupczewska-Dobecka M, Czerczak S, Jakubowski M (2011) International Journal of Occupational Medicine and Environmental Health 2011;24(2) pp. 208 – 217

Lamb J, van Tongeren M, Rashid S, Hesse S (2014) eteam Project Deliverable D12: Description of Exposure Situations Used in the External Validation Exercise

Lamb J, Galea KS, Miller BG, Spankie S, van Tongeren M, Hazelwood G (2013) eteam Project Deliverable D22: Report on Between-User Reliability Exercise (BURE) and Workshop

Lee EG, Harper M, Bowen RB, Slaven J (2009) ‘Evaluation of COSHH Essentials: Methylene Chloride, Isopropanol, and Acetone Exposures in a Small Printing Plant’ Ann Occup Hyg 2009 53 (5): pp. 463-474.

Lee EG, Slaven J, Bowen RB, Harper M (2011) 'Evaluation of the COSHH Essentials Model with a Mixture of Organic Chemicals at a Medium-sized Paint Producer' Ann. Occup. Hyg., 2011 55 (1): pp. 16-29

Maidment SS (1998) Occupational hygiene considerations in the development of a structured approach to select chemical control strategies. Ann Occup Hyg. 1998 Aug;42(6): pp. 391-400.

Rajan B, Alesbury R, Carton B, Gerin M, Litske H, Marquart H, Olsen E, Scheffers T, Stamm R and Woldbaek T. (1997) European Proposal for Core Information for the Storage and Exchange of Workplace Exposure Measurements on Chemical Agents. Applied Occupational and Environmental Hygiene 12 (1) pp. 31-39.

Saltelli A, Tarantola S, Campolongo F, Ratto M. Sensitivity analysis in practice: A guide to assessing scientific models. Chichester: John Wiley and Sons.

Schinkel J, Fransman W and Heussen H (2010) ‘Cross-validation and refinement of the Stoffenmanager as a first tier exposure assessment tool for REACH’ Occup. Environ. Med. (67): pp. 125-132;

Tielemans E, Warren N, Fransman W, van Tongeren M, McNally K, Tischer M, Ritchie P, Kromhout H, Schinkel J, Schneider T and Cherrie JW (2011) ‘Advanced REACH Tool (ART): Overview of Version 1.0 and Research Needs’ Ann. Occup. Hyg., 2011 55 (9), pp. 949-956.

Tischer M, Bredendiek- Kamper, Poppek U (2003) 'Evaluation of the HSE COSHH Essentials Exposure Predictive Model on the Basis of BAuA Field Studies and Existing Substances Exposure Data' Ann. Occup. Hyg. 2003 47(7), pp. 557-569

Appendix 1 eteam Project user guides to entering inhalation and dermal data

IOM

Fraunhofer
ITEM

eteam Project-
Guide to Entering Inhalation Exposure Data

RESEARCH CONSULTING SERVICES
Multi-disciplinary specialists in Occupational and Environmental Health and Hygiene

www.iom-world.org

OUR IMPACT ON THE ENVIRONMENT

At IOM we seek to minimise our environmental impact. We produce thousands of reports every year and these consume a large quantity of paper. To minimise our impact on the environment, we prefer to only provide an electronic copy of reports, although we can provide a paper copy on request. If you have any additional requirements please let us know.

User Guide for Entering Inhalation Exposure Data

1. Before you start

The Institute of Occupational Medicine (IOM) has been commissioned by the German Federal Institute of Occupational Safety and Health, (BAuA) to carry out a comprehensive evaluation of the exposure assessment models identified as suitable for use in tier 1 assessments under REACH- the ECETOC TRA, MEASE, EMKG-Expo-tool, RISKOFDERM and Stoffenmanager.

In collaboration with colleagues at the Fraunhofer Institute of Toxicology and Experimental Medicine (ITEM), the IOM is carrying out an investigation of the underlying concepts of each of the models, assessing their user-friendliness and comparing model predictions with real workplace inhalation and dermal measurement data.

As part of the project, we would therefore like to gather information from a range of sources covering a variety of exposure situations.

An exposure situation can be defined as a set of workplace circumstances within which exposures occur, for example spraying of isocyanate paints in a car body repair facility. The exposure situation description should only cover tasks which are directly related to the activity for example filling of spray gun, spraying and cleaning out of gun. Where tasks take place in different exposure circumstances, (such as mixing of materials in another area with a different local exhaust ventilation system), and so occur separately rather than as an integral part of the process, these should be described as a different exposure situation on a separate worksheet.

All of the data gathered will be stored securely, used solely for the purposes stated, i.e. the validation of exposure assessment models. To do this, we have also sent you a Microsoft Excel template (ETEAM Project_Inhalation Data Collection Template) to allow you to enter information concerning **inhalation exposure** data you would like to share.

A separate Microsoft Excel template and guide to entering **dermal exposure** data has also been provided.

As the data required are sensitive, to prevent any unauthorised access to the template during the collection and submission process, you should:

a) Protect the template with a password. On the top menu go to **Tools>>Options**, then the **Security** tab, and enter a password in the 'password to open' field and press OK. It will prompt you to re-enter your password and then click on the OK button. You should then save the file to ensure the security changes are kept. The template will now require a password to be entered any time it is opened.
b) On submission of your data, please email the completed updated and password protected file to either Judith Lamb or Anne Sleeuwenhoek. In addition, and in a separate email, please send a copy of your password for the file to allow us to unlock and retrieve the documents.

The following sections of this document provide guidance on how to enter **inhalation exposure** data into the template.

If you have any questions concerning data entry, security and usage of the data please contact Judith Lamb (project leader) on Judith.lamb@iom-world.org or by telephone on +44 (0) 131 449 8030 or Anne Sleeuwenhoek on anne.sleeuwenhoek@iom-world.org or by telephone on +44 (0) 131 449 8049.

All data provided to us will be stored on the secure IOM server and will only be accessed by designated project team members. No data will be shared with other organisations. The identities of individuals or organisations providing data will not be disclosed.

2. Using the template

There are three different worksheets:

1. Introduction and instructions – this page will appear each time you open the template. It contains a brief introduction about the data collection process and condensed information on how to enter your data.
2. Data Provider Contact Details – [Please complete with your personal details]
3. ES_DE_Template01 – this is a master worksheet which should be used to create a blank copy, which can then be used to enter your exposure situation data (See Entering Data into the Template). The master sheet should not be changed.

3. Entering inhalation exposure data into the template

3.1 Starting a new worksheet

Sheet 'ES_DE_Template01' is a master sheet with sample data and you **must not** make any changes within it (Fig. 1).

You will need to create copies of this master worksheet for each exposure situation that you have inhalation exposure data for, which you can then complete. Please see the instructions below on how to create a copy of the master sheet and enter data.

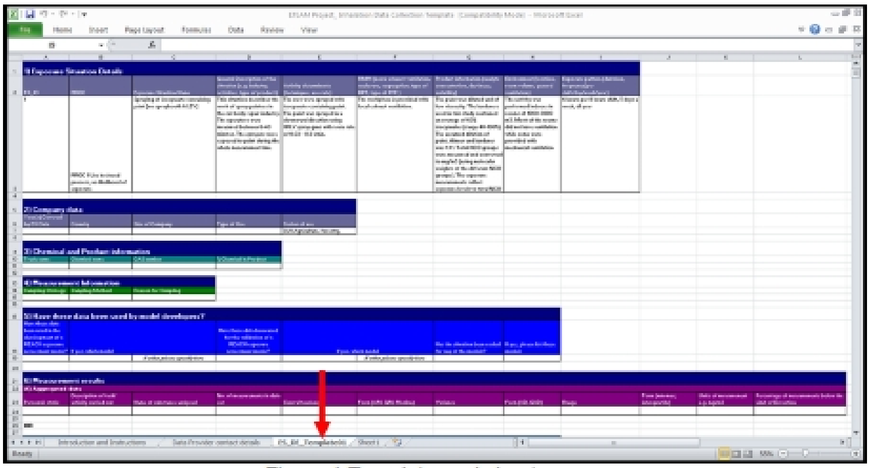

Figure 1 Template worksheet

Right click on 'ES_DE_Template01' (Fig 1)

Select (Move or Copy...) (Fig 2)

Select (Move to end from the list) (Fig 2)

Tick (Create a Copy) (Fig 2)

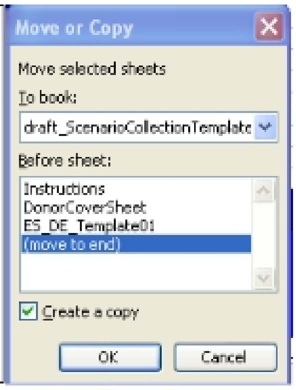

Figure 2

A new worksheet will be created. Rename the worksheet with a unique name e.g. Exposure Situation ID etc.

Before you start entering your own data onto the new sheet, you will need to clear the example data from it. Following this, you can use it to enter your own exposure situation details and measurement results.

The new empty worksheet contains the fields that you should fill in for each separate exposure situation.

You can directly write or paste data into the cells. If you have trouble pasting the data into the cell, then click on the cell and paste the data into the **Insert Function** field at the top of the screen (Fig. 3). There are some cells where you must select an option from a drop down pick-list.

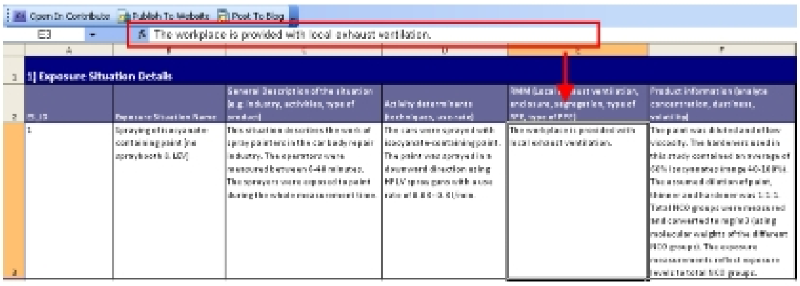

Figure 3 Alternative means of pasting data

Please repeat the steps above for each new exposure situation data entry.

More detailed instructions on the exact entry requirements for each data field are provided in the following sections.

