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Development of a Practical Guide for Determination of Conditions of Safe Use of Chemicals with the Aid of Scaling

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Development of a Practical Guide for Determination of Conditions of Safe Use of Chemicals with the Aid of Scaling

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Abstract

Scaling in the context of REACH implies the application of simple mathematics to examine whether chemicals are used in a safe way, even when certain conditions of use deviate from the exposure scenario.

Scaling offers downstream users the opportunity in selected cases to demonstrate at little cost that their specific conditions of use comply with an exposure scenario.

In this Report we describe the statutory obligation of downstream users to examine their conditions of use. We define scaling in relation to REACH and describe the objectives and results of scaling. Available scaling tools that facilitate scaling are characterized in a structured way. Options for further development and harmonization of scaling tools are also described.

Making use of experience with existing tools, we have developed a practical guide to scaling, in which, on the basis of three examples from different industries, we illustrate in five steps how scaling functions. This practical guide is directed at persons who use chemical substances in industrial or professional applications; that is, downstream users in terms of REACH. The practical guide is additionally directed at manufacturers of substances and formulators that wish to develop scaling tools for their customers.

The Report includes a spreadsheet for environment-related scaling (REACH Scale Environment). It also includes a template for generation of product-specific scaling tools.

The Report focuses solely on scaling related to environmental exposure assessment. Scaling is also possible in relation to exposure of workers and consumers. Literature on the topic of scaling is discussed in Chapter 7.

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Abbreviations and Acronyms

CLP	EU Regulation on Classification, Labelling and Packaging
CSA	Chemical Safety Assessment
CSR	Chemical Safety Report
DNEL	Derived no-effect level
ECETOC TRA	ECETOC Targeted Risk Assessment
ECHA	European Chemicals Agency
ES	Exposure scenario
eSDS	Extended Safety Data Sheet (eSDS)
OC	Operational conditions
MNQ	low-flow rate of receiving waters
PEC	Predicted environmental concentration
PNEC	Predicted no-effect concentration
RCR	Risk characterization ratio
RMM	Risk-management measures
REACH	EU Regulation on the Registration, Evaluation, Authorization and Restriction of Chemical Substances
SDS	Safety Data Sheet
ScIDeEX	Scaling tool for inhalative and dermal exposure
ZVO	Zentralverband der Oberflächentechnik – German Federation of Surface Technology Industries

1 Scaling: Definition, Objectives and results, target groups

Definition

In the ECHA guidance document "Guidance for downstream users"[1] (Section 5.2.5) the possibility of scaling for downstream users is mentioned as an alternative to conduct of a chemical safety assessment. The term "scaling" is used in different fields of technology, including process engineering, for the resizing – scaling-up – of installations from laboratory scale to pilot plant scale. The terms "scaling-up" and "scaling-down" describe a true-to-scale increase and true-to-scale decrease, respectively.

Scaling, in the context of REACH, is understood to mean the modification of a given exposure assessment in relation to particular variables. The predetermined exposure assessment is contained in the exposure scenario of the supplier. Such a modification is carried out by downstream users. A prerequisite for this is that downstream users are provided with information on scaling. This information (in the form of "scaling aids", "scaling tools") indicates the exposure assessment values that are modifiable (applied quantity, for example), and how such a modification can be executed.

Scaling is defined in Annex G-1 ("Methodology on Scaling") of Part G of ECHA "Guidance on Information Requirements and Chemical Safety Assessment". Part G deals with the extending of safety data sheets (SDS) pursuant to REACH[2].

> „Scaling in this context means the use of simple equations in the exposure scenario (ES), by which the downstream user (DU) can demonstrate that he operates within the conditions of the ES provided by the registrant."

Objective of scaling

The objective of scaling is simple examination of whether the user's use of chemical substances or preparations is safe, even when certain application conditions deviate from information in the exposure scenario.

Scaling should ensure, on the one hand, that with particular applications problematical exposure of humans and the environment does not arise, and that predetermined effect concentrations are not exceeded. On the other hand, scaling should enable the downstream user to verify the safe use of chemicals without complex chemical safety assessments.

Scaling is not required by law (in other words, it is not mandatory), but for downstream users it is in many cases an interesting option for compliance with a prescribed exposure

[1] http://echa.europa.eu/documents/10162/17226/du_en.pdf

[2] http://echa.europa.eu/documents/10162/17224/information_requirements_part_g_en.pdf.

scenario. Article 37 (4) REACH requires a downstream user of a substance on its own or in a preparation to prepare a chemical safety assessment for any use outside the conditions communicated to him by his supplier in an exposure scenario (or for any use his supplier advises against).

Outcome of scaling

The outcome of scaling is the statement whether or not application can be continued when particular application conditions deviate from the exposure scenario.

Depending on the structure of scaling, this statement can be made in different forms, as shown in the following two examples:

- The ratio between predicted environmental concentration (PEC) and the accompanying predicted no-effect concentration (PNEC) can be stated (risk ratio, PEC/PNEC). If the risk ratio has a value smaller than 1 the application is classified as safe and can be continued.
- A maximum quantity to be used can be calculated. The user's application is safe when the quantity used does not exceed the maximum level.

Target groups for scaling

The target group for scaling is downstream users who themselves handle substances and preparations, by which exposure of humans and the environment can occur. This is the case with formulators who manufacture preparations from substances, and with downstream users who ultimately apply such substances and preparations in different processes.[3]

Depending on role and background of experience, three groups of users can be distinguished:

- Downstream users with an extensive background of experience with environmental exposure assessment and knowledge of relevant tools such as EUSES or ECETOC TRA. This user group comprises not only downstream users but also substance manufacturers and importers. This applies for many manufacturers of preparations who themselves manufacture a part but not all of their base materials.

[3] Under REACH, a downstream user is any natural or legal person established within the Community, other than the manufacturer or importer, who uses a substance, either on its own or in a mixture, in the course of his industrial or professional activities. Distributors and consumers are not downstream users (Article 3(14) REACH). Distributors that refill or repack substances are downstream users. It is unlikely that exposure occurs in such procedures, which constrains downstream users to conduct their own assessments.

- Downstream users who are not themselves obligated to register substances, but have a background of experience with environmental exposure assessment and themselves prepare safety data sheets with exposure scenarios. This is the case with many formulators.
- Downstream users finally who employ chemicals in different processes in industrial or professional applications. In most cases, such users have little or no experience with environmental exposure assessment.

Expectations of scaling tools and the possibilities of their use vary depending on the user group.

Practical tip: The maximum quantity to be used as stated in exposure scenarios and safety data sheets should, where possible, not be fully utilized by companies. It could be that the same substance is discharged by another company into the same receiving water. Greater clearance to maximum quantities also means greater certainty that problematical loading does not occur in the receiving water.

2 Summary of available approaches

REACH-related scaling tools have been developed in recent years at both a national and a European level.

- On the initiative of the Confederation of Danish Industry (DI), and with the support of the Danish Environmental Protection Agency, the so-called Exposure Scenario Modifier (ES-Modifier) has been available since May 2010.
- Scaling tools have been developed by companies, which relate directly to exposure assessment tools such as ECETOC TRA and the exposure-modifying factors they contain.
- Scaling tools have also been developed in Germany by individual industrial associations – for example, by the textile and leather industries – within the scope of preparation of exposure scenarios.
- Excel-based scaling tools have been developed by Öko-Institut in research projects on behalf of the Federal Environment Agency: *Umsetzungshilfen für ein erfolgreiches Risikomanagement im Rahmen von REACH, 2007* (http://www.reach-help-desk.info/fileadmin/reach/dokumente/REACH_Umsetzungshilfen_Endbericht_final_070228.pdf), and *Konkretisierung von Expositionsszenarien und/oder Expositionskategorien für Textilhilfsmittel, 2004* (http://www.reach-info.de/expoanalyse.htm). An English summary of the latter report is available under the title "Screening tool supporting environmental exposure assessment under REACH for substances used in textile finishing Short Project Report1 (December 2004)" at: http://www.reach-info.de/dokumente/textile_finishing_industry_project_summary.pdf. They have

been further developed within the scope of the project "REACH Practical Guide on Exposure Assessment and on Communication in the Supply Chains" concerning the "REACH Scale" tool.

Currently available tools are listed below in Table 1 together with their source and date of publication. Tools that do not relate to environmental exposure are printed in *italics*. A more detailed characterization of individual tools is to be found in Chapter 3, where the focus is on environment-related tools.

Table 1: Publicly available scaling tools

	Scaling Tools	**Publication**	**Source**
1	*ECHA equation for scaling of consumer exposure*	*2008*	*ECHA Guidance on Information Requirements, Part G*
2	ECHA equation for scaling environmental exposure, textile industry	2008	ECHA Guidance on Information Requirements, Part G
3	ECETOC TRA v2, exposure-modifying factors	2009	ECETOC
4	ES-Modifier	2010	DHI
5	Textile table for scaling wastewater loading, textiles, v1 + v2	2004, 2007	German Federal Environment Agency / Textile Industry Assoc.
6	Matrix access tool for exposure assessment	2006	OECD Matrix Project, German Federal Environment Agency
7	Scaling aid for electroplating processes, ZVO	2007	German Federal Environment Agency / ZVO
8	Equation for scaling solvent-loading of wastewater	April 2009	Merck AG, Example in VCI 2010, REACH Practical Guide
9	*Equation for scaling exposure at workplaces on the example of solvents*	*February 2010*	*Merck AG, example for training purposes*
10	*Excel Table ScIdEEx, inhalative and dermal exposure*	*April 2010*	*VCI 2010, REACH Practical Guide*
11	REACH Scale, Environment	April 2010	Öko-Institut e.V., VCI 2010, REACH Practical Guide
12	Wastewater tool	August 2010	Leather Industry Assoc. / TEGEWA

In addition, there are company-owned scaling tools that have not yet been published.

It has also been investigated within the framework of this project whether comparable scaling approaches are to be found within the scope of legislation on biocidal products, pesticides and medicinal products. No examples have been found for the modification of a prescribed exposure assessment by a user of biocidal products, pesticides or medicinal products.