3.2 Exposure Situation Details

Please use this section (Fig 4) to enter the data for the parameters listed in Table 1, which give general details about the exposure situation of interest:

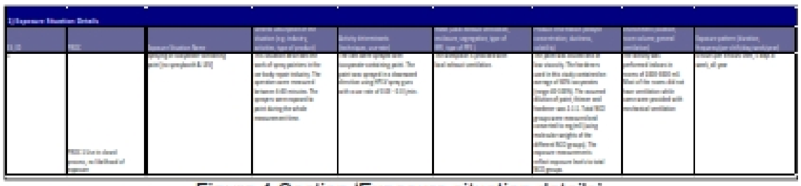

Figure 4 Section 'Exposure situation details'

Table 1: Exposure situation parameters

Parameter	Description	Example of required text
ES_ID	Please enter your unique identifying number for the exposure situation	1
PROC CODE (if available)	PROC code and description as per standard REACH process categories.	Drop down list options provided, e.g. PROC 7 – Industrial Spraying
Exposure Situation Name	Short descriptive name of the exposure situation	Spraying of isocyanate containing paint
General description of the situation (e.g. industry, activities, type of product)	A short description of the industry sector/ branch, particular circumstances of use, type product used,	This situation describes the work of spray painters in the car body repair industry. The sprayers were exposure to paint during the whole measurement time. Samples were taken over periods of between 6-40 minutes.

Activity determinants (techniques, use-rate)	A description of what was done- e.g. how were the activities carried out/details of the task/ equipment used/amount of product used per minute.	The cars were sprayed with isocyanate-containing paint. The paint was sprayed in a downward direction using HPLV spray guns with a use rate of 0.03-0.3 l/min.
RMM (Local exhaust ventilation, enclosure, segregation, type of RPE, type of PPE)	A description of the risk management measures in place in the work area, e.g. LEV (integrated or separate), use of cabins, segregation of work, containment, type of respiratory protective equipment used, type of personal protective equipment used (gloves, aprons, face shield etc)	The workplace is provided with local exhaust ventilation. The spraying activities are carried out in a separate room from other workers.
Product information (analyte concentration, dustiness, volatility)	A description of the product used- the percentage range of any active ingredients, an indication of the volatility or dustiness. A brief summary of any relevant information on the measurement analytes can also be included here	The paint was diluted and of low viscosity. The hardeners used in this study contained an average of 60% isocyanates (range 40-100%). The assumed dilution of paint, thinner and hardener was 1:1:1. Total NCO groups were measured and converted to mg/m3 (using molecular weights of the different NCO groups). The exposure measurements reflect exposure levels to total NCO groups.
Environment (location, room volume, general ventilation)	A description of the work area- indoors or outdoors; volume of the work room; is general ventilation provided (e.g. open windows/ doors/ roof vents/ mechanical ventilation fans)?	The activity was performed indoors in rooms of 1000-3000 m3. The rooms had mechanical ventilation.
Exposure pattern (duration, frequency(per shift/day/week/year)	A description of the manner/work pattern by which the workers are exposed in the situation.	The painters work 6 hours per 8 hours shift, 5 days a week, all year.

3.3 Company Data

Please use this section (Fig. 5) to enter the data for the parameters which relate to the company where the exposure took place (Table 2)

2) Company data				
Year(s) Covered by ES Data	Country	Size of Company	Type of Use	Sector of use
				SU1 Agriculture, forestry, fishery

Figure 5 Section 'Company data'

Table 2: Company data parameters

Parameter	Description of parameter	Example of required text
Year(s) Covered by ES Data	Year(s) over which measurement data were obtained.	Drop down list options provided
Country	Country in which the exposure situation takes place	Drop down list options provided
Size of Company	Description of the size of organisation in which the exposure takes place – micro/small/medium or large.	Drop down list options provided
Type of Use	Description of the general type of use during which the exposure takes place- manufacturing/ downstream industrial or downstream professional	Drop down list options provided
Sector of use	Description of the industry sector in which the exposure takes place- from the standard REACH categories	Drop down list options provided

3.4 Chemical and Product Information

Please use this section (Fig. 6) to enter the data for the parameters which relate to the product and/or components which have been measured (Table 3)

3) Chemical and Product information			
Trade name	Chemical name	CAS number	% Chemical In Product

Figure 6 Section 'Chemical and product information'

Table 3: Product or component parameters

Parameter	Description of parameter	Example of required text
Trade name	The trade name of the product or material used if available.	Acme IsoPaint
Chemical name	The chemical name of the substance of concern to which the worker is exposed	Methyl di-isocyanate
CAS number	The CAS number of the chemical of concern	101-68-8
% Chemical In Product	The percentage of the chemical of concern in the product.	60% (ranges from 40-100%)

3.5 Measurement Information

Please use this section (Fig. 7) to enter the data for the parameters which relate to the reasons that the inhalation sampling exercise was carried out and the general approach and measurement methods used (Table 4).

Figure 7 Section 'Inhalation measurement information'

Table 4: Inhalation measurement information parameters

Parameter	Description of parameter	Example of required text
Sampling Strategy	A description of the strategy by which the measurements were obtained- i.e. were they designed to measure a reasonable worst case exposure, were they representative of a typical exposure or were they randomly taken on any available worker?	Drop down list options provided
Sampling Method	A description of what general sampling method was used- e.g. active or passive/ respirable or inhalable dust?	Drop down list options provided
Reason for Sampling	A description of the reason for which the samples were taken- regulation/ to check compliance with an occupational exposure limit/ for research/ other purpose	Drop down list options provided

3.6 Have data been used by model developers?

Please use this section (Fig. 8) to enter information on parameters which will allow us to identify whether or not data can be used for validating a particular model (Table 5).

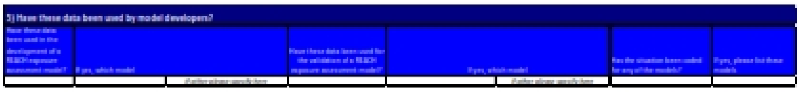

Figure 8 Section 'Have data been used by model developers?'

Table 5 Use of data in model development and validation- parameters

Parameter	Description of parameter	Example of required text
Have these data been used in the development of a REACH exposure assessment model?	We would like to determine if the data have been used in the development and/or calibration of any exposure assessment models (either for REACH or other purposes).	Yes/ No
If yes, which model	Name of REACH exposure assessment or other model	As per drop down list options for REACH exposure

		assessment models. For other "non-REACH" models select "other" and enter name as free text.
Have these data been used for the validation of a REACH exposure assessment model?	Please indicate if the data have been used for any other validation studies of REACH or other exposure assessment models.	Yes/ No
If yes, which model	Please enter the name of the REACH exposure assessment or other model for whose validation the data has been used.	As per drop down list options for REACH exposure assessment models. For other "non-REACH" models select "other" and enter name as free text.
Has the situation been coded for any of the models?	Please indicate whether the data have been coded previously for use with an exposure assessment model.	Yes/ No
If yes, please list these models	Please enter the name of the REACH exposure assessment or other model for which the data have been coded.	ECETOC TRA v2

3.7 Measurement Results

The measurements section of the Excel worksheet allows you to enter your inhalation exposure data for the given exposure situation in two ways; firstly as aggregated data and/or secondly as individual measurements.

A) Aggregated data

Where you have data which is aggregated across a number of workers, we need to gather some additional descriptive statistics to allow us to use the information fully. Please use this section (Figure 9) to enter the information about the necessary parameters (Table 6).

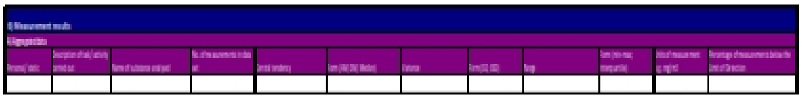

Figure 9 Section 'Measurements results. Aggregated data'

Table 6 Aggregated data parameters

Parameter	Description of parameter	Example of required text
Personal/Static	Please indicate the type of measurement, i.e. personal sample taken on the worker or static sample taken in area.	Personal
Description of Task/activity Carried out	A short description of the task that was carried out during the measurement period	Cleaning of spray equipment
Name of Substance(s) analysed	Please give the name of the substance for which analysis was carried out.	Total isocyanate groups

Parameter	Description of parameter	Example of required text
No. of measurements in data set	The number of measurements taken in the dataset. Please enter the number.	26
Central tendency	Please enter the numerical value for the indicator of central tendency for the dataset, e.g. the calculated value of the arithmetic mean (AM), geometric mean (GM) or median.	7.5
Form (AM, GM, Median)	What measure of central tendency has been used to describe the data- i.e. the AM/GM/ median?	Drop down list options provided
Variance	Please enter the numerical value of the measure of variance, e.g. the standard deviation (SD) or the geometric standard variation (GSD)	0.2
Form (SD, GSD)	What measure of variance has been used to describe the data- SD or GSD?	Drop down list options provided.
Range	Please enter the numerical values for the range of measurements within the dataset.	2.0- 12.5
Form (min-max; interquartile)	What type of range has been used to describe the dataset e.g. minimum – maximum or interquartile range?	Drop down list options provided.
Units of measurement e.g. mg/m^3	The units of measurement used in the dataset, e.g. ppm/ mgm^{-3}	Drop down list options provided.
Percentage of measurements below the Limit of Detection	Please enter the percentage of measurements which were below the limit of detection for the sampling method.	15

B) Individual Sample Results

Where you have collected inhalation measurement data which relate to individual workers' exposures, please use this section (Figure 10) to enter the information for the following parameters (Table 7).

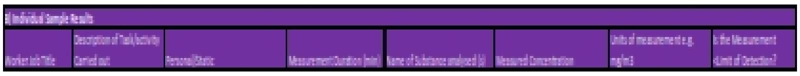

Figure 10 Section 'Measurements results. Individual sample results'

Table 7 Individual data parameters

Parameter	Description of parameter	Example of required text
Worker Job Title	The job title of the worker to whom the measurement relates.	Spray painter
Description of Task/activity Carried out	A short description of the task that was carried out during the measurement period	Cleaning of spray equipment
Personal/Static	Please indicate the type of measurement, i.e. personal sample taken on the worker or static sample taken in area.	Personal
Measurement Duration (min)	Please give the duration of the measurement period in minutes.	240
Name of Substance analysed	Please give the name of the substance for which analysis was carried out.	Total isocyanate groups
Measured Concentration	Please give the numerical value of the measured concentration for the sample	2.8
Units of measurement e.g. mg/m^3	The units of measurement used for the sample, e.g. ppm/ mgm^{-3}	Drop down list options provided.
Is the measurement below the limit of detection?	Please indicate if the measurement was below the limit of detection for the sampling method.	Yes/ No

4. Amending and deleting existing data

If you need to amend a record already entered, identify the sheet you wish to change and select the required cell. Next, amend the required information in the **Insert Function** area at the top of the sheet (Figure 11) and press {**Save**}. Please note that writing directly into a cell will overwrite the previous text.

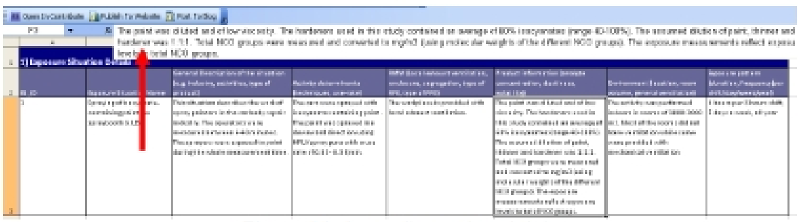

Figure 11: Amending entered data

You can delete the text from the cell by simply selecting the required cell and pressing {**Del**} button on your keyboard or by overwriting it.

IOM

Fraunhofer ITEM

eteam Project-
Guide to Entering Dermal Exposure Data

RESEARCH CONSULTING SERVICES
Multi-disciplinary specialists in Occupational and Environmental Health and Hygiene
www.iom-world.org

OUR IMPACT ON THE ENVIRONMENT

At IOM we seek to minimise our environmental impact. We produce thousands of reports every year and these consume a large quantity of paper. To minimise our impact on the environment, we prefer to only provide an electronic copy of reports, although we can provide a paper copy on request. If you have any additional requirements please let us know.

User Guide for Entering Dermal Exposure Data

1. Before you start

The Institute of Occupational Medicine (IOM) has been commissioned by the German Federal Institute of Occupational Safety and Health, (BAuA) to carry out a comprehensive evaluation of the exposure assessment models identified as suitable for use in tier 1 assessments under REACH- the ECETOC TRA, MEASE, EMKG-Expo-tool, RISKOFDERM and Stoffenmanager.

In collaboration with colleagues at the Fraunhofer Institute of Toxicology and Experimental Medicine (ITEM), the IOM is carrying out an investigation of the underlying concepts of each of the models, assessing their user-friendliness and comparing model predictions with real workplace inhalation and dermal measurement data.

As part of the project, we would therefore like to gather information from a range of sources covering a variety of exposure situations.

An exposure situation can be defined as a set of workplace circumstances within which exposures occur, for example spraying of isocyanate paints in a car body repair facility. The exposure situation description should only cover tasks which are directly related to the activity for example filling of spray gun, spraying and cleaning out of gun. Where tasks take place in different exposure circumstances, (such as mixing of materials in another area with a different local exhaust ventilation system), and so occur separately rather than as an integral part of the process, these should be described as a different exposure situation on a separate worksheet.

All of the data gathered will be stored securely, used solely for the purposes stated, i.e. the validation of exposure assessment models. To do this, we have also sent you a Microsoft Excel template (ETEAM Project_Dermal Data Collection Template) to allow you to enter information concerning **dermal exposure** data you would like to share.

A separate Microsoft Excel sheet and guide to entering **inhalation exposure** data has also been provided.

As the data required are sensitive, to prevent any unauthorised access to the template during the collection and submission process, you should:

a) Protect the template with a password. On the top menu go to **Tools>>Options,** then the **Security** tab, and enter a password in the 'password to open' field and press OK. It will prompt you to re-enter your password and then click on the OK button. You should then save the file to ensure the security changes are kept. The template will now require a password to be entered any time it is opened.
b) On submission of your data, please email the completed updated and password protected file to either Judith Lamb or Anne Sleeuwenhoek. In addition, and in a separate email, please send a copy of your password for the file to allow us to unlock and retrieve the documents.

The following sections of this document provide guidance on how to enter **dermal exposure** data into the template.

If you have any questions concerning data entry, security and usage of the data please contact Judith Lamb (project leader) on Judith.lamb@iom-world.org or by telephone on +44 (0) 131 449 8030 or Anne Sleeuwenhoek on anne.sleeuwenhoek@iom-world.org or by telephone on +44 (0) 131 449 8049.

All data provided to us will be stored on the secure IOM server and will only be accessed by designated project team members. No data will be shared with other organisations. The identities of individuals or organisations providing data will not be disclosed.

2. Using the template

There are three different worksheets:

1. Introduction and instructions – this page will appear each time you open the template. It contains a brief introduction about the data collection process and condensed information on how to enter your data.
2. Data Provider Contact Details – [Please complete with your personal details]
3. ES_DE_Template01 – this is a master worksheet which should be used to create a blank copy, which can then be used to enter your exposure situation data (See Entering Data into the Template). The master sheet should not be changed.

3. Entering dermal exposure data into the template

3.1 Starting a new worksheet

Sheet 'ES_DE_Template01' is a template with sample data and you **must not** make any changes within it (Fig 1)

You will need to create copies of this master worksheet for each exposure situation that you have dermal exposure data for, which you can then complete. Please see the instructions below on how to create a copy of the template sheet and enter data.

Figure 1 Template worksheet

Right click on 'ES_DE_Template01' (Fig 1)
Select {Move or Copy...} (Fig 2)
Select {Move to end from the list} (Fig 2)
Tick {Create a Copy} (Fig 2)
Click {OK} (Fig 2)

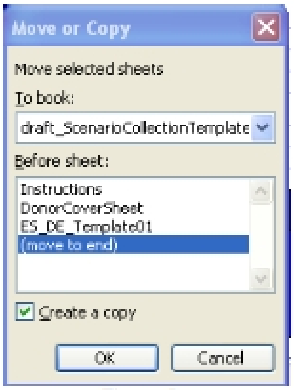

Figure 2

A new worksheet will be created. Rename the worksheet with a unique name e.g. Exposure Situation ID etc.

Before you start entering your own data onto the new sheet, you will need to clear the example data from it. Following this, you can use it to enter your own exposure situation details and measurement results.

The new empty worksheet contains the fields that you should fill in for each separate exposure situation.

You can directly write or paste data into the cells. If you have trouble pasting the data directly into the cell, then click on the cell and paste the data into the **Insert Function** field at the top of the screen (Fig. 3). There are some cells where you must select an option from a drop down pick-list.

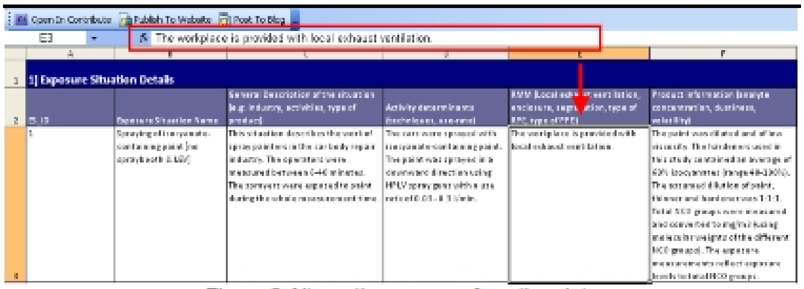

Figure 3 Alternative means of pasting data

Please repeat the steps above for each new situation data entry.

More detailed instructions on the exact entry requirements for each data field are provided in the following sections.

3.2 Exposure Situation Details

Please use this section (Fig 4) to enter the data for the parameters listed in Table 1, which give general details about the exposure situation of interest:

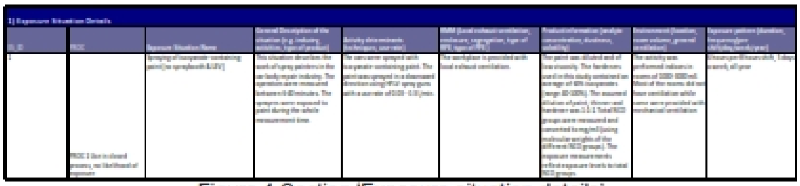

Figure 4 Section 'Exposure situation details'

Table 1: Exposure situation parameters.

Parameter	Description	Example of required text
ES_ID	Please enter your unique identifying number for the exposure situation	1
PROC CODE (if available)	PROC code and description as per standard REACH process categories.	Drop down list options provided, e.g. PROC 7 – Industrial Spraying
Exposure Situation Name	Short descriptive name of the exposure situation	Spraying of isocyanate containing paint
General description of the situation (e.g. industry, activities, type of product)	A short description of the industry sector/ branch, particular circumstances of use, type product used,	This situation describes the work of spray painters in the car body repair industry. The sprayers were exposure to paint during the whole measurement time. Samples were taken over periods of between 6-40 minutes.

Activity determinants (techniques, use-rate)	A description of what was done- e.g. how were the activities carried out/details of the task/ equipment used/amount of product used per minute.	The cars were sprayed with isocyanate-containing paint. The paint was sprayed in a downward direction using HPLV spray guns with a use rate of 0.03-0.3 l/min.
RMM (Local exhaust ventilation, enclosure, segregation, type of RPE, type of PPE)	A description of the risk management measures in place in the work area, e.g. LEV (integrated or separate), use of cabins, segregation of work, containment, type of respiratory protective equipment used, type of personal protective equipment used (gloves, aprons, face shield etc)	The workplace is provided with local exhaust ventilation. The spraying activities are carried out in a separate room from other workers.
Product information (analyte concentration, dustiness, volatility)	A description of the product used- the percentage range of any active ingredients, an indication of the volatility or dustiness. A brief summary of any relevant information on the measurement analytes can also be included here	The paint was diluted and of low viscosity. The hardeners used in this study contained an average of 60% isocyanates (range 40-100%). The assumed dilution of paint, thinner and hardener was 1:1:1. Total NCO groups were measured and converted to mg/m3 (using molecular weights of the different NCO groups). The exposure measurements reflect exposure levels to total NCO groups.
Environment (location, room volume, general ventilation)	A description of the work area- indoors or outdoors; volume of the work room; is general ventilation provided (e.g. open windows/ doors/ roof vents/ mechanical ventilation fans)?	The activity was performed indoors in rooms of 1000-3000 m3. The rooms had mechanical ventilation.
Exposure pattern (duration, frequency(per shift/day/week/year)	A description of the manner/work pattern by which the workers are exposed in the situation.	The painters work 6 hours per 8 hours shift, 5 days a week, all year.