The reason for this can be that application conditions in the case of biocidal products, pesticides and medicinal products are generally laid down precisely, and are adhered to by users. By contrast, with many products that are used in the chemicals industry, and by its downstream users, the range of application conditions is wide. In many cases it will not be possible to cover the whole range through the exposure assessments of suppliers. Here, it is therefore expedient to describe standard uses in exposure scenarios, and to make scaling tools available for adaptation of these scenarios.

3 Description and examination of individual concepts

The scaling tools briefly presented in Chapter 2 differ considerably with regard to objective, user group and complexity. Individual scaling tools are analysed and assessed below on the basis of key issues.

In so doing, we restrict ourselves to the tools listed in Table 2, which relate directly to environmental exposure assessment, and which have been developed for downstream users.

Table 2: Scaling tools relating to environmental exposure estimation

	Environment-related scaling approaches / Tools for downstream users	Publi-cation	Source
1	ECHA equation for scaling environmental exposure, textile industry	2008	ECHA Guidance on Information Requirements, Part G
2	ES-Modifier	2010	DHI
3	Textile table for scaling wastewater loading, textiles, v1 + v2	2004, 2007	German Federal Environment Agency / Textile Industry Association
4	Scaling aid for electroplating processes	2007	German Federal Environment Agency / ZVO
5	Equation for scaling solvent-loading of wastewater	April 2009	Merck AG, Example in VCI 2010, REACH Practical Guide
6	REACH Scale, Environment	April 2010	Öko-Institut e.V.,
7	Wastewater tool	August 2010	Leather Industry Association / TEGEWA

Tools are not further considered that

- have no relation to environmental exposure assessment (in Table 1 the tools SciDeEx and ECHA Tables), or
- have been primarily developed as exposure assessment tools for the registrant, and are too complex for downstream users without knowledge of exposure assessment (ECETOC TRA version 2, exposure assessment tool from the OECD Matrix Project).

In the Annex to this Report we provide interested readers with a description of exposure assessment tools (ECETOC TRA v2 and the Matrix tool) that are not considered below, as well as a more detailed description of the ES-Modifier.

The following central questions have been raised for characterization of the tools described below:

- By which stakeholder has the tool been developed, and with what purpose?
- For which user group has the tool been developed?
- Which areas of application are addressed?
- Are particular application circumstances – for example, direct discharger / indirect discharger – addressed?
- Which environment compartments are covered?
- Which input parameters are required?
- In which form is the outcome presented?
- How great is the tool's complexity?
- Does the possibility of direct transfer to other industries exist?
- Does the possibility of transfer following adaptation exist?

Important assessment criteria are:

- substantive accuracy of the underlying equations,
- consideration of upper limits for exposure-defining variables,
- consideration of effects on other environmental compartments,
- appropriateness of tools for the intended user group, and
- particular strengths and weaknesses of the tool, also in comparison with other tools.

The **need and possibilities of further development** are described on the basis of this characterization.

All considered tools for environment-related scaling fall back on exposure assessments and risk characterisation pursuant to ECHA guidelines (Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.8 (PNEC derivation), Chapter R.16 (environmental exposure estimation) and Part G (risk characterization).

The following equation is used for calculation of the environmental concentration to be expected:

$$PEC_{local} = \frac{Q_{product} \cdot C_{substance} \cdot (1 - F_{fix}) \cdot (1 - Red_{min}) \cdot (1 - F_{STP})}{Q_{water} \cdot 10^{-6}}$$

Abbreviations used:

PEC_{local}	Predicted local environmental concentration, stated in micrograms per litre [µg/l]
$Q_{product}$	Average quantity of substance or formulation used per day, stated in kilograms per day [kg/d]
$C_{substance}$	Concentration of the chemical in the preparation (for example, concentration: 40%, input value for the calculation: 0.4). As a rule, with substances a concentration of 100% is assumed.
F_{fix}	So-called degree of fixation. This is the proportion of the substance used that is fixed to the

	substrate or consumed in the process, and therefore not discharged into wastewater (for example, fixation: 80%, input value in the calculation: 0.8).
Red_{min}	Effectiveness of additional emission reduction measures (for example, reduction of 95%, input value for the calculation: 0.95).
F_{STP}	The proportion of the substance that is "removed" by varied processes from water in the treatment plant, and is therefore not discharged into the receiving water (for example, removal of 55%, input value for the calculation: 0.55.
Q_{water}	The quantity of water into which residues of the substance used are released, composed of the volume flow of the wastewater treatment plant that takes in the quantity of the substance released from the process into the wastewater, and the volume flow of the receiving water (average low-flow discharge). These values are stated in cubic metres per day ([m^3/d]). In exposure assessments it is assumed as a standard value that the volume of wastewater passing through the treatment plant amounts to 2,000 cubic metres per day, and that in the receiving water dilution to the factor of 10 occurs (to 20,000 cubic metres per day).
10^{-6}	This value is merely a conversion factor. The predicted local environmental concentration is stated in "micrograms per litre. Previous input values were such that without the conversion factor the calculated value would have the analytically uncommon unit "kg/m^3".

In some scaling tools exhaustive exposure assessment and risk characterization is carried out (for example, in the ES-modifier; see Section 3.2). In other scaling tools no separate exposure assessment is undertaken, but rather individual variables abstracted from an exposure assessment that has already been undertaken and employed in the scaling tool (for example, in the ECHA equation for environmental scaling, see Section 3.1).

3.1 The ECHA equation for environmental scaling

Examples of scaling are provided in ECHA Guidance on Information Requirements and Chemical Safety Assessment, Part G (Extending the Safety Data Sheet) (ECHA 2008). The following equation stems from the example concerning environmental scaling:

$$RCR_{actual} = RCR_{ES} \cdot \frac{Q_{actual}}{Q_{ES}} \cdot \frac{F_{water,actual}}{F_{water,ES}} \cdot \frac{(1 - f_{abatement,actual})}{(1 - f_{abatement,ES})} \cdot \frac{T_{emission,ES}}{T_{emission,actual}}$$

Abbreviations used:

RCR	Risk characterization ratio: The ratio of predicted exposure level and the predicted no-effect concentration (PNEC). Use is regarded as safe when the RCR is smaller than 1.
Q	Average quantity of preparation used per year.[4]
C	Concentration of the substance in the preparation.
F	Release factor: The proportion of the substance that does not remain in the process, but rather enters process wastewater.
$f_{abatement}$	Proportion of the substance that is removed from process wastewater by additional emission reduction measures.
$T_{emission}$	Number of days per year on which the substance is used.
Addendum "actual"	The items refer to the actual application circumstance of the downstream user.

[4] Note: At this point in the ECHA Guidance Document, Part G, "quantity used per day" is stated as an explanation. It should, however, be "quantity used per year"; otherwise, the final part of the equation (days used per year) would have to be omitted.

Addendum "ES" The values relate to data in the exposure scenario (ES).

The RCR is not calculated in the scaling equation, but rather taken from the exposure scenario. The use of the equation is shown on the basis of an example in the following table from the ECHA guidance document.

(Note: In the exemplary table, in calculation of the RCR ("Safety Ratio", 4th column) a value of 1,000 kg is applied in the second line for the quantity used according to the exposure scenario (Q_{ES}). In the cell to its left, a value of 10,000 kg is erroneously given for this item; the other preconditions from the Exposure Scenario remained unchanged).

Table 3: Exemplary presentation of environmental scaling using the scaling equation. Source: ECHA Guidance Document on Information Requirements and Chemical Safety Assessment, Part G (Extending the Safety Data Sheet) (ECHA 2008). Extract from the table published therein.

Parameter	Actual	ES	Safety Ratio	Comment
Q (kg)	750	10,000	Q_{actual} / Q_{ES} = 750 / 1,000 = 0.75	
C (-)	0.1	0.1	C_{actual} / C_{ES} = 0.1 / 0.1 = 1	In the standard evaluation the pure substance (100%) is evaluated. The specific product contains 20% of the risk-determining substance.
f_{water} (-)	0.35	0.3	$f_{water,actual} / f_{water,ES}$ = 0.35 / 0.3 = 1.16	
RCR	RCR_{actual}	0.3	RCR_{actual} = $RCR_{ES} \cdot 0.3 \cdot 0.75 \cdot 1.16 \cdot 0.4 \cdot 1.33$ = 0.14	The calculated actual overall RCR_{actual} is below 1. Hence, the specific conditions of use are considered safe.

Additional information on the above table:

1. In the equation, the quantity used is stated in kilograms per day, although the calculation is based on the quantity used per year (and the number of days of use per year). This should be rectified on using the equation.
2. In line 3 of the table it is stated that concentration of the substance amounts to 10% not only in the exposure scenario but also with the user. This does not correspond with information in the commentary. In calculating the actual risk ratio in line 7 the correct ratio of 0.4 is applied.

By means of the scaling equation the following variables can be scaled: quantity used, concentration of the substance in the product, proportion of the quantity used that is released into process wastewater, effectiveness of operational emission reduction measures and the duration of release (in days per year). The emission factor for discharge from the process into wastewater must also take into account emissions from cleaning and maintenance processes.

Calculated variable:

The risk characterisation ratio is calculated under the operational conditions entered by the user (RCR_{actual}).

Outcome of estimation:

If the risk ratio is smaller than 1 the application is regarded as safe (that is, covered by the exposure scenario). If the risk ratio is greater than 1 the application is regarded as unsafe (that is, not covered by the exposure scenario).

Target group for the scaling tool:

In the example the user is a textile finisher; that is, the final user of the product. The scaling equation is also, however, of interest to formulators, since it is possible to modify the concentration of substances in preparations.

Substantive basis:

Modelling of wastewater loading is generally carried out, in accordance with the ECHA Guidance Document on Environmental Exposure Estimation (Chapter R.16), for determination of risk ratios in the exposure scenario.

Features:

Duration of use is stated, as scaling parameter, in working days per year. An alternative would be quantity used per day. Modification of the volume flow of the receiving water is not possible, although this value would vary greatly among downstream users. Modification of degradation efficiency in municipal or industrial wastewater treatment plants is not possible; which in most cases is also reasonable.

Ratios are formed for the five influencing variables and then multiplied. There is no calculator support for execution of individual steps and multiplication of individual ratios. Experience shows that there is a substantial risk of calculating errors occurring.

Table 4: Profile: Features of the ECHA equation for environmental scaling

The ECHA equation for environmental scaling	
1	**By which stakeholder has the tool been developed, and for what purpose?**
	The equation was developed by public authorities and companies within the framework of the REACH implementation project RIP 3.2. The objective is clarification of scaling on the basis of an example that can be adopted by registrants.
2	**For which user group has the tool been developed?**
	Registrants, formulators and end-users.
3	**Which areas of application are addressed?**

The ECHA equation for environmental scaling	
	Textile finishing
4	**Are particular application circumstances addressed?**
	Application in an open equipment with occurring emissions into the environment
5	**Which environmental compartments are covered?**
	Surface waters (fresh waters)
6	**Which input parameters are required?**
	Concentration of the substance in the product, degree of release, effectiveness of operational measures for emission reduction, duration of release (in days per year), quantity of the substance used (with the above parameters, the standard assumptions of the registrant and company-specific values in each case) and risk characterization ratio from the chemical safety assessment.
7	**In which form is the outcome presented?**
	The risk characterization ratio is calculated for the particular circumstance of the user.
8	**Complexity of the tool**
	An average degree of complexity (creation of several ratios is required as well as subsequent multiplication of individual ratios). High probability of error.
9	**Possibility of direct transfer to other industries**
	The equation is directly transferable to similarly-structured applications.
10	**Possibility of transfer following adaptation**
	The equation is directly transferable.
11	**Substantive correctness of the underlying equations**
	Linear dependencies are correctly given. The risk characterization ratio under standard conditions is not calculated in the tool itself, but is taken from an existing calculation.
12	**Consideration of upper limits for exposure-defining variables**
	Upper limits are not considered.
13	**Consideration of effects on other environmental compartments**
	No such consideration.
14	**Appropriateness of the tool for the intended user group**
	The tool is appropriate; however, there is a high probability of errors in calculations.
15	**Particular strengths and weaknesses of the tool, also in comparison with other tools**
	Advantage: direct traceability of the calculation. Disadvantage: no computer support, therefore high probability of error.
16	**Need and possibilities of further development**
	Inclusion of volume flow in the receiving water on site as a variable quantity (average low –water discharge). Implementation in spreadsheets (see tools in Sections 3.3, 3.6 and 3.7).

3.2 The ES-Modifier

The ES-Modifier is primarily an IT tool for exposure estimation. Its objective therefore goes beyond scaling and the modification of individual values of an exposure scenario. The ES-Modifier enables direct calculation of risk characterization ratios for industrial, professional and private use of substances.

The following figure displays certain elements of the ES-Modifier.

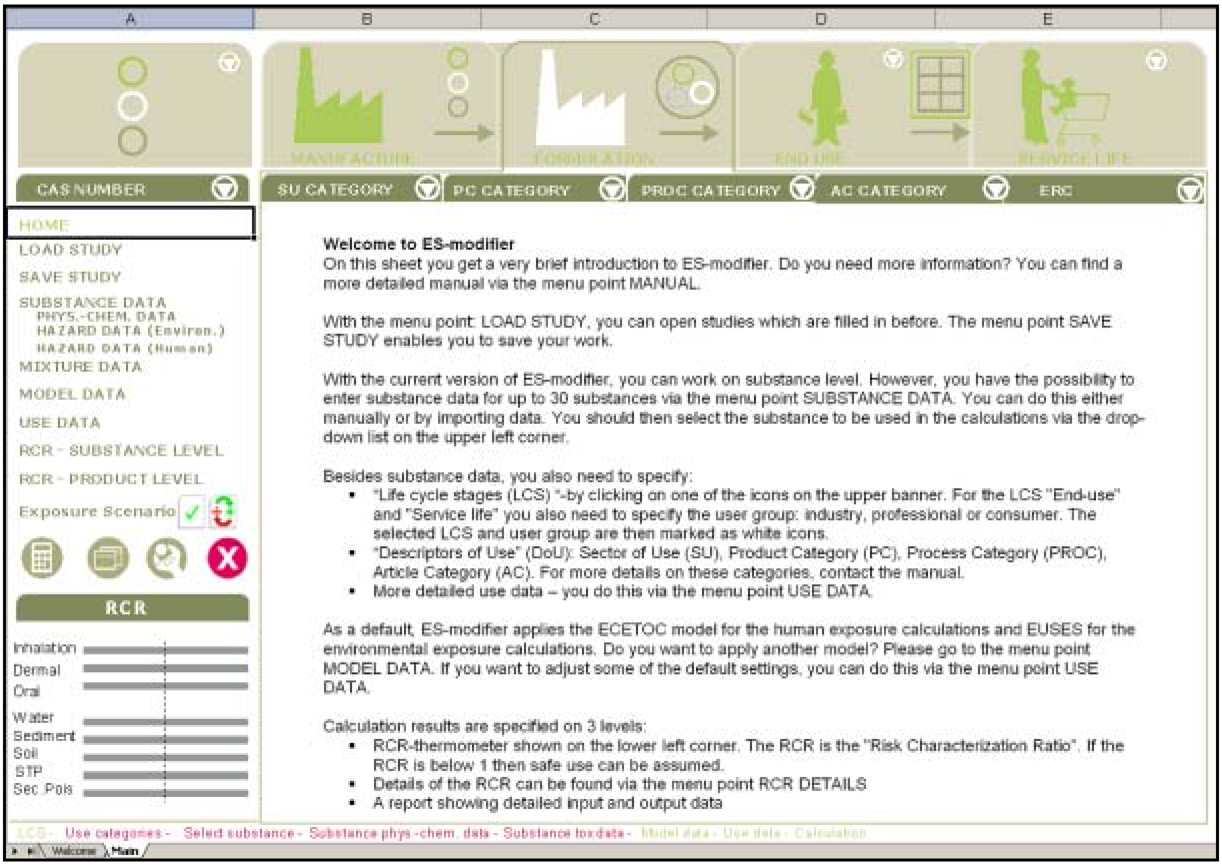

Figure 1: The structure of the ES-Modifier

Calculated variable

With the aid of the ES-Modifier risk characterization ratios are calculated for different environmental compartments (e.g. water, soil).

Outcome of estimation

Risk characterization ratios are displayed in the form of a scale that is termed "thermometer". In Figure 1 this "RCR thermometer" can be seen in the bottom left-hand corner. The thermometer (an easily understandable presentation of the outcome!) provides eight items of information: values for three exposure pathways for people at their workplace, for four environmental compartments and for indirect human exposure via environmental media and the food chain.

Target group of the ES-Modifier

The target group of the ES-Modifier is registrants and formulators that use substances in preparations. The ES-Modifier is probably too complicated for most downstream users.

Substantive basis

The presently most common exposure estimation tools are incorporated in the ES-Modifier: EUSES (environmental exposure), ECETOC TRA Version 2 (environmental, consumer and worker exposure), the Dutch "Stoffen Manager" model by RIVM/TNO and "EMKG-Expo-Tool", the simple concept of measures of the German Federal Institute for Occupational Safety and Health (BAuA) (the two last-mentioned for estimation of worker exposure) as well as "ConsExpo" (consumer exposure). In the ES-modifier, exhaustive modelling of environmental exposure is undertaken, pursuant to ECHA Guidance in Chapter R.16, using the EUSES exposure estimation tool.

Features:

The ES-Modifier enables exhaustive exposure estimations on the basis of the currently most common exposure estimation tools. Exposure scenarios for preparations can also be prepared, which are based on the DPD+ method for determination of lead substances[5].

Further information on the ES-Modifier is provided in the Annex, Section 8.2.2.

Table 5: Profile: Features of the ES-Modifier

The ES-Modifier	
1	**By which stakeholder has the tool been developed and for what purpose?**
	The ES-Modifier has been developed by European research institutes (DHI, TNO) to facilitate the preparation of exposure scenarios.
2	**For which user group has the tool been developed?**
	Registrants, formulators and end-users of chemicals.

[5] The DPD+ method is a methodical proposal for establishing risk-determining components in mixtures. It has been developed and published by Cefic (http://cefic.org/templates/shwPublications.asp?HID=750). It is based on the Dangerous Preparations Directive (DPD) and additionally includes the vapour pressure of substances for assessment of inhalative exposure (for this reason, the "+" in DPD+). A description of the method and recommendations for application are provided in Part 3 of the REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains (https://www.vci.de/Themen/Chemikaliensicherheit/REACH/Seiten/REACH-Praxisfuehrer.aspx#). The ES-Modifier can define so-called lead substance indicators (LSI) for mixtures and thus the lead substance of the mixture in accordance with the DPD+ method, and it lists these in a table. In addition, substances whose LSI make up at least 10% of the LSI of the lead substance are identified with another colour ("sub-lead substances"). The RCR of lead substances and "sub-lead substances" are added in respect of each exposure pathway in order to assess possible additive effects.

The ES-Modifier	
3	**Which areas of application are addressed?**
	All areas in which chemicals are used.
4	**Are particular application circumstances addressed?**
	No, all ascertainable processes in common exposure estimation tools can be reproduced.
5	**Which environmental compartments are covered?**
	Water (freshwater and seawater), sediment (freshwater and seawater), soil, air, microorganisms in sewage sludge and effects by way of environmental media (secondary poisoning).
6	**Which input parameters are required?**
	Not only data on substance properties (for example, molecular weight, vapour pressure and solubility) but also ecotoxicological impact data and data on processes.
7	**In which form is the outcome presented?**
	The risk characterization ratio is calculated.
8	**Complexity of the tool**
	There is a high degree of complexity. Experience in dealing with exposure estimation tools is a prerequisite for meaningful use.
9	**Possibility of direct transfer to other industries**
	Transfer is not necessary, since the tool, in terms of its structure, is applicable in all industries.
10	**Possibility of transfer following adaptation**
	Adaptation is not necessary (see 9 above).
11	**Substantive correctness of underlying equations**
	Calculations for environmental exposure are based on EUSES. The use descriptor system with corresponding environmental release categories is utilized.
12	**Consideration of upper limits for exposure-defining variables**
	Upper limits are not considered.
13	**Consideration of effects on other environmental compartments**
	See 5 above. All environmental compartments covered in EUSES are represented.
14	**Appropriateness of the tool for the intended user group**
	Registrants will easily understand the tool. For downstream users it is too complicated (formulators who themselves register substances are the exception).
15	**Particular strengths and weaknesses of the tool, also in comparison with other tools**
	The ES-Modifier enables quick and convenient application of the most common exposure estimation tools. This makes it attractive for experienced users.
16	**Need and possibilities of further development**
	One interesting further development would be the possibility, as registrant, to set default values and to provide the downstream user with a "prepared" ES-Modifier. The downstream user would then only have to modify a few values. Consideration of upper limits.