3.3 Company Data

Please use this section (Fig. 5) to enter the data for the parameters which relate to the company where the exposure took place (Table 2)

2) Company data				
Year(s) Covered by ES Data	Country	Size of Company	Type of Use	Sector of use
				SU1 Agriculture, forestry, fishery

Figure 5 Section 'Company data'

Table 2: Company data parameters

Parameter	Description of parameter	Example of required text
Year(s) Covered by ES Data	Year(s) over which measurement data were obtained.	Drop down list options provided
Country	Country in which the exposure situation takes place	Drop down list options provided
Size of Company	Description of the size of organisation in which the exposure takes place – micro/small/medium or large.	Drop down list options provided
Type of Use	Description of the general type of use during which the exposure takes place- manufacturing / downstream industrial or downstream professional	Drop down list options provided
Sector of use	Description of the industry sector in which the exposure takes place- from the standard REACH categories	Drop down list options provided

3.4 Chemical and Product Information

Please use this section (Fig. 6) to enter the data for the parameters which relate to the product and/or components which have been measured (Table 3)

3) Chemical and Product information			
Trade name	Chemical name	CAS number	% Chemical In Product

Figure 6 Section 'Chemical and product information'

Table 3: Product or component parameters

Parameter	Description of parameter	Example of required text
Trade name	The trade name of the product or material used if available.	Acme IsoPaint
Chemical name	The chemical name of the substance of concern to which the worker is exposed	Methyl di-isocyanate
CAS number	The CAS number of the chemical of concern	101-68-8
% Chemical In Product	The percentage of the chemical of concern in the product.	60% (ranges from 40-100%)

3.5 Measurement Information

Please use this section (Fig. 7) to enter the data for the parameters which relate to the reasons that the dermal sampling exercise was carried out and the general approach and measurement methods used (Table 4).

4) Dermal Measurement Information		
Sampling Strategy	Sampling Method	Reason for Sampling

Figure 7 Section 'Dermal measurement information'

Table 4: Dermal measurement information parameters

Parameter	Description of parameter	Example of required text
Sampling Strategy	A description of the strategy by which the measurements were obtained- i.e. were they designed to measure a reasonable worst case exposure, were they representative of a typical exposure or were they randomly taken on any available worker?	Drop down list options provided
Sampling Method	A description of what general sampling method was used- e.g. skin wipe, skin strip, glove etc	Drop down list options provided
Reason for Sampling	A description of the reason for which the samples were taken- regulation/ to check compliance with an occupational exposure limit/ for research/ other purpose	Drop down list options provided

3.6 Have data been used by model developers?

Please use this section (Fig. 8) to enter information on parameters which will allow us to identify whether or not data can be used for validating a particular model (Table 5).

5) Have these data been used by model developers?							
Have these data been used in the development of a REACH exposure assessment model?	If yes, which model		Have these data been used for the validation of a REACH exposure assessment model?	If yes, which model		Has the situation been coded for any of the models?	If yes, please list these models
		If other please specify here			If other please specify here		

Figure 8 Section 'Have data been used by model developers?'

Table 5 Use of data in model development and validation- parameters

Parameter	Description of parameter	Example of required text
Have these data been used in the development of a REACH exposure assessment model?	We would like to determine if the data have been used in the development and/or calibration of any exposure assessment models (either for REACH or other purposes).	Yes/ No
If yes, which model	Name of REACH exposure assessment or other model	As per drop down list options for REACH exposure assessment models. For other "non-REACH" models

		select "other" and enter name as free text.
Have these data been used for validation of a REACH exposure assessment model?	Please indicate if the data have been used for any other validation studies of REACH or other exposure assessment models.	Yes/ No
If yes, which model	Please enter the name of the REACH exposure assessment or other model for whose validation the data has been used.	As per drop down list options for REACH exposure assessment models. For other "non-REACH" models select "other" and enter name as free text.
Has the situation been coded for any of the models?	Please indicate whether the data have been coded previously for use with an exposure assessment model.	Yes/ No
If yes, please list these models	Please enter the name of the REACH exposure assessment or other model for which the data have been coded.	ECETOC TRA v2

3.7 Measurement results

The measurements section of the Excel worksheet allows you to enter your dermal exposure data for the given exposure situation in two ways; firstly as aggregated data and/or secondly as individual measurements.

A) Aggregated data

Where you have data which are aggregated across a number of workers, we need to gather some additional descriptive statistics to allow us to use the information fully. Please use this section (Figure 9) to enter the data for the information about the necessary parameters (Table 6).

Figure 9 Section 'Measurement results. Aggregated data'

Table 6 Aggregated data parameters

Parameter	Description of parameter	Example of required text
No. of measurements in data set	The number of measurements taken in the dataset. Please enter the number.	26
Description of Task/activity Carried out	A short description of the task that was carried out during the measurement period	Cleaning of spray equipment
Name of Substance analysed	Please give the name of the substance for which analysis was carried out.	Total isocyanate groups
Measurement type	A description of whether actual or potential dermal exposure was being assessed	Drop down list options provided

Central tendency	Please enter the numerical value for the indicator of central tendency for the dataset, e.g. the calculated value of the arithmetic mean (AM), geometric mean (GM) or median.	7.5
Form (AM, GM, Median)	What measure of central tendency has been used to describe the data- i.e. the AM/GM/ median?	Drop down list options provided
Variance	Please enter the numerical value of the measure of variance, e.g. the standard deviation (SD) or the geometric standard variation (GSD)	0.2
Form (SD, GSD)	What measure of variance has been used to describe the data- SD or GSD?	Drop down list options provided.
Range	Please enter the numerical values for the range of measurements within the dataset.	2.0- 12.5
Form (min-max; interquartile)	What type of range has been used to describe the dataset e.g. minimum – maximum or interquartile range?	Drop down list options provided.
Units of measurement e.g. µg/cm²	The units of measurement used in the dataset, e.g. mg/cm², µg /cm²	Drop down list options provided.
Percentage of measurements below the Limit of Detection	Please enter the percentage of measurements which were below the limit of detection for the sampling method.	15

B) Individual Sample Results

Where you have collected dermal measurement data which relate to individual workers' exposures, please use this section (Figure 10) to enter the information for the following parameters (Table 7).

Figure 10 Section 'Measurements results. Individual sample results'

Table 7 Individual sample results parameters

Parameter	Description of parameter	Example of required text
Worker Job Title	The job title of the worker to whom the measurement relates.	Spray painter
Description of Task/activity Carried out	A short description of the task that was carried out during the measurement period	Cleaning of spray equipment
Duration of task/activity	Please give the typical duration of the tasks /activity which was sampled in minutes	240
Measurement type	A description of whether actual or potential dermal exposure was being assessed	Drop down list options provided
Body part	Please indicate the body part from which the sample was collected	Drop down list options provided.
Were gloves worn during the measurement period?	Please indicate if protective gloves were worn during the measurement period	Yes / No
Measurement Duration (min)	Please give the duration of the measurement period in minutes.	240
Name of Substance(s) analysed	Please give the name of the substance for which analysis was carried out.	Total isocyanate groups
Measured Concentration	Please give the numerical value of the measured concentration for the sample	2.8
Units of measurement e.g. µg/cm^2	The units of measurement used in the dataset, e.g. mg/cm^2, µg /cm^2	Drop down list options provided.
Is the measurement below the limit of detection?	Please indicate if the measurement was below the limit of detection for the sampling method.	Yes / No

4. Amending and deleting existing data

If you need to amend a record already entered, identify the sheet you wish to change and select the required cell. Next, amend the required information in the **Insert Function** area at the top of the sheet (Figure 11) and press {**Save**}. Please note that writing directly into a cell will overwrite the previous text.

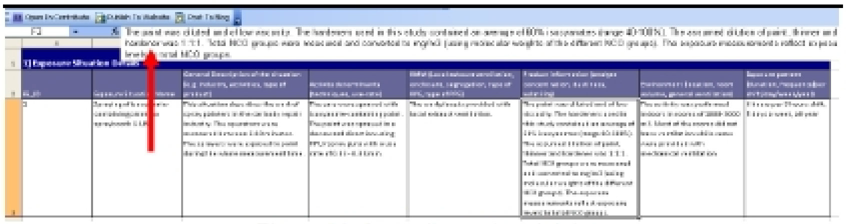

Figure 11: Amending entered data

You can delete the text from the cell by simply selecting the required cell and pressing {**Del**} button on your keyboard or by overwriting it.

Appendix 2 extract from eteam project quality control manual

The following extract from the eteam Project Quality Control Manual details the decision making process for assigning tool inputs during the coding process.

Table 5: Level of Parameter Uncertainty and Example Circumstances

Level of Uncertainty	Circumstances where this level of uncertainty would be allocated
No uncertainty	Where the choice of required input parameter was clear to the coder with no other sensible options.
Minor uncertainty	Where the coder was almost certain about the required input option, however some limited uncertainty existed as to a possible alternative
Major uncertainty	Where the coder could not be certain that one option was any more applicable/ "correct" than any other option or
	Where the coder was not certain from the description given and had to choose between two options (for example "yes/ no") or
	Where the range for a particular parameter as given in the contextual information for the exposure situation covered more than one range of the tool (for example a range of concentration within the description which goes across more than one concentration range in the tool)

5 CODING OF PHYSICO-CHEMICAL PROPERTIES INTO TOOLS

5.1 FUGACITY - VAPOUR PRESSURE

From discussions with tool users during the between-user reliability exercise, it was indicated that in general they would use the vapour pressure value for the pure substance rather than the partial vapour pressure over a mixture.

As such, and because of the very significant difficulty in identifying partial vapour pressures for mixtures without detailed compositional and process information, the vapour pressure of the pure substance at 20 °C will be used during coding, other than situations where the process is operating at higher temperatures. This temperature has been chosen as being appropriate with regard to both the scope of all of the tools and standard reference materials for this parameter.

Where there is a range given for vapour pressure (for example for mixed hydrocarbon solvents), the median value should be used for the estimation. A second choice of using the highest value of vapour pressure should then be made, with a designation of "minor uncertainty" noted if both values lie within the same vapour band category of the tool, and "major uncertainty" if the choice of highest value in the range requires a higher volatility band to be chosen within the tool.

Where there are mixtures of hydrocarbon solvents present in a situation, a randomised selection process as outlined previously will be used to identify the substance for which the pure vapour pressure will be used in the exposure estimation.

It is recognised that using this approach may lead to an under- or overestimation of the vapour pressure because of uncertainty in the concentration of the substance in the mixture and the effect of activity coefficients on component vapour pressures in non-ideal mixtures. However it is considered to be a pragmatic approach in the observed absence of detailed information on all other substances present in the particular situation. (please see section 5.3 below for further information on correcting for the concentration of a particular substance in a mixture)

To ensure standardisation across the coding team, a list of vapour pressures at 20 °C from the GESTIS-database has been provided by IFA, and will be used for frequently-occurring substances in the database, for example organic solvents such as toluene, ethyl acetate etc. In the event that the substance of interest is not included in the GESTIS-database list, the coding team will also be provided with a set of preferred reference sources for vapour pressures of less common substances. The source used for vapour pressure will be noted by the coders in their coding log for future reference.