3.3 Spreadsheet for textile finishers

The spreadsheet was developed in a research project of the Federal Environment Agency together with the *Verein Deutscher Textilveredlungsfachleute* and the *Verband der Nordwestdeutschen Textil- und Bekleidungsindustrie*. The following figure displays the structure of this scaling tool (only available in German language).

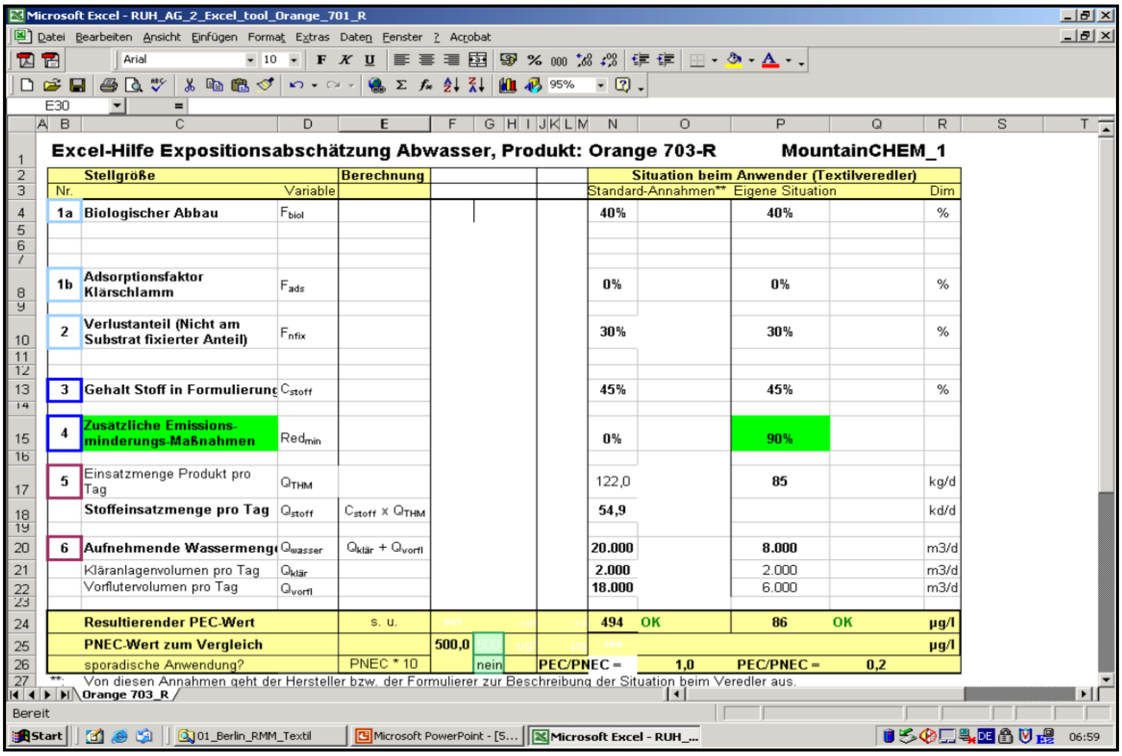

Figure 2: Structure of the spreadsheet for textile finishers

The assumptions of the supplier on exposure-defining variables are entered in the spreadsheet. These variables are shown in the left half of the spreadsheet and are designated "Standard-Annahmen".

The downstream user enters his values in the right half of the table in the column "Eigene Situation". The scaling tool requires the entry of the following variables:

Degree of biological degradation (“F_{biol}”), adsorption factor to sewage sludge (“F_{ads}”), proportion that is not fixed to the substrate (the so-called share of loss, which remains in the wastewater and is discharged in the case of indirect dischargers into the next municipal wastewater treatment plant; “F_{nfix}”), concentration of the substance in the preparation (“C_{stoff}”), quantity of the product used per day (from the last two variables the quantity of substance used per day is calculated; “Q_{THM}”), volume flow per day of the wastewater treatment plant (“$Q_{klär}$”) and volume flow per day of the receiving water (“Q_{vorfl}”). The supplier also enters the PNEC value (freshwater) of the substance, which in the majority of cases is decisive for environmental exposure in the effluent.

Calculated variable

The risk characterization ratio PEC/PNEC for surface waters is calculated in the spreadsheet.

Outcome of estimation

The PEC/PNEC ratio is directly stated. In the case of values above 1 a warning notice in red appears to the effect that the respective application is not covered.

Target group of the spreadsheet

The spreadsheet has been developed for textile finishers as downstream users of chemicals.

Substantive basis

Modelling of environmental exposure is directly undertaken in the spreadsheet. For this reason entry of the PNEC value for surface waters (freshwater) is required. Modelling takes place in accordance with the equations in ECHA guidelines on environment-related exposure estimation (ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.16: http://guidance.echa.europa.eu/docs/guidance_document/information_requirements_r16_en.pdf?vers=27_05_10**).**

However, it is not the result of modelling the different processes that take place in a wastewater treatment plant (biological degradation, adsorption to sewage sludge, release of a proportion of the substance into the atmosphere) that is entered in the spreadsheet in respect of the behaviour of substances in a treatment plant.[6] Instead, individual factors are applied for biological degradation and adsorption to effluent sludge. In the calculation, these factors are multiplied by each other. This leads to miscalculations in the case of substances with which additional processes take place in the wastewater treatment plant; for instance, release into the atmosphere in the case of volatile substances.

In reworking the spreadsheet, the two factors mentioned above should be replaced by one factor for substance reduction in the wastewater treatment plant, which takes account of all processes that are important for such reduction.

Features:

The spreadsheet enables direct comparison between the assumptions that the registrant or formulator has made and actual application conditions with the textile finisher. In practical tests with finishers it has been shown, however, that the multitude of possible input options and information contained in the spreadsheet demand too much of many users.

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[6] Such modelling is carried out, for example, in the EUSES environment-related exposure estimation tool using the SimpleTreat calculation module.

Table 6: Profile: Features of the spreadsheet for textile finishers

Spreadsheet for textile finishers	
1	**By which stakeholder has the tool been developed, and for which purpose?**
	Developed by Öko-Institut together with the *Verein Deutscher Textilveredlungsfachleute* and the *Verband der Nordwestdeutschen Textil- und Bekleidungsindustrie*. Objective: Support for textile finishers in risk management and in the review of exposure scenarios.
2	**For which user group has the tool been developed?**
	Downstream users who themselves apply preparations or substances as such.
3	**Which application areas are addressed?**
	Textile finishing.
4	**Are particular application circumstances addressed?**
	Application in an open equipment with occurring emissions into the environment
5	**Which environmental compartments are covered?**
	Surface waters (freshwater)
6	**Which input requirements are required?**
	Degree of biological degradation, adsorption to sewage sludge, (initial) release factor from process, concentration of the substance in the preparation, quantity of the product used per day, treatment plant volume flow per day, receiving-water volume flow per day and PNEC value (freshwater) of the substance.
7	**In which form is the outcome presented?**
	The risk characterization ratio PEC / PNEC is calculated.
8	**Complexity of the tool**
	Average complexity. Many entries are required.
9	**Possibility of direct transfer to other industries**
	Transferability to other industries.
10	**Possibility of transfer following adaptation**
	See 9 above. The spreadsheet can also be used in other industries. The terminology (for example, "degree of fixation") might have to be adapted to the respective industry.
11	**Substantive correctness of underlying equations**
	The spreadsheet calculation is based on equations from the ECHA guidelines on environment-related exposure estimation. Data on degradability and behaviour on sewage sludge should be replaced by the results of wastewater treatment plant modelling (single value for emission reduction).
12	**Consideration of upper limits for exposure-defining variables**
	Upper limits are not used.
13	**Consideration of the effects on other environmental compartments**
	No other environmental compartments are considered.
14	**Appropriateness of the tool for the intended user group**
	For most downstream users the tool will be difficult to use, due to the multitude of input options.
15	**Particular strengths and weaknesses of the tool, also in comparison with other tools**
	Advantage: comparative presentation of entries by the formulator and the user. Disadvantage: Multitude of entry options.
16	**Need and possibilities of further development**

Spreadsheet for textile finishers	
	For downstream users the focus can be set on the variables that he can modify (see REACH Scale Environment tool). Consideration of upper limits.

3.4 Scaling aid for galvanization processes

Scaling tables have been developed within the framework of a research project of the Federal Environment Agency together with the German Federation of Surface Technology Industries (ZVO). They are reproduced in the three tables below, which relate to organic process chemicals.

Calculated variables

The tables show the quantity of a process chemical that can be used per day, depending on the size of the receiving water (Table 7), the toxicity of the substance for aquatic organisms (Table 8, PNEC value) and the abatement of substance release via the wastewater treatment plant (Table 9).

The tables are based on exposure estimation and risk characterization undertaken with the EUSES exposure estimation tool and the equations it contains. This estimation was carried out for a substance under consideration of the following assumptions:

$PNEC_{aquatic,\ surface\ waters}$: 1 mg / l

Logarithm of the partition coefficient octanol/water (LogPow): < 4.5

The substance is biologically degradable in the wastewater treatment plant (assuming inherent biodegradability).

The volume flow of the receiving water amounts to 20,000 cubic metres per day (average low water discharge).

Under consideration of these assumptions, the possible maximum quantity of the substance to be used is 33 grams per day. This value is displayed in the following three tables with a yellow background.

Table 7: Maximum quantity to be used depending on the volume flow of the receiving water

PNEC ≥ 1 mg/l, $LogP_{OW}$ < 4.5 At least inherently biodegradable **Variation: receiving water volume flow [m³/d]**	**≥ 5,000**	**≥ 20,000**	**≥ 50,000**	**≥ 100,000**	**≥ 200,000**	**≥ 500,000**
Maximum quantity used [g/d]	8	33	82	165	330	820

Table 8: Maximum quantity used and PNEC value of substances

LogP$_{OW}$ < 4.5 At least inherently biodegradable, **Receiving water volume flow** ≥ 20,000m^3/d **Variation: PNEC [mg/l]**	≥ 0,1	≥ 1	≥ 10	≥ 100
Maximum quantity used in [g/d]	3	33	330	3,300

Table 9: Quantity used and degree of elimination [7] of substances in the wastewater treatment plant

PNEC ≥ 1 mg/l, Receiving water volume flow ≥ 20,000m^3/d Degradability and LogP$_{OW}$ variable **Variation: Elimination degree [%]**	≥ 40	≥ 60	≥ 80	≥ 90	≥ 95	≥ 99
Maximum quantity used in [g/d]	33	50	100	200	400	2,000
Iteration factor	1	1.5	3	6	12	60

Outcome of use of tables

Maximum quantities to be used are stated in grams per day.

Target group

Formulators who themselves wish to prepare exposure scenarios for their products, from which tables are created that can be made available to downstream users of products.

Substantive basis

The maximum useable quantity of a substance is not calculated in the table for a given set of default options, but rather entered directly. Modelling of environmental exposure is carried out to determine the respective value in accordance with equations in ECHA guidance on environment-related exposure estimation (Chapter R.16).

Features:

Special feature: With the aid of these tables

- the PNEC value and
- abatement of substance discharge via the wastewater treatment plant

– that is, substance properties – can also be modified. These properties are prescribed in other tools. In general, process and ambient parameters are scaled.

[7] The abatement of substance discharge into the receiving water can be effected in the wastewater treatment plant by means of mechanical processes, biological degradation, adsorption to the sewage sludge or volatilization of the substance in the atmosphere.

Values are preset in the spreadsheets; own entries cannot be made. In a comparable form, non-linear dependencies could also be described.

Upper limits are not envisaged.

Table 10: Profile: features of the scaling spreadsheet for organic chemicals in electroplating

Scaling spreadsheet for organic chemicals in electroplating	
1	**By which stakeholder has the tool been developed, and for what purpose?**
	Development: Ökopol together with the German Federation of Surface Technology Industries (ZVO). Purpose: Support in the development of exposure scenarios.
2	**For which user group has the tool been developed?**
	Formulators who prepare exposure scenarios.
3	**Which areas of application are addressed?**
	Surface finishing.
4	**Are particular application circumstances addressed?**
	Use of organic substances in electrolytes.
5	**Which environmental compartments are covered?**
	Surface waters (freshwater)
6	**Which input parameters are required?**
	Volume flow of the receiving water, PNEC value (special feature of this tool!), emission abatement in wastewater treatment plants.
7	**In which form is the outcome presented?**
	The maximum permissible quantity of substance to be used is stated.
8	**Complexity of the tool**
	Low.
9	**Possibility of direct transfer to other industries**
	In terms of its structure, the spreadsheet can also be used in other industries.
10	**Possibility of direct transfer following adaptation**
	Direct transfer is possible.
11	**Substantive correctness of underlying equations**
	The linear dependency of variables is correctly reproduced. The maximum possible quantity used under standard conditions is not calculated in the tool itself, but is taken from an existing calculation.
12	**Consideration of upper limits for variables that affect exposure**
	Upper limits are not considered.
13	**Consideration of effects on other environmental compartments**
	No such consideration.
14	**Appropriateness of the tool for the intended user group**
	The tool is appropriate for formulators who prepare exposure scenarios.
15	**Particular strengths and weaknesses of the tool, also in comparison with other tools**
	Advantage: simple structure, easy to use. Disadvantage: less convenient when more than one variable is changed.
16	**Need and possibilities of further development**
	Consideration of upper limits.

3.5 Scaling equation for solvent loading in wastewater

The REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains[8] (first edition, 2009) contains an equation for calculation of acetonitrile effluent load with, which is taken from an exposure scenario for acetonitrile. The equation is reproduced in the following table.

Table 11: Scaling equation for acetonitrile effluent load. Source: REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains, April 2009.

Information on estimated exposure and DU guidance	
8	**Exposure estimation and reference to its source**
9	**Guidance to DU to evaluate whether he works inside the boundaries set by the ES** **The exposure is inside the boundaries set by the ES if the following requirements are met:** **Environment:** • Wastewater: ○ The maximum release to wastewater can be calculated by the following equation: ▪ Maximum release [kg/day] = 0.120 * 0.1 * (F_R + E_D) / E_D F_R = low-flow rate of river E_D = STP effluent discharge ○ The RMM in section 6.2 and 7 are followed.

F_R: Volume flow of the receiving water; E_D: Volume flow of the wastewater treatment plant

The equation enables calculation of how many kilograms of acetonitrile may be released per day with process effluent into a wastewater treatment plant, depending on the volume flow of the receiving water and the volume flow of the treatment plant.

The data is based on exposure estimation and risk characterization. The outcome is that release of 0.12 kg of acetonitrile per day is permissible when the volume flow of the treatment plant is 2,000 cubic metres per day and the volume flow of the receiving water is at least 18,000 cubic metres per day. These stipulations are also stated in the exposure scenario (from the ratio between volume flow of the treatment plant and that of the receiving water there arises a factor of 0.1 in the equation for calculation of maximum permissible release in Table 12). The corresponding extract from the exposure scenario is shown in the following table.

[8] The REACH Practical Guide is published by the German Chemical Industry Association (VCI) and the European Chemical Industry Council (Cefic) (https://www.vci.de/Themen/Chemikaliensicherheit/REACH/Seiten/REACH-Praxisfuehrer.aspx#).

Table 12: Extract from the exposure scenario with additional information on the scaling equation

Risk Management Measures	
6.1	Risk management measures related to human health
6.2	Risk management measures related to the environment: ▪ Waste water: - Any potential releases to water should be avoided as far as possible - Wastewater should be directed to an STP - Maximum daily release to wastewater per site[1]: 0.120 kg/day ▪ Air: Any potential releases to air should be avoided as far as possible ▪ Soil: Direct release to soil should be avoided [1] STP effluent discharge = 2000 m^3/day; Flow rate of effluent receiving river = 18000 m^3/day; see section 9 for an equation to calculate the maximum release to wastewater on the basis of a known effluent discharge and a known flow rate of the receiving river.

Two variables can be modified: the capacity of the wastewater treatment plant (purified water volume in cubic metres per day) and the volume flow of the receiving water (in cubic metres per day).

Calculated variable

With the scaling equation for solvent loading of effluent, the maximum quantity of solvent that may be released into the wastewater treatment plant can be calculated.

Outcome of estimation:

The maximum quantity that may be released into the wastewater is stated in kilograms per day.

Target group of the scaling tool:

Formulators who apply the substance in preparations, or downstream users who themselves apply the substance or a preparation containing the substance.

Substantive basis:

The maximum permissible quantity used under standard conditions is not calculated in the equation, but directly entered. Modelling of effluent load is carried out for determination of this parameter in accordance with ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.16 Environmental Exposure Estimation.

Features:

Merely the volume flow of the wastewater treatment plant and the volume flow of the receiving water are given as scaling parameters. No upper limits are considered. With this tool, the outcome is not the maximum possible quantity of substance used, but rather the maximum permissible quantity that may be released into wastewater.

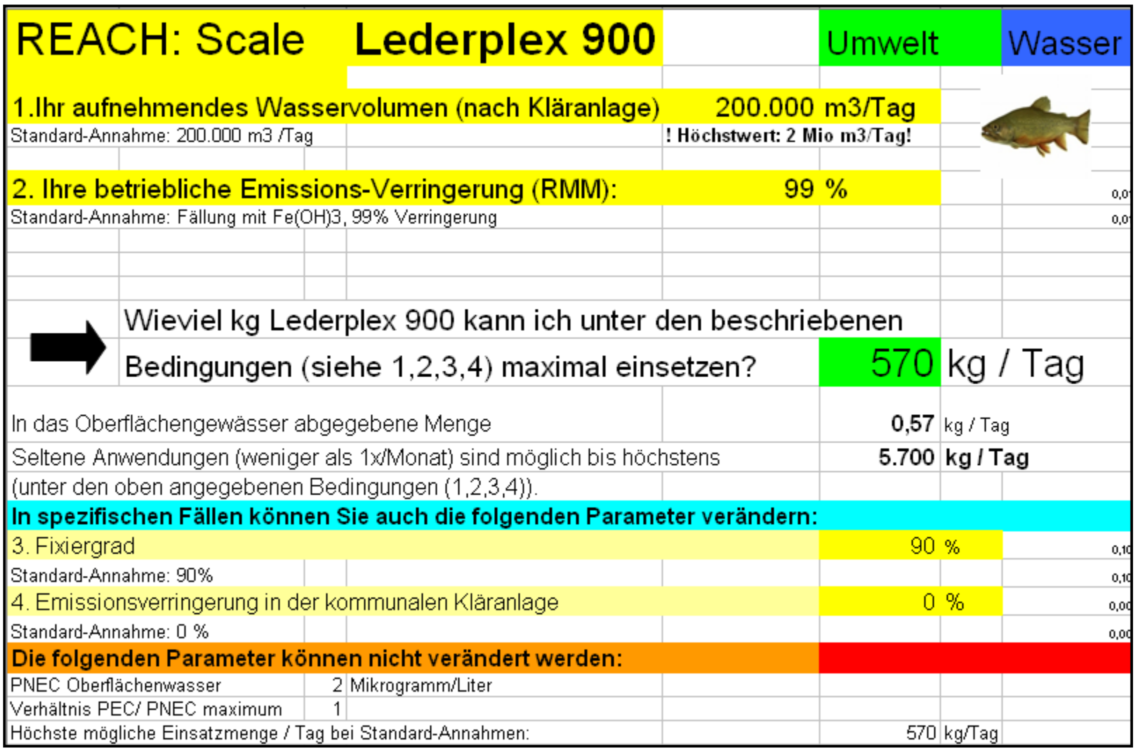
Table 13: Profile: Features of the scaling equation for solvent loading of effluent

Scaling equation for solvent loading of effluent	
1	**By which stakeholder has the tool been developed and for what purpose?**
	The tool was developed by a substance manufacturer to support scaling by its customers.
2	**For which user group has the tool been developed?**
	Industrial and profession users of solvents.
3	**Which areas of application are addressed?**
	Industrial applications of solvents.
4	**Which particular application circumstances are addressed?**
	Closed applications and batch production.
5	**Which environmental compartments are covered?**
	Surface waters (freshwater).
6	**Which input parameters are required?**
	Volume flow of the wastewater treatment plant and volume flow of the receiving water.
7	**In which form is the outcome presented?**
	The quantity that may be released per day into wastewater is stated.
8	**Complexity of the tool**
	Low.
9	**Possibility of direct transfer to other industries**
	Transferability exists
10	**Possibility of direct transfer following adaptation**
	Transferability exists
11	**Substantive correctness of underlying equations**
	The equation correctly describes the ratio between exposure level and the receiving water volume. The maximum possible quantity to be used under standard conditions is not calculated in the tool, but is taken from an existing calculation.
12	**Consideration of upper limits for exposure-defining variables**
	Upper limits are not considered.
13	**Consideration of effects on other environmental compartments**
	Only the water compartment is considered.
14	**Appropriateness of the tool for the intended user group**
	The tool can be used by formulators and end-users.
15	**Particular strengths and weakness of the tool, also in comparison with other tools**
	Advantage: limited number of input parameters. Disadvantage: no direct link to the quantity used.
16	**Need and possibilities of further development**
	Description of input form (data in cubic metres per day). Explanation of how the "released" quantity can be calculated.