Within the RISKOFDERM tool, dermal operation unit (DEO) "Spraying" there is an option to select the volatility of the carrier liquid. Where the choice is not clear, the option of "not highly volatile" should be chosen in the first instance as the more conservative option for dermal exposure and "highly volatile" as the second choice, with a "major uncertainty" assigned.

5.2 FUGACITY – INTRINSIC DUSTINESS AND METAL ABRASIVE PROCESSES

Information on intrinsic dustiness is very limited within the data available to the eteam project. Therefore, an educated guess at the dustiness of the substance will often need to be made based on the descriptions given and other available authoritative information for example discussions with the relevant data provider and/ or manufacturers' safety data sheets. The source used for identifying the dustiness will be recorded in the coding log book for future reference.

Where there is no clear authoritative information on the appropriate level of dustiness, a "medium" score should be given for the first option and then a "high" dustiness category for the second option. A "major" level of uncertainty should be allocated to this parameter. In these circumstances, the dustiness categories should be coded in the various tools as below:

Table 6: Allocation of Dustiness Category

Tool	"Medium" dustiness category	"High" dustiness category
EMKG-EXPO-TOOL	medium	high
ECETOC TRA v2 and ECETOC TRA v3	medium	high
MEASE	solid medium dustiness	solid high dustiness
Stoffenmanager	"a cloud of dust is generated in the air and stays visible for a while, e.g. like flour dust or talcum powder"	"a cloud of dust is formed in the air and stays visible for a long time"
RISKOFDERM	low/ moderately dusty solid	highly dusty solid

The dustiness of abrasive metal processes may also be unclear from the exposure situation description. In these cases, the guidance in the applicable tools (ECETOC TRA v2, ECETOC TRAv3 and MEASE) was followed regarding allocation of dustiness.

Within MEASE, where there is no clear information on the dustiness of the process, the first option will be "medium" fugacity followed by "high" for the second choice.

The fugacity of abrasive metal processes is handled differently in the ECETOC TRAv2 and ECETOC TRAv3 tools. The guidance in the ECETOC TRA tools and supporting documentation recommends that for PROCs 21- 25, thus including PROC 24a/b/c, the fugacity category should be identified by a comparison of the process temperature with the melting point of the metal, i.e. melting point < activity temperature (where abrasion is the main source of the dust), low fugacity should be chosen. It was not possible to determine the point of contact temperature for the relevant exposure situations collected within the eteam project database, thus all considered to fall within the low fugacity category and were coded as PROC 24a.

For metal abrasive processes, as for all of the coding activity, the decision on the most appropriate category will be made from the description given in the situation: in some cases the coders may have to rely on other sources, for example professional judgement/ experience of similar situations or internet searches relating to similar activities.

5.3 CONCENTRATION OF SUBSTANCE IN PREPARATION

Where there is a range of concentration of a substance given in the exposure situation description, the median value should be used for the first option and the upper limit of the range used for the second option. .

Where the use of the upper limit of the range requires the next highest concentration category in the tool to be chosen (for example where a range of 10- 40% is given in a situation, requiring the ">25%" option to be chosen in the tool for the upper end of the range), this should be designated as having "major" uncertainty.

Where there is no information given in the situation on the concentration of the substance, the following procedure should be used.

- If there is information available on the manufacturer and the product name, an internet search will be carried out to gather any useful information. Failing this, information will be sought on similar products and a best estimate of the concentration of the substance for the type of product will be made. Where a range of concentration is given, the median value will be used as the first choice and the highest values for the second choice. Uncertainty will be allocated as outlined above.

- If no sensible information is available, then an assumed concentration of 5-25% should be the first choice option for MEASE, the ECETOC TRA v2 and the ECETOC TRA v3, with a second choice of >25% and a "major uncertainty" allocated.

- For Stoffenmanager, where no sensible information is found, a first option concentration of 50% should be chosen, with a second choice of 100% and a "major uncertainty" allocated in these cases.

For the ECETOC TRA v2 and v3, MEASE and Stoffenmanager, corrections for the amount of substance in a mixture will be done using the relevant concentration correction factors within the tools themselves, whilst for the EMKG-EXPO-TOOL, this will be done retrospectively following the estimation process and prior to the comparison with the relevant workplace measurements.

6 CODING OF OPERATIONAL CONDITIONS

6.1 PROCESS CATEGORY/ HANDLING DESCRIPTION

For those tools which use the REACH descriptor system (ECETOC TRA v2, ECEOC TRA v3 and MEASE), the choice of PROC code is an important determinant in the calculation of the final exposure estimate. Our initial assessment of the findings from the between-user reliability remote completion exercise and workshop suggests that tool-users on occasion find the choice of PROC code very challenging. Within Stoffenmanager, similar task characterisation choice issues were suggested by the between-user reliability study. We expect the coding team to experience similar difficulties in assigning some PROC codes and handling descriptions. The following approach will therefore be taken.

Information describing the PROC codes and tasks (from ECHA, ECETOC, MEASE and Stoffenmanager guidance) will be provided to the coders to assist them in choosing the closest code/ handling category.

Where it is unclear which PROC code or handling description should be chosen, the one deemed most appropriate should be chosen as the first option, with the second closest option given as the second choice. The parameter should then be designated as having "major uncertainty" associated with it. Additional information relating to the choice made will be noted in the coding log book.

Some data providers (EBRC, NIOSH, SECO and industry) have allocated PROC codes prior to submission. These will be entered as the second choice option in cases in which the coders disagree with the suggested PROCs with the input template, with an appropriate level of uncertainty allocated. Any discrepancies between the provider and coder choices will also be noted in the coder's log book for future investigation.

6.2 TYPE OF SETTING/ DOMAIN OF ACTIVITY/ SCALE OF OPERATION

6.2.1 ECETOC TRA v2, ECETOC TRA v3, MEASE

For those tools which use the REACH descriptor system (ECETOC TRA v2, ECETOC TRA v3 and MEASE), the choice of domain of activity/ scale of operation can also have a significant effect on the final exposure estimate obtained. The domains are designated in the different tools as follows:

Table 7: Allocation of Domain of Activity/ Scale of Operation

Tool	Options for domain of activity/ scale of operation
ECETOC TRA v2	Industrial or public/ professional
ECETOC TRA v3	Industrial or professional
MEASE	Industrial or professional

However; there is no definitive guidance from ECHA in the REACH documentation as to the nature of these two categories, for example if the decision should be made on the basis of process size/ throughput (e.g. large scale production= industrial), location (e.g. factory or domestic) or process type (e.g. manufacture vs end use of product).

The ECHA document "Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system" (ECHA, 2010) indicates that information on the Sector of Use "industrial use" (SU 3) and "professional use" (SU 22) can be taken into consideration in deciding on the appropriate category.

These designations will be allocated where such information is available; however as for other input parameters, where a prior judgement has been made by the data provider, to ensure consistency and to allow comparison, the final choice will be made independently by the coding team. The domain/ setting allocated by the data provider, if it is different from that of the coding team, will be used as the second option and a level of uncertainty assigned accordingly.

Within ECHA document "Guidance on information requirements and chemical safety assessment Chapter R.14: Occupational exposure estimation" (ECHA, 2012), the following descriptions are also given:

- Industrial use: Application of the substance, mixture/product in an industrial process
- Professional use: Application of mixtures/products in skilled trade premises

The R14 document includes a suggestion that the choice can be difficult, and suggests that, where a domain of use is unclear, "professional" should be chosen as a conservative option as this reflects a higher final exposure estimate. Bearing in mind the above, the following method will be followed.

- Where the process clearly takes place in a plant, workshop or factory setting as part of an industrial process, "industrial" will be chosen, otherwise the coder will choose "professional/ public" domain.
- Where the domain is not clearly stated, a best guess will be made by comparison with similar known work activities, and consideration of other relevant factors, for example the size of the company, where small enterprises may be more likely to be professional and larger ones industrial.
- In situations where a suitable work activity for comparison cannot be identified, the domain will initially be coded as professional, with the second option as industrial, and "major uncertainty" assigned to this parameter.

6.2.2 EMKG-EXPO-TOOL

Within the EMKG-EXPO-TOOL, the scale of use is given in volume bands for liquids and in weight bands for solids. Where a stated point value quantity of substance is given (e.g. 10kg), this value should be used in the allocation of scale of use band. Where a range of amounts is given, for example 0.5- 10l, the median value should be used to allocate the band for the first option. The highest value in the range should be chosen for the second best option.
Where the upper end of the range lies within a higher band for scale of use within the tool, a designation of "major uncertainty" for this parameter should be made.

Within EMKG-EXPO-TOOL, there is an option to input information on tasks where a liquid (more than 1l) is applied to a surface > 1 m^2 in area. This option should be chosen only when it is considered to be appropriate, for example in application by roller, brushing or otherwise spreading over large surface areas, otherwise the "no" option should be selected. Within this parameter, the scale of use (>1l) refers to the amount used per event, thus for tasks carried out many times over an 8 hour shift, the total amount may in fact be larger than this.

6.2.3 Stoffenmanager

The domain of activity is implicit within the handling descriptions of Stoffenmanager chosen during task characterisation, thus does not require a separate choice to be made.

6.2.4 RISKOFDERM

Within RISKOFDERM, there is no specific parameter relating to domain of use, thus no choice has to be made. The amount of material is expressed in parameters related to use rate or application rate dependent on the DEO being used. The allocation of a value to these parameters will reflect as closely as possible the situation, however discussion between the coding team members and/ or the tool developer may be required on the best option for cases where the choice is not clear.

As a general rule, the coder should use best or median choice (e.g median use/ application rate), with the second choice option reflecting a high rate, and an appropriate level of uncertainty allocated.

6.3 DURATION OF EXPOSURE

The duration of exposure options differ between tools in numerical value and in the degree of effect that the choice makes on the final exposure estimate generated. For example the TRA v2 and v3 provides an 8 hour time weighted average estimate that can then be adjusted using actual task duration, whilst Stoffenmanager generates a task-based estimate. The facility within the Stoffenmanager tool to calculate 8 hour time weighted averages will not be used in the Project. The EMKG-EXPO-TOOL also allows for estimation of exposures in tasks lasting less than 15 minutes per day. The required coding options for each tool to accommodate these differences are outlined below.

6.3.1 ECETOC TRA v2 and ECETOC TRA v3

Where the measurement data relates to a task-based measurement, an assumption should be made that the exposure occurs for the whole of this period. The duration option of >4 hrs should be chosen in the tool to reflect this.