3.6 The REACH Scale Environment spreadsheet

The REACH Scale Environment spreadsheet has been developed by Öko-Institut together with companies from the textile industry within the framework of the REACH Practical

Guide.[9] It represents further development and simplification of the spreadsheet (see Section 3.3), the structure of which is reproduced in the following figure.



REACH: Scale Lederplex 900	Umwelt	Wasser	
1.Ihr aufnehmendes Wasservolumen (nach Kläranlage)	200.000 m3/Tag		
Standard-Annahme: 200.000 m3 /Tag	! Höchstwert: 2 Mio m3/Tag!		
2. Ihre betriebliche Emissions-Verringerung (RMM):	99 %		0,0
Standard-Annahme: Fällung mit Fe(OH)3, 99% Verringerung			0,0
Wieviel kg Lederplex 900 kann ich unter den beschriebenen Bedingungen (siehe 1,2,3,4) maximal einsetzen?	570	kg / Tag	
In das Oberflächengewässer abgegebene Menge	0,57	kg / Tag	
Seltene Anwendungen (weniger als 1x/Monat) sind möglich bis höchstens (unter den oben angegebenen Bedingungen (1,2,3,4)).	5.700	kg / Tag	
In spezifischen Fällen können Sie auch die folgenden Parameter verändern:			
3. Fixiergrad	90 %		0,1
Standard-Annahme: 90%			0,1
4. Emissionsverringerung in der kommunalen Kläranlage	0 %		0,0
Standard-Annahme: 0 %			0,0
Die folgenden Parameter können nicht verändert werden:			
PNEC Oberflächenwasser	2 Mikrogramm/Liter		
Verhältnis PEC/ PNEC maximum	1		
Höchste mögliche Einsatzmenge / Tag bei Standard-Annahmen:	570	kg/Tag	

Figure 3: Structure of the REACH Scale Environment spreadsheet

Four variables that affect exposure can be entered in the spreadsheet by downstream users: Water volume/unit of time of the receiving water (downstream of the wastewater treatment plant, more precisely, the average low-flow rate), effectiveness of operational emission reduction measures, degree of fixation (data on the proportion of chemicals present in the dyeing bath that is applied to textile fibres) and emission abatement in the municipal wastewater treatment plant.

The data is entered in the lines that begin with the numbers 1 to 4 and have a dark- or light-yellow background.

Calculated variable

The quantity of the product that downstream users may use per day is directly calculated in the REACH Scale Environment spreadsheet.

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[9] The REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains is published by the German Chemical Industry Association (VCI) and the European Chemical Industry Council (Cefic) (https://www.vci.de/Themen/Chemikaliensicherheit/REACH/Seiten/REACH-Praxisfuehrer.aspx#).

Outcome of estimation

The maximum permissible quantity of the product is stated in the cells in the centre of the spreadsheet that have a green background (in Figure 4 the quantity is 570 kilograms per day).

In addition, the quantity is stated that is possible with "intermittent application", which is defined in the ECHA guidance document with "less than one application per month, **with a duration of less than 24 hours** (ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.10, Section 10.3.3).

Target group of the scaling tool:

REACH Scale Environment has been developed for downstream users of chemicals that have no previous experience in environmental exposure estimation (but not for formulators).

Substantive basis:

The maximum possible quantity used is not calculated in the spreadsheet; instead a value determined by the registrant is entered. Modelling of effluent load is generally carried out to determine this value, in accordance with ECHA guidelines on environmental exposure estimation (Chapter R.16).

A distinction is not made in the scaling tool between the volume flow of the treatment plant and the volume flow of the receiving water upstream of the treatment plant.

Features:

Input options in this tool have been deliberately limited to variables, which in the case of downstream users of substances or preparations, can deviate from data of the supplier in the exposure scenario.

An upper limit has been set for volume flow of the receiving water. The highest possible input value is 2,000,000 cubic metres. This corresponds, with a standard value 2,000 m^3 for volume flow in the wastewater treatment plant, to a receiving-water dilution factor of 1000. This maximum value is laid down in Chapter R.16 (environmental exposure estimation) of the ECHA Guidance on Information Requirements and Chemical Safety Assessment. http://guidance.echa.europa.eu/docs/guidance_document/information_requirements_r16_en.pdf?vers=27_05_10).

A distinction is made between two key parameters that are generally variable (volume flow of the receiving water and effectiveness of operational risk-management measures), and two further scaling variables, which should only be modified when additional data exists: degree of fixation and emission abatement in the municipal wastewater treatment plant. Emission abatement in those wastewater treatment plants is understood to be mechanical removal, biological degradation, adsorption to effluent sludge and release into the atmosphere which depends on the substance properties.

With this scaling tool the preset starting values are permanently displayed.

Table 14: Profile: Features of the REACH Scale Environment spreadsheet

REACH Scale Environment spreadsheet	
1	**By which stakeholder has the tool been developed, and for what purpose?**
	REACH Scale Environment was developed by Öko-Institut to support end-users with little or no experience with exposure estimation tools.
2	**For which user group has the tool been developed?**
	Downstream users of chemicals (substances and preparations) .
3	**Which areas of application are addressed?**
	Textile finishing.
4	**Are particular application circumstances addressed?**
	Continuous and discontinuous processes (batch production).
5	**Which environmental compartments are covered?**
	Surface waters (freshwater).
6	**Which input parameters are required?**
	Volume flow of the receiving water, effectiveness of operational emission reduction measures, degree of fixation and emission abatement in the municipal wastewater treatment plant.
7	**In which form is the outcome presented?**
	Maximum quantity of daily use and maximum possible quantity of use in the case of intermittent applications are stated.
8	**Complexity of the tool**
	Low to medium complexity (spreadsheet).
9	**Possibility of direct transfer to other industries**
	Transfer to other industries is possible.
10	**Possibility of transfer following adaptation**
	The spreadsheet can also be used in other industries; where necessary, the terminology (for instance, "degree of fixation") should be adapted to the respective industry.
11	**Substantive correctness of the underlying equations**
	Linear dependencies are correctly reproduced. The maximum possible quantity used under standard conditions is not calculated in the spreadsheet itself, but is taken from an existing calculation.
12	**Consideration of upper limits for variables that affect exposure**
	Upper limits are included in the water volume of the receiving water.
13	**Consideration of effects on other environmental compartments**
	There is no consideration of environmental compartments other than water.
14	**Appropriateness of the tool for the intended user group**
	The tool is appropriate for end-users.
15	**Particular strengths and weaknesses of the tool, also in comparison with other tools**
	Advantage: Limitation to a few input parameters. Weakness: No consideration of the volume flow of the wastewater treatment plant.
16	**Need and possibilities of further development**

REACH Scale Environment spreadsheet	
	Inclusion of further upper limits. Consideration of the volume flow of the wastewater treatment plant. Development of similarly-structured tools for other environmental compartments.

3.7 REACH Wastewater tool of the TEGEWA Association

The REACH wastewater tool has been developed by the TEGEWA Association, which represents manufacturers of, among others, textile auxiliaries and tanning agents. The wastewater tool represents further development and simplification of the spreadsheet, which has been developed together with companies from the textile industry (see Section 3.3). The structure of the tool is reproduced in the following figure.

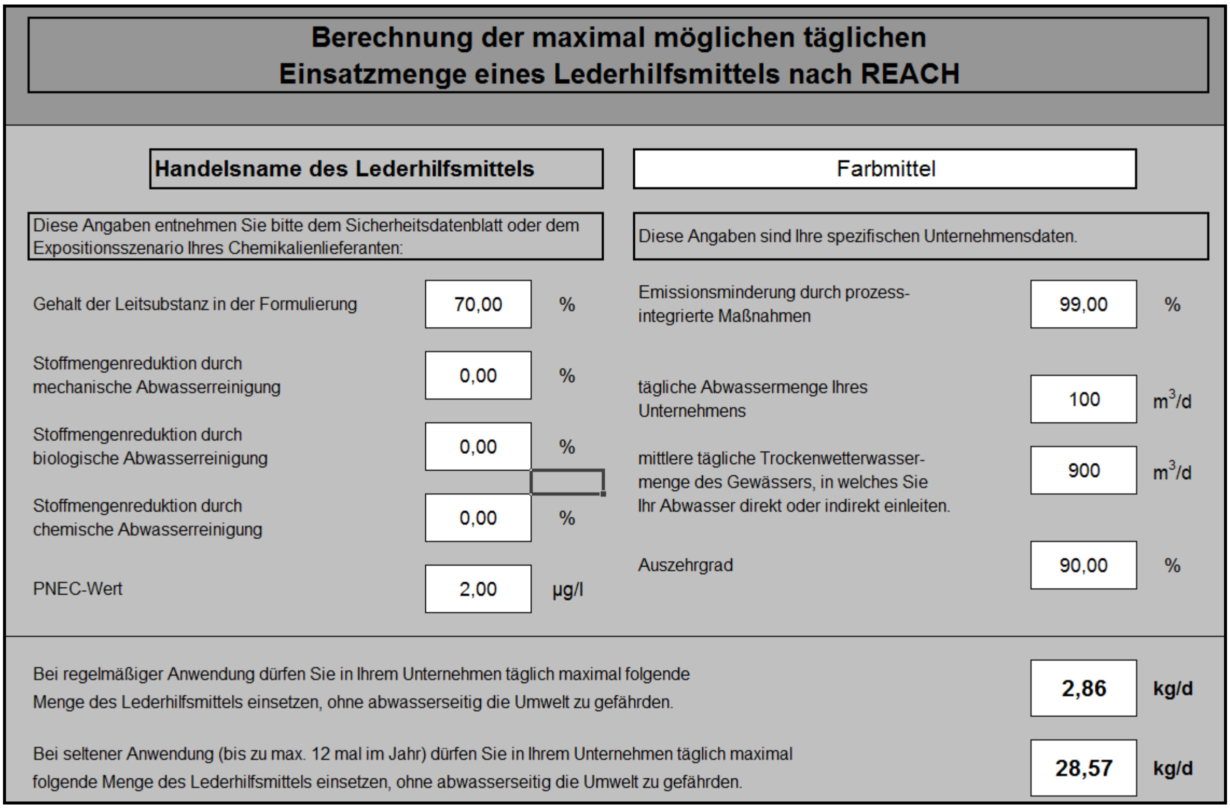

Figure 4: Structure of the REACH wastewater tool of the TEGEWA Association

In the REACH wastewater tool a total of 9 variables can be modified. The tool thus enables exhaustive estimation of environmental exposure on the basis of the equation described in this chapter. The values are entered in the boxes with a white background in the upper part of the tool.

Calculated variable

The maximum quantity of the product that the downstream user may apply per day is calculated directly in the REACH wastewater tool.

Outcome of use of tables

In the lower third of the spreadsheet the maximum permissible quantity of the product is stated. In addition, the quantity that may be used in intermittent applications is also stated.

Target group of the scaling tool

The wastewater scaling tool has been developed for formulators and tanners (downstream users of tanning chemicals).

Substantive basis

Direct modelling of effluent load is carried out in the scaling tool in accordance with the equation shown in Table 3. The procedure corresponds to the description in ECHA guidance on environmental exposure estimation.[10] A distinction is made in the scaling tool only between the wastewater volume flow of the company and the volume flow of the receiving water. The standard settings for water volumes of wastewater treatment plants and receiving waters, as laid down in Chapter R.16 of ECHA Guidance on Information Requirements and Chemical Safety Assessment (treatment plant capacity: 2,000m^3 per day; receiving-water dilution factor: 10), have not been adopted. TEGEWA assumes that the spreadsheet will be used by both direct and indirect dischargers.

In the scaling tool, the behaviour of substances in the wastewater treatment plant is not based on the result of modelling the different processes that occur in such a plant (biodegradation, adsorption to effluent sludge and release of a proportion of the substance into the atmosphere[11]). Instead, individual factors for mechanical, biological and chemical reduction of substance quantities should be stated. These values are in many cases not available. In reworking the scaling tool, the individual factors mentioned should be replaced by a factor for substance reduction in the treatment plant that takes account of all relevant important processes.

The term "intermittent application" is defined in the scaling tool as "up to 12 times per year". This should be replaced by the stipulation contained in the ECHA guidance document; namely, less than once a month, with a duration of less than 24 hours (ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.10, Section 10.3.3).

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[10] http://echa.europa.eu/documents/10162/17224/information_requirements_r16_en.pdf.

[11] Such modelling is undertaken, for example, in the EUSES environmental exposure estimation tool with the aid of the "SimpleTreat" calculation module.

Features

A large number of parameters can be entered in the REACH wastewater tool. Input options for the concentration of a substance in the product and for the PNEC value of an ingredient are important for formulators, but of no significance for downstream users of chemicals.

No upper limits are prescribed for input values.

With this scaling tool, default values are not permanently displayed, but are overwritten with the tool user's own values. This makes it difficult to comprehend the original assessment of the supplier after initial use.

REACH Wastewater tool of the TEGEWA Association	
1	**By which stakeholder has the tool been developed and for what purpose?**
	The TEGEWA Association, together with the Leather Industry Association
2	**For which user group has the tool been developed?**
	Formulators of preparations and downstream users of chemicals.
3	**Which areas of application are addressed?**
	Industrial and professional applications with discharge into the environment.
4	**Are particular application circumstances addressed?**
	Use of chemical substances for manufacture of leather (in tanneries).
5	**Which environmental compartments are covered?**
	Surface waters (freshwater)
6	**Which input parameters are required?**
	Concentration of the substance in the product, substance reduction in the product, substance reduction by means of wastewater purification by mechanical, biological and chemical processes, effectiveness of operational emission reduction measures, volume of company wastewater, volume flow of the receiving water, degree of fixation and PNEC value
7	**In which form is the outcome presented?**
	Maximum permissible quantity used per day and quantity used per day with intermittent applications are stated.
8	**Complexity of the tool**
	Average complexity.
9	**Possibility of direct transfer to other industries**
	Transfer is possible.
10	**Possibility of transfer following adaptation**
	Transfer is possible; where necessary, with adaptation of terminology (for example, "degree of fixation").
11	**Substantive correctness of underlying equations**
	Calculations are based on EUSES. Data on degree of degradation in individual stages of wastewater treatment should be replaced by SimpleTreat modelling. The term "intermittent applications" should be supplemented in accordance with the ECHA guidance document.
12	**Consideration of upper limits for exposure-defining variables**
	There are no upper limits.

13	**Consideration of effects on other environmental compartments**
	Other environmental compartments are not considered.
14	**Appropriateness of the tool for the intended user group**
	Based on experience, the aid is appropriate for the target group of formulators and tanners.
15	**Particular strengths and weaknesses of the aid, also in comparison with other tools**
	Advantage: User-friendly structure. Disadvantage: Default values are overwritten with user-entered values.
16	**Possibility and need of further development**
	Inclusion of upper limits. Documentation of default values.

Table 15: Profile: Features of the REACH Wastewater tool of the TEGEWA Association

4 Required parameters and existing scaling tools developed by stakeholders

Scaling tools have already been developed by stakeholders. In this chapter, the parameters employed in existing tools are described and commented upon. Recommendations are also made concerning the parameters that have to be considered in scaling tools and the minimum standards that have to be met in order that scaling does not lead to incorrect assessments. In addition, advice is given on meaningful supplementation for further development of scaling tools.

A total of 19 different parameters are applied in the seven scaling tools under examination.

Certain of the parameters are related to each other. Terms such as degree of fixation, application and consumption all relate to the proportion of the quantity of substance used that remains on the processed material. Related parameters are arranged in seven groups in the table. Where required, a brief annotation is provided for individual parameters.

Table 16: Changeable parameters that are mentioned in scaling tools

	Parameter	Annotation
1	Concentration of a substance in the product	This value can be changed only by formulators, and not by users of chemicals
2	Consumption of a substance in the process	
2.1	Degree of fixation	In different industries different terms are used to express the same subject matter
	Degree of consumption	
2.2	Proportion of the quantity used that is released	This value arises from the total quantity minus the value from 2.1
3	Quantity used and number of days of use per year	
3.1	Quantity used per day	
3.2	Quantity used per year	Parameter 3. 1 is calculated from these two parameters
	Days of use per year	
4	Effectiveness of operational emission reduction measures	
5	Substance behaviour and fate in municipal wastewater treatment plants	
5.1	Elimination degree in the treatment plant / emission abatement in the municipal wastewater treatment plant / substance reduction in the treatment plant	Summarizing value that links the individual processes that are addressed in 5.2
5.2	Elimination in mechanical treatment	The processes that occur in mechanical, biological and chemical wastewater purification can generally not be separately designated with factors
	Biodegradability	
	Adsorption to effluent sludge	
6	Receiving water volume	
6.1	Daily wastewater volume of the company	
6.2	Capacity (wastewater volume) of the wastewater treatment plant	Standard assumption: 2,000 m^3 (ECHA R.16)
6.3	Volume of the receiving water	
6.4	Average daily low-flow rate of the receiving water / Average low water discharge (MNQ)	More precise description of 6.3 (R.16: 18,000 m^3 per day)
6.5	Dilution factor in the receiving water	With standard calculations = 10
6.6	Total receiving water volume	Sum of 6.2 and 6.3; standard: 20,000 m^3
7	Parameters that relate to ecotoxicological properties of substances	
	PNEC aquatic	Substance parameter, not scaleable

4.1 Upper limits for possible input values

With most of the parameters it is useful to specify upper limits in the calculation to avoid errors. Proposals for such limits are made in the right-hand column of the following table.

Table 17: Upper input limits for modifiable parameters in scaling tools

Parameter		Proposed upper limit
1	Concentration of the substance in the product	100%
2	Consumption of a substance in the process	
	Degree of fixation	100%
	Degree of consumption	100%
	Proportion of the quantity used that is released	100%
3	Quantity used and number of days of use per year	
	Days of use per year	365
	Quantity used per day	-
	Quantity used per year	-
4	Effectiveness of operational emission reduction measures	99.5%
5	Substance fate in the municipal wastewater treatment plant	
	Elimination degree in the treatment plant / emission abatement in the municipal wastewater treatment plant / substance reduction in the wastewater treatment plant	100%
	Elimination in mechanical treatment	100%
	Biodegradability	100%
	Adsorption to effluent sludge	100%
6	Receiving water volume	
	Daily wastewater volume of the company	-
	Volume flow of the wastewater treatment plant	20,000 m^3/day
	Volume flow of the receiving water (average low-flow rate (MNQ))	2,000,000 m^3/day
	Dilution factor in the receiving water	1000
	Total receiving-water volume	2,000,000 m^3

In the calculation of local concentration in the receiving water, according to ECHA Guidance, Chapter R.16 the dilution factor should not exceed a value of 1,000 (standard value: 10) (ECHA Chapter R.16, Section 16.6.6.2). The outcome is a maximum value for volume flow of the receiving water of 2 million m^3 per day (standard assumption: treatment plant effluent volume: 2,000 m^3/day).