Where it is not clear how long the task lasted in comparison with the measurement duration, and there is an 8 hour (or more than 4 hour) measurement value, the option of "1-4 hours" should be chosen. A "major uncertainty" should be assigned to the parameter.

Where the actual time of exposure is given, and an 8 hour measurement is provided (i.e. the measurement time is > task duration), the relevant option on the tool should be chosen for the task time, e.g. <15 mins/ 15mins-1 hour etc.

Where the exposure time is given as range, the median value should be used as the first option, then the highest value of the range entered as the second choice. Where the upper value is within a higher duration band, the parameter should be coded as having "major uncertainty, otherwise a "minor uncertainty" should be assigned.

6.3.2 MEASE

In case of a task-based measurement, an assumption should be made that the exposure occurs for the whole of this period. The duration option of ">240 mins" should be chosen in the tool to reflect this.

Where it is not clear how long the task lasted in comparison with the measurement duration, and there is an 8 hour (or more than 4 hour) measurement value, the option of 60- 240 mins" should be chosen. A "major uncertainty" should be assigned to the parameter.

Where the actual time of exposure is given, and an 8 hour measurement is provided (i.e. the measurement time is > task duration), the relevant option on the tool should be chosen for the task time, e.g. <15 mins/ 15mins-60 mins.

Where the exposure time is given as range, the median value should be used as the first option, then the highest value of the range given as the second choice. Where this upper value is then within a higher duration band, the parameter should be coded as having "major uncertainty".

6.3.3 Stoffenmanager

The task duration options in Stoffenmanager do not affect the final exposure estimate therefore a default option of "4-8 hours per day" should be chosen for the sake of consistency.

During comparison of the Stoffenmanager estimates with the workplace data for the situations where a measurement duration > task duration is given, a correction factor will be applied to prevent apparent overestimation on the part of this tool. The correction factors applied will be matched to those used in the TRAv2, v3 and MEASE to account for shorter task durations within an 8 hour measurement period.

The frequency of task option within Stoffenmanager does not impact on the final exposure assessment so should be set to 4-5 days per week in all cases for consistency.

6.3.4 EMKG-EXPO-TOOL

The EMKG-EXPO-TOOL also generates a task-based estimate of exposure. Where the measurement data relate to a task-based measurement, an assumption should be made that the exposure occurs for the whole of this period. The estimate from the EMKG-EXPO-TOOL should be considered to reflect the exposure over the period of the task.

The EMKG-EXPO-TOOL does not allow for adjustment for task durations which are >15 minutes but <8 hours. Before comparison with the tool-generated estimates is made, a correction factor will be applied to the workplace measurement data for those situations where the sampling duration is greater than the task duration. This will prevent an apparent overestimation by this tool.

The correction factors applied will be matched to those used in the TRAv2, TRAv3 and MEASE to account for shorter task durations within an 8 hour measurement period.

Within EMKG-EXPO-TOOL, there is an option of <15 minutes task duration within an 8 hour shift. This option gives a significant reduction in the overall exposure estimate, therefore should be chosen only in situations where this is clearly stated as being the case.

6.3.5 RISKOFDERM

The task duration for the cumulative duration of the task (in minutes) should match the task duration given in the contextual information for the situation.

If no task duration is given, an informed assumption of duration should be made, and a "major uncertainty" assigned to the parameter. These instances will be discussed on an individual basis with the coding team and/ or tool developer as necessary.

As a general rule, the initial coding will reflect an "average" approach (i.e. a median cumulative duration), with the second choice option reflecting a longer task time. A "major uncertainty" will be allocated. Where applicable for a particular DEO, the choice for application rate will also be considered in conjunction with that for task time. A median value for application rate will also be chosen as the first option followed by a higher application rate for the second choice, and a "major uncertainty" allocated.

6.4 PROCESS TEMPERATURE

In relation to metal processing, the MEASE tool allows input of the process temperature and melting point of the metal or mineral. For a number of PROCs relating to hot processes, the exposure estimate is determined in part by the ratio of the process temperature to the material melting point.

In the event that the process temperature is unavailable for a particular exposure situation, the project database will be examined to identify similar activities. If necessary, where the exposure situation is unique in the database, i.e. no suitable comparator situations are available, internet searches will be carried out to identify an appropriate typical process temperature.

6.5 RISK MANAGEMENT MEASURES- TOOLS USED FOR INHALATION EXPOSURE ASSESSMENT

6.5.1 Local Exhaust Ventilation (LEV), Containment and General Ventilation

i) ECETOC TRA v2

The TRA v2 requires the user to state if LEV is present or not. For this, where it is not clear from the situation description that LEV is present, the first option chosen should be that it is not present "no", the second that it is present "yes". A designation of "major uncertainty" should be assigned to this parameter.

There is no choice given in this tool for general ventilation or containment.

ii) ECETOC TRA v3

The TRA v3 requires a choice between different combinations of indoors/ outdoors/LEV (present or not) and general ventilation (whether present and its effectiveness). The most appropriate option for the situation should be chosen from the list.
Where there is doubt about the presence of LEV, the conservative option "indoors" should be chosen, with "indoors with LEV" being chosen as the second choice and a "major uncertainty" allocated.

Where there is no indication about the level of general ventilation, the option "indoors" should be chosen. The option of "indoors with good general ventilation" should be chosen as the second option, with a designation of "minor uncertainty" allocated.

There is no separate option in this tool relating to process containment, however this is included in the level of containment assumed for several PROC codes, for example PROCs 1-4.

iii) MEASE

Within MEASE, the tool guidance suggests that the lower confidence level of the efficiency of local exhaust ventilation systems and other Risk Management Measures as indicated by Fransman et al (2008) should be chosen as a conservative option. In the absence of any additional information in the exposure situation description, which suggests higher efficiencies, this option shall be chosen as the first option. A second option of the median efficiency should be used with a designation of "major uncertainty" allocated.

Where clear information on the efficiency of a particular system is provided, the appropriate choice should be made from the list, e.g. the ECETOC 2009 default, median or upper confidence limit from the Fransman study.

The option for general ventilation within MEASE is included in this set of parameters (Implemented RMMs).

iv) EMKG-EXPO-TOOL

The most appropriate control level should be chosen with the section "Control Strategies", which includes options for general ventilation, LEV and containment.

Where it is not clear from the situation that there is LEV present, then "control approach 1" should be chosen, with "control approach 2" chosen as the second best choice and "major uncertainty" assigned to the parameter.

Similarly, where containment is mentioned in the description of the situation, but no detail is given about the level of containment, "control option 2" should be chosen as the first option and then "control level 3" as the second, and a designation of "major uncertainty" allocated.

v) Stoffenmanager

There are a number of combined options for Stoffenmanager that relate to LEV and containment within the section "available control measures".

Where the description given is unclear regarding the presence or not of LEV with or without containment these parameters will require consideration on a case by case basis. In general the first option chosen will reflect a sensible middle option, for example "LEV". In these circumstances, a "major uncertainty" will be allocated.

For Stoffenmanager, where general ventilation is considered separately to local controls, in situations where there is no information given on this parameter, a sensible best guess will be made, and a "major uncertainty" allocated.

6.5.2 Respiratory Protective Equipment (RPE)

As all of the measurement data are likely to have been collected outside of any RPE worn, with the possible exception of samples taken for welding fume, the option of "no RPE" should be chosen. For welding fume, the sampling method should first be checked to determine if the sample was taken inside or outside of any RPE. If there is no information on the method used, then it should be assumed that no RPE was worn, and the relevant "no RPE" option chosen from the tool.

For welding fume samples and other situations where it is stated clearly that the sample has been obtained inside RPE, the option chosen should match that given in the description. Where there is no detailed information given on the type of RPE, the lowest Assigned Protection Factor option available in the tool should be used as the conservative option.

6.5.3 Volume of Room

Within Stoffenmanager, in the absence of clear information about room size a best guess at the size of room will be made in the first instance for example via comparison with similar known workplace settings/ processes (either within the database or elsewhere), the following options should be chosen, depending on the domain of operation.

Table 7: Allocation of Room Volume

Domain	1st choice	2nd Choice option	Level of uncertainty
Industrial	100-1000m^3	>1000m^3	major
Professional/ Public	<100m^3	100-1000m^3	major

6.5.4 Other Risk Management Measures: e.g. Suppression, Use of cabins, Suppression at source/ Cleaning of workroom/ Inspection and Maintenance of Equipment.

Within MEASE and Stoffenmanager, there are options for a variety of other risk management measures. It is not possible within this document to identify the best and second option for all of these parameters for every potential situation.

A general approach of choosing a best guess / "average" option for the first choice and an appropriate more conservative option for the second option will be used, and uncertainty will be allocated accordingly.

For example, where there is a "yes/ no" option, in the absence of any clear information, the option of "no" will be chosen in the first instance, "yes" chosen for the second and a "major uncertainty" allocated.

7 PARAMETERS SPECIFIC TO DERMAL EXPOSURE ASSESSMENT TOOLS

7.1 PERSONAL PROTECTIVE EQUIPMENT - GLOVES

There are limited numbers of dermal data within the database, which have been collected using a variety of methods. The majority of these measurements represent actual dermal exposure, obtained using either interception or removal techniques. The Tier 1 tools generate estimates of potential exposure i.e. that which lands on the outer surfaces of workwear or on exposed areas of skin.

The glove option chosen for a particular situation will depend on the measurement method used. The "no gloves" option should be chosen where the measurement is taken directly from the skin using interception or removal techniques and where no protective gloves have been worn.

Where the measurement is of actual dermal exposure, i.e. carried out directly from the skin via removal or interception from under a protective glove, then the option for a glove being worn should be chosen as follows:

Table 8: Allocation of Glove Type

MEASE	Properly designed/ selected gloves
ECETOC TRA v3	Closest option to glove type given in sampling method/ description (gloves APF5 or gloves APF10) otherwise choose (gloves APF5) as a conservative option

7.2 Other Parameters related to Dermal Exposure

There are a number of parameters which are specific to assessing dermal exposure, within MEASE, RISKOFDERM, and in relation to the ECETOC TRA v3, consideration of the effect of LEV.
Where the choice of option is not clear for a particular parameter, the situation will require consideration/ discussion between the team on an individual basis, as it is not possible to cover every potential variation within this document.

In general the same approach will be taken as above- where the choice is not clear, the first option chosen will reflect an average / median exposure, and the second a less controlled activity/ higher estimated exposure, with the related degree of uncertainty allocated accordingly.

8 QUALITY CONTROL - CODING

As the allocation of input parameters to the tools is dependent in part on experience and professional judgment, initial training, regular feedback and mechanisms to check the appropriateness of the chosen inputs are required to ensure consistency amongst the coding team.

A training session for the team will be held prior to the start of coding to allow the details of this document to be fully discussed, with trial situations being coded and group reviewed.

Within each coding template, a tick box to indicate that all required inputs have been completed and checked for plausibility will be included.

Regular meetings will be held by the coding team to allow discussion of issues or areas of uncertainty.

In addition, we will double code approximately 10% of the exposure situations, during which the plausibility of the choices, for example vapour pressure, will also be checked.

Differences will be resolved via group discussion and significant variation will trigger a more thorough review of the data.

9 IMPLEMENTATION OF SEMI-AUTOMATED METHODS OF RUNNING TOOLS- ACCESS FUNCTIONS AND BATCH MODE ROUTINES

To facilitate handling of the large numbers of exposure situations within the database, and reduce the risk of data entry errors during manual coding of contextual information into the tool parameters, semi-automated methods of implementing the various tools within the database have been developed and are detailed below.

For EMKG-EXPO-TOOL and Stoffenmanager, the project team has incorporated the decision process and algorithm for the tools into the database.

Similarly, a routine has been written by the project team to run the Excel-based MEASE, RISKOFDERM and ECETOC TRA v2 tools in batch mode. This involves the data being exported from the database in a batch, single-line Excel format, then run through the tools and re-imported. A record of the exposure estimate generated is therefore stored with its respective exposure situation description in the database.

The ECETOC TRA v3 tool contains an in-built batch-run facility which accepts data in batches of up to 60 situations, with 15 situations per substance. An Access query has been designed to extract data in the input format of the tool from the eteam database. The data are then transformed to reformat them and run through the TRA v3. Following completion, the results are copied back into the database and stored with the situation description.

9.1 QUALITY CONTROL - WITHIN-DATABASE IMPLEMENTATION OF TOOLS

To verify that the EMKG-EXPO-TOOL process and Stoffenmanager algorithm have been correctly incorporated into the database, and are functioning as the respective "standalone" tool would, a number of test situations will be run through the original tools for cross-checking. These situations will be chosen to reflect a range of activities, substances and tool parameters, thus ensuring as far as reasonably practicable that the database versions of the tools are operating properly.

The eteam routines used do not affect the exposure estimation process of the TRA v2, TRA v3, RISKOFDERM and MEASE, however we will also run test/ cross-check batches as described above to verify that the system is functioning correctly in terms of the export and import mechanisms from these tools.

There are many safeguards built into the original tools to guide and assist the user to verify the "sense" of their inputs, for example logic checks between combinations of physical form and fugacity or process. The project scope does not allow for reproduction of all of these safeguards in the within-database implementation of the tools, therefore the plausibility checks carried out by the original and duplicate coders of the inputs mentioned above will be of great importance in ensuring sensible outputs. This is especially the case for Stoffenmanager and the EMKG-EXPO-TOOL where the tool processes themselves are incorporated within the database.

In addition, as the routines used to run the ECETOC TRA v2, ECETOC TRA v3 and MEASE tools within the database do not alter their actual operation, these internal safeguards and checks will still operate and will result in the programme flagging up any inconsistencies which will then be addressed through a review of the input parameters.

10 DOCUMENT REVIEW

This document will be reviewed as necessary in the light of the initial coding training session and experience gained during the exercise itself.

Appendix 3 quality control of coding process- summary of blind recoding exercise

Appendix 3, Table 1 Quality control of coding process- blind re-coding of situations

Tool/ (number of situations double coded)	Number of situations with differences	Difference			Comments/ examples of differences	Action taken
		Initial coding correct	Second coding correct	Neither coding correct		
ECETOC TRAv3 (90)	26	20	5	1	Situations where initial coding was deemed correct related primarily to pathology work where differences in PROC code were noted (PROC 13 for initial coding and PROC 15 for the second).	All relevant situations were reviewed and standardised as PROC 13 to reflect quantities and nature of task.
					Other situations where the initial coding was deemed correct related to choice of transfer PROC rather than mixing PROC where the task involved use of a mixer.	All relevant situations were reviewed and PROC codes verified as to whether filling/ loading task or mixer operation.
					Situations where the second coding was correct related primarily to 4 situations where the measurement was for inhalable dust but a concentration reduction for a specific substance had been made.	All inhalable dust measurement situations reviewed and concentration set to >25%/ not in preparation for relevant tools.
					A situation where the professional setting had been chosen with enhanced ventilation plus LEV was identified. All professional situations were reviewed.	Situations where combination of LEV and enhanced ventilation in professional setting had been chosen were identified and corrected.
					A situation where both the original and second codings were deemed incorrect which related to mixer feeding was identified.	As above: all relevant situations were reviewed and PROC codes verified as to whether filling/ loading task or mixer operation.
ECETOC TRAv2 (90)	46	41	5	0	Situations where initial coding was correct related primarily to pathology work where differences in PROC code were noted (PROC 13 for initial coding and PROC 15 for the second).	All relevant situations were reviewed and standardised as PROC 13 to reflect quantities and nature of task.
					Situations where the initial coding was deemed correct related to use of solvents for cleaning in professional premises (as per initial coding), rather than industrial (second coding)	Initial coding correct but all relevant situations reviewed to verify correct choice had been made.
					Situations relating to filling and sieving had been coded correctly compared with mixing as chosen by the second coder.	All relevant situations were reviewed and PROC codes verified as to whether filling/ loading task or mixer operation.
					Differences between initial coding of PROC 8b for dedicated filling points and second coding choice PROC	Initial coding correct, but all relevant situations checked.

					8a (non-dedicated) identified.	
EMKG-EXPO-TOOL (55)	24	22	2	0	Situations where initial coding related to millilitre- 1l quantities deemed correct for quantities used per task in opticians- second coding chose 1-1000l option.	Relevant situations checked to make sure coding was consistent.
					Situations involving mixer dosing with powder were identified where the “large” quantity had been chosen for the initial coding and “medium” for the second coding, during industrial scale manufacturing processes. Initial coding deemed correct.	Relevant situations checked to make sure coding was consistent.
					Situations involving pathology processes originally coded as 1-1000l quantity, second coding was “millilitres-1l”. Original coding deemed correct from description.	None
					Situations were noted where the original coding was correct for the vapour pressure category but the second coding was incorrect.	None- however cross checking of vapour pressures across all tools was subsequently carried out as described in Section 2.3.4.2.
					Situation noted where the original coding of “1-1000l” was correct rather than millilitres-1l for second coding.	None
					Situations where the original quantity was correct, whilst the second coding was deemed incorrect.	None.
					Situation noted where the second coding quantity was “small” and deemed to be correct whilst the original coding was “medium”.	Original coding changed accordingly.
					Situation noted where original coding did not include application on surfaces> 1m^2, whilst second coding (correctly) did.	Original coding changed accordingly.
MEASE (40)	18	12	6	0	Situations where the original coding was PROC 26, whilst the second coding was non-MEASE specific i.e. PROC 8a/8b, or in one case related to mixing rather than handling of powder.	Original coding verified. Cross checking across relevant tools of PROCs to make sure that PROC 26 used where appropriate for MEASE (as outlined in Section 2.3.4.2).
					Situation which was soldering (original coding) rather than grinding (second coding).	Similar situations checked for consistency. Coding of all of the hot metal processes was subsequently reviewed to make sure that the options chosen were correct for the situation and in comparison with the tool guidance.
					Situation where LEV was present, however second coder had missed it from inputs.	None.
					Situation noted where PROC 8a chosen by second coder, original coding was PROC 19.	Original coding changed as maintenance task

					One situation noted where the original coding was professional (correct) whereas the second coding was industrial.	None
					One situation where the original coding was enclosure whilst the second coder had chosen LEV.	Original coding kept.
					One situation where the original coding was PROC 2 for sampling task whilst second coding was better (8a).	Original coding corrected.
					Two situations where the original metal processing PROC was inconsistent with the MEASE guidance: PROC 25 instead of PROC 22 for casting and PROC 23 instead of PROC 25 for a large scale soldering process,	Coding of all of the hot metal processes was reviewed to make sure that the options chosen were appropriate for the situation and in comparison with the tool guidance, e.g. process temperatures / melting points.
					Situation where massive object had been chosen originally instead of medium dustiness (second coding) identified.	Relevant similar situations checked for dustiness choice.
					Situation noted where the PROC 27a had been chosen for a metal spraying process, whereas the second coder had chosen PROC 7, which fitted the description better.	Original coding changed and similar situations checked.
STOFFEN-MGR (90)	50	43	6	1	Situations where the handling description was correct in original coding, but incorrect in second coding (e.g. addition of powder to vessel original coding “handling of products with relatively high speed/ force which may lead to some dispersion of dust” with second coding “handling of products with low speed or little force in medium quantities”.	Original coding kept.
					Situations where the original room size was correct, second coding incorrect e.g. default option for room size used where there was no information on dimensions- 100-1000m^3 for original coding, $< 100m^3$ for second coding	Original coding kept.
					Situations where original handling description incorrect, second coding correct-original coding low speed spraying, second coding correct- “handling of liquids at high pressure resulting in substantial generation of mist or spray haze”	Original coding changed for spray processes- all spraying situations checked for handling description, presence of spraybooth, LEV option and room size.
					Situations where the original room size was incorrect, second coding correct (spraybooth $< 100m^3$)	All situations relating to spraybooths checked for size, LEV option and handling description to ensure consistency.

Appendix 4 impact of specific input parameter combinations on level of conservatism by exposure category

Appendix 4, Table 1 Impact of PROC in combination with input parameters on level of tool conservatism: percentage of measurements exceeding tool estimate/ (number of measurements) – Powders

Tool	PROC	Input parameter										
		Dustiness			Domain		LEV		Concentration in mixture			
		Low	Med	High	Industrial	Professional	LEV	no LEV	<1%	1-5%	6-25%	>25%
TRAv2	5	-	10 (n=63)	-	75 (n=8)	0 (n=55)	30 (n=20)	0 (n=43)	-	-	0 (n=2)	10 (n=61)
TRAv3		-	10 (n=63)	-	75 (n=8)	0 (n=55)	30 (n=20)	0 (n=43)	-	-	0 (n=2)	10 (n=61)
MEASE		-	5 (n=63)	-	38 (n=8)	0 (n=55)	15 (n=20)	0 (n=43)	-	-	0 (n=2)	5 (n=61)
EMKG		-	51 (n=63)	-	38 (n=8)	53 (n=55)	60 (n=20)	47 (n=43)	-	-	0 (n=2)	52 (n=61)
STM		-	0 (n=63)	-	0 (n=8)	0 (n=55)	0 (n=20)	0 (n=43)	-	-	0 (n=2)	0 (n=61)
TRAv2	8a	-	50 (n=54)	90 (n=20)	62 (n=53)	57 (n=21)	10 (n=10)	69 (n=64)	-	-	-	61 (n=74)
TRAv3		-	41 (n=54)	90 (n=20)	62 (n=53)	33 (n=21)	10 (n=10)	61 (n=64)	-	-	-	54 (n=74)
MEASE		-	42 (n=50)	95 (n=20)	65 (n=49)	38 (n=21)	10 (n=10)	65 (n=60)	-	-	-	57 (n=70)
EMKG		-	57 (n=54)	95 (n=20)	58 (n=53)	90 (n=21)	80 (n=10)	66 (n=64)	-	-	-	68 (n=74)
STM		-	6 (n=54)	35 (n=20)	19 (n=53)	0 (n=21)	0 (n=10)	16 (n=64)	-	-	-	14 (n=74)
TRAv2	8b	100 (n=1)	18 (n=22)	0 (n=31)	13 (n=38)	0 (n=16)	14 (n=36)	0 (n=18)	-	-	-	9 (n=54)
TRAv3		100 (n=1)	18 (n=22)	0 (n=31)	13 (n=38)	0 (n=16)	14 (n=36)	0 (n=18)	-	-	-	9 (n=54)
MEASE		0 (n=1)	18 (n=22)	0 (n=31)	11 (n=38)	0 (n=16)	11 (n=36)	0 (n=18)	-	-	-	7 (n=54)
EMKG		0 (n=1)	45 (n=22)	3 (n=31)	11 (n=38)	44 (n=16)	11 (n=36)	39 (n=18)	-	-	-	20 (n=54)
STM		0 (n=1)	0 (n=22)	0 (n=31)	0 (n=38)	0 (n=16)	0 (n=36)	0 (n=18)	-	-	-	0 (n=54)
TRAv2	14	-	50 (n=24)	-	50 (n=24)	-	100 (n=2)	45 (n=22)	-	-	-	50 (n=24)
TRAv3		-	88 (n=24)	-	88 (n=24)	-	100 (n=2)	86 (n=22)	-	-	-	88 (n=24)
MEASE		-	75 (n=8)	-	75 (n=8)	-	100 (n=2)	67 (n=22)	-	-	-	75 (n=8)
EMKG		-	63 (n=24)	-	63 (n24)	-	0 (n=2)	68 (n=22)	-	-	-	63 (n=24)
STM		-	0 (n=24)	-	0 (n=24)	-	0 (n=2)	0 (n=22)	-	-	-	0 (n=24)

Appendix 4, Table 2 Impact of PROC in combination with input parameters on level of tool conservatism: percentage of measurements exceeding tool estimate/ (number of measurements) - Volatile liquids

Tool	PROC	Input parameter										
		Vapour pressure			**Domain**		**LEV**		**Concentration in mixture**			
		Low	Med	High	Industrial	Professional	LEV	no LEV	<1%	1-5%	6-25%	>25%
TRAv2		67 (n=9)	3 (n=40)	40 (n=10)	20 (n=56)	0 (n=3)	60 (n=15)	5 (n=44)	-	0 (n=26)	37 (n=30)	0 (n=3)
TRAv3		67 (n=9)	8 (n=40)	60 (n=10)	27 (n=56)	0 (n=3)	73 (n=15)	9 (n=44)	-	0 (n=26)	50 (n=30)	0 (n=3)
MEASE	4	-	-	-	-	-	-	-	-	-	-	-
EMKG		33 (n=9)	21 (n=14)	20 (n=10)	20 (n=30)	67 (n=3)	47 (n=15)	6 (n=18)	-	-	20 (n=30)	67 (n=3)
STM		11 (n=9)	0 (n=40)	10 (n=10)	4 (n=56)	0 (n=3)	13 (n=15)	0 (n=44)	-	0 (n=26)	7 (n=30)	0 (n=3)
TRAv2		100 (n=3)	21 (n=47)	10 (n=10)	23 (n=60)	-	24 (n=17)	23 (n=43)	0 (n=2)	-	20 (n=15)	26 (n=43)
TRAv3		100 (n=3)	32 (n=47)	10 (n=10)	32 (n=60)	-	29 (n=17)	33 (n=43)	0 (n=2)	-	53 (n=15)	26 (n=43)
MEASE	5	-	-	-	-	-		-	-	-	-	-
EMKG		0 (n=3)	0 (n=47)	0 (n=10)	0 (n=60)	-	0 (n=17)	0 (n=43)	0 (n=2)	-	0 (n=15)	0 (n=43)
STM		100 (n=3)	13 (n=47)	0 (n=10)	15 (n=60)	-	12 (n=17)	16 (n=43)	0 (n=2)	-	13 (n=15)	16 (n=43)
TRAv2		78 (n=9)	37 (n=65)	74 (n=121)	-	62 (n=195)	69 (n=174)	0 (n=21)	-	0 (n=4)	41 (n=87)	81 (n=104)
TRAv3		89 (n=9)	57 (n=65)	82 (n=121)	-	74 (n=195)	83 (n=174)	0 (n=21)	-	25 (n=4)	59 (n=87)	88 (n=104)
MEASE	7	-	-	-	-	-	-	-	-	-	-	-
EMKG		-	-	-	-	-	0 (n=21)	-	-	-	0 (n=20)	0 (n=1)
STM		22 (n=9)	3 (n=65)	6 (n=114)	6 (n=188)	-	7 (n=167)	0 (n=21)	-	0 (n=4)	5 (n=87)	7 (n=97)
TRAv2		11 (n=19)	28 (n=148)	1 (n=78)	20 (n=188)	12 (n=57)	74 (n=34)	9 (n=211)	100 (n=3)	0 (n=1)	27 (n=59)	14 (n=182)
TRAv3		16 (n=19)	33 (n=148)	4 (n=78)	28 (n=188)	5 (n=57)	74 (n=34)	14 (n=211)	100 (n=3)	0 (n=1)	39 (n=59)	16 (n=182)
MEASE	10	-	-	-	-	-	-	-	-	-	-	-
EMKG		5 (n=19)	5 (n=147)	3 (n=78)	5 (n=187)	2 (n=57)	24 (n=33)	1 (n=211)	0 (n=3)	0 (n=1)	5 (n=58)	4 (n=182)
STM		0 (n=19)	9 (n=148)	0 (n=78)	7 (n=188)	0 (n=57)	30 (n=34)	2 (n=211)	0 (n=3)	0 (n=1)	7 (n=59)	5 (n=182)

Appendix 4, Table 2 Impact of PROC in combination with input parameters on level of tool conservatism: percentage of measurements exceeding tool estimate/ (number of measurements) - Volatile liquids (continued)

Tool	PROC	Input parameter										
		Vapour pressure			Domain		LEV		Concentration in mixture			
		Low	Med	High	Industrial	Professional	LEV	no LEV	<1%	1-5%	6-25%	>25%
TRAv2		7 (n=73)	18 (n=28)	28 (n=29)	25 (n=36)	10 (n=94)	24 (n=63)	4 (n=67)	-	33 (n=15)	16 (n=67)	4 (n=48)
TRAv3		10 (n=73)	43 (n=28)	45 (n=29)	47 (n=36)	16 (n=94)	40 (n=63)	10 (n=67)	-	47 (n=15)	31 (n=67)	8 (n=48)
MEASE	13	80 (n=10)	-	-	80 (n=10)	-	100 (n=5)	60 (n=5)	-	-	80 (n=10)	-
EMKG		5 (n=73)	18 (n=28)	17 (n=29)	6 (n=36)	13 (n=94)	16 (n=63)	6 (n=67)	-	27 (n=15)	6 (n=67)	13 (n=48)
STM		0 (n=73)	7 (n=28)	0 (n=29)	-	-	2 (n=63)	1 (n=67)	-	0 (n=15)	3 (n=67)	0 (n=48)
TRAv2		-	88 (n=171)	0 (n=7)	-	85 (n=178)	90 (n=168)	0 (n=10)	0 (n=2)	-	0 (n=10)	91 (n=166)
TRAv3		-	91 (n=171)	14 (n=7)	-	88 (n=178)	91 (n=168)	30 (n=10)	50 (n=2)	-	30 (n=10)	92 (n=166)
MEASE	14	-	-	-	-	-	-	-	-	-	-	-
EMKG		-	12 (n=171)	0 (n=7)	-	12 (n=178)	13 (n=168)	0 (n=10)	0 (n=2)	-	0 (n=10)	13 (n=166)
STM		-	78 (n=171)	0 (n=7)	-	-	79 (n=168)	0 (n=10)	0 (n=2)	-	0 (n=10)	80 (n=166)

Appendix 4, Table 3 Impact of PROC in combination with input parameters on level of tool conservatism: percentage of measurements exceeding tool estimate/ (number of measurements) - Metal abrasion

Tool	**PROC**	**Input parameter**										
		Dustiness			**Domain**		**LEV**		**Concentration in mixture**			
		Low	**Med**	**High**	**Industrial**	**Professional**	**LEV**	**no LEV**	**<1%**	**1-5%**	**6-25%**	**>25%**
TRAv2		20 (n=41)	66 (n=41)	-	45 (n=78)	0 (n=4)	74 (n=35)	19 (n=47)	-	-	0 (n=7)	47 (n=75)
TRAv3	24	20 (n=41)	68 (n=41)	-	46 (n=78)	0 (n=4)	74 (n=35)	21 (n=47)	-	-	0 (n=7)	48 (n=75)
MEASE		12 (n=41)	53 (n=43)	-	33 (n=83)	0 (n=1)	56 (n=39)	13 (n=45)	-	-	0 (n=7)	36 (n=77)

Appendix 4, Table 4 Impact of PROC in combination with input parameters on level of tool conservatism: percentage of measurements exceeding tool estimate/ (number of measurements) - Non-volatile liquids

Tool	**PROC**	**Input parameter**							
		Domain		**LEV**		**Concentration in mixture**			
		Industrial	Professional	LEV	no LEV	<1%	1-5%	6-25%	>25%
MEASE	11	-	43 (n=7)	-	43 (n=7)	-	-	100 (n=3)	0 (n=4)
STM		-	17 (n=233)	67 (n=6)	16 (n=227)	13 (n=71)	30 (n=73)	15 (n=26)	8 (n=63)