In the case of risk reduction measures we propose specification of a maximum value of 99.5%. Should in isolated cases greater effectiveness be achieved, the value can be changed (for example, to 99.9%).

The quantity of substance used and the reference value $PNEC_{aquatic}$ are dependent on the company and the substance. Here, no proposals for upper limits can be made.

Other proposed upper limits shown in the table arise directly from the respective parameter. The quantity of a substance absorbed by fabric can thus not exceed the quantity applied in the process. The degree of consumption, which indicates the proportion of the quantity used that remains on the fabric, is therefore a maximum of 100%.

4.2 Use of standard parameters

The use of different parameters for the same exposure-defining variable complicates comprehension and application of scaling tools. We therefore propose that the parameters mentioned in the following table be used in scaling tools for exposure in surface waters (freshwater). Here it should be borne in mind that it can be useful for suppliers to adapt scaling tools to the terminology common in their industry (for instance, substitution of the term "consumption of the substance in the process" with "degree of fixation").

The proposed upper limits correspond to the values in Table 17. Since the input of 100% would have the effect with certain variables that calculations are no longer carried out (division by 0 is not permissible), the value "100%" should here be replaced by 99.9%.

Table 18: Standard designations for input variables in scaling tools

	Parameter	Unit; where applicable, upper limit
1	Concentration of the substance in the product	100%
2	Consumption of the substance in the process (degree of fixation, degree of consumption)	99.9%
3	Quantity used per day	kg
4	Effectiveness of operational emission reduction measures	99.5%
5	Substance reduction in the wastewater treatment plant	99.9%
6	Volume flow of the wastewater treatment plant in cubic metres per day	cubic metre/day (m^3/day)
7	Volume flow of the receiving water (without influent flow of the wastewater treatment plant), stated as average low -water discharge (MNQ) of the receiving water.	Maximum of 2,000,000 m^3/day

It can be assumed in respect of all the above-mentioned parameters that a linear correlation exists, at least to a certain extent, between a parameter and the environmental concentration that is later to be expected. No parameters are used in existing environment-related scaling tools that are non-linear (for example, process temperature and its influence on degree of fixation).

With precise knowledge of the correlation between influencing variable and emission / exposure these parameters, too, could be adopted in a scaling aid (see Section 4.4 Need for Further Development).

4.3 Minimum demands on scaling tools

From examination of existing scaling tools the following minimum demands on such tools can be deduced:

4.3.1 Substantive correctness of the underlying equations and assumptions

Scaling tools are ultimately based on models for environmental exposure assessment. The content of these models should conform to the relevant ECHA guidance document (ECHA

Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.16). The model employed should be named. As a rule, the EUSES model is involved.

4.3.2 Comprehensibility of the tool on the part of the target group

Existing scaling tools differ considerable in their extent and comprehensibility for persons without expert knowledge. The most intricate tool is the ES-Modifier, which demands at least fundamental knowledge of environmental exposure estimation. Most downstream users of chemicals do not dispose of such knowledge.

The easiest tables to use are those in which value ranges are predefined for a given parameter (such as in the scaling tool for electroplating in Section 3.4).

Where several exposure-defining variables can be modified, clearly structured spreadsheets represent the simplest solution.

Comprehensibility of a scaling tool on the part of the respective target group should be checked and ensured by means of tests carried out with a number of companies.

4.3.3 Unequivocal identification of upper limits for scaling

Where spreadsheets are offered as scaling tools, upper limits for possible input values should be applied. Should this not be the case, calculation errors can easily occur. Moreover, the area can be quit in which linear dependence exists between exposure-defining variables and exposure. Scaling then results in erroneous estimations.

4.3.4 Support of users by means of examples and background information

Scaling is not self-explanatory. Scaling tools should therefore be properly explained. We further recommend provision in each case of an example that illustrates application.

Background information should also explain the options that exist when scaling reveals that the intended use is not covered.

4.4 Need and possibilities of further development

There are a number of aspects of environmental risk assessment that have not, or have only rarely been considered:

1. Existing scaling tools are predominantly concerned with surface waters (freshwater). Other environmental compartments, such as activated sludge micro-organisms, marine ecosystems and accompanying sediment, air and soil, are not yet represented in simply-applicable tools. Here, there is a need for further development.
2. In scaling tools, input possibilities exist in each case for one risk management measure. It should be shown on the basis of examples how scaling can be conducted when several risk management measures exist.
3. There is presently no scaling tool for preparations having several substances that represent a risk, where in conclusion varied risk management measures are required.

4. Through integration of tables with default values in the case of non-linear dependencies the area of scaling application would be usefully extended.
5. Up to now, exposure measurements have not been utilized in scaling tools. Here, significant possibilities for further development presumably exist.
6. Available scaling tools are targeted at organic chemicals. Inorganics, metals and special substance groups (for example, tensides) are not yet covered. Here, further exposure-defining variables could be included in scaling (for example, bioavailability depending on pH value).

5 Practical guide to scaling

Up to now a practical guide to scaling for downstream users is lacking. Such a guide has been developed within the scope of this research project, on the basis of information and experiences described in previous chapters.

The Practical Guide is directed – also in terms of the level of communication - at small- and medium-sized businesses that have little or no experience with exposure assessment. On the other hand, it also supports registrants and formulators who wish to provide their customers with scaling aids in exposure scenarios.

An important part of the Practical Guide is a revised and extended version of the "REACH Scale Environment" spreadsheet, which is described in Section 3.6.

The Practical Guide is structured as follows:

- Introduction for users: Why scaling?
- How does scaling work?
- Examples.
- Exemplary Spreadsheet: *"REACH_Scale_Environment_Lederplex_900"*.
- Information for registrants and formulators.
- A formatting template that facilitates preparation of a product-specific scaling tool.
- Supplementary information on scaling.

The Practical Guide and the "REACH Scale Environment" spreadsheet are available as separate documents. In this report, reference to both is made in the Annex, Section 8.3.

The examples presented below in Chapter 6 are included (in condensed form) in the Practical Guide.

Practical Guide to Scaling available at: www.reach-info.de/dokumente/scaling/reach_scaling_practical_guide.pdf

6 Implementation of scaling in three industries, with documentation of the outcome

In this chapter, environment-related scaling is documented for three industries. The selected applications differ in respect of their exposure-defining variables. The fields of application are electroplating, leather manufacturing and textile finishing.

In the three examples, three scaling tools are employed that differ in terms of their circle of users and address the three stakeholders mentioned in Work Step 1 (registrants, formulators and users of chemicals).

In the example for electroplating a table with default values is used. This tool is appropriate for users of chemicals by which just one parameter is modified (here degree of fixation is irrelevant).

In the example for textile finishing a spreadsheet is used that enables modification of a limited number of parameters, and is therefore particularly appropriate for end-users of chemicals. On the basis of this example, it is further shown how a supplier can use the given general format of a scaling aid to prepare a product-specific tool for his customers.

In the example for leather manufacture a spreadsheet is used that allows modification of substance concentration and the choice of another PNEC value in the product. It is therefore particularly suitable for formulators who develop and bring preparations onto the market.

These examples, which are uniformly structured, are explained in the following three subchapters:

- Starting point for all examples is the circumstance of the user in practice. The user receives an extended safety data sheet with an exposure scenario. In the exposure scenario information on scaling is provided. Those parts of the exposure scenario are reproduced that contain scaling information and exposure-defining variables.
- We document the assumptions of the registrant on exposure-defining variables and the resulting outcome of risk characterization.
- We describe the actual circumstance of the downstream user. This relates to the variable for which scaling is proposed.
- We describe the steps required for implementation of scaling recommendations contained in the exposure scenario as well as the outcome. In so doing, we apply the method recommended in the Practical Guide. In a given case, several runs can be required before safe use is proven.
- In the second example, textile finishing, we initially describe how the supplier can prepare a product-specific scaling tool. We then show use of the aid by the downstream user (corresponding to examples 1 and 3).

Implementation of the Practical Guide is demonstrated on the basis of examples.

6.1 Exemplary scaling for electroplating

1. Characterization of application and of the substance to which the exposure scenario relates.

For the electroplating of materials organic compounds are used as process chemicals in watery electrolytes. In the example, an alkylsulfonate (chain length C10-18, sodium salt) is used, which is added to lower surface tension.

The alkylsulfonate is not depleted by way of reactions. In surface treatment, however, a proportion of the electrolyte is transported into the next bath and discharged into wastewater. In order to offset this loss, alkylsulfonate is continuously added. In the product used in electroplating the alkylsulfonate concentration is 50%.

Alkylsulfonate is readily biodegradable, has low vapour pressure (5 pascals at 20 ^{o}C) and does not have the tendency to bioaccumulate. The $PNEC_{aquatic,freshwater}$ amounts to 8 microgram/l.

SimpleTreat modelling shows that the substance is for the most part degraded in the sewage plant. Merely 13% of the substance quantity discharged into the wastewater treatment plant reaches the receiving water.

2. Exposure defining variables and the outcome of risk characterization by the registrant

For exposure assessment and risk characterization the registrant proceeds on the assumption of the following values:

- Quantity of product used per day: 2.46 kg
- Concentration of alkylsulfonate in the product: 50%
- Emission abatement in the wastewater treatment plant: 87%
- Effectiveness of operational partial-flow treatment: 0%
- Volume flow of the wastewater treatment plant: 2,000 m^3/day
- Volume flow of the receiving water: 20,000 m^3 /day (average low-flow rate (MNQ))
- $PNEC_{aquatic,freshwater}$ 8 micrograms/l
- Resulting risk ratio: 0.99

Outcome: The application is safe

Note: In practice, the risk ratio should show a value of clearly below 1, since in a company the same substance can be used in several products. In this case, the substance represents a higher total burden on the environment.

Receiving water volumes, in particular, can greatly differ among customers. For this reason, the registrant prepares a table as a scaling aid, in which the maximum possible daily quantities used in respect of several receiving water volumes are stated.

Note: With galvanization processes the shape and number of treated parts as well as the number of processed flight bars have an influence of the quantity of retained process solution. The downstream user has the task of checking whether the application he undertakes is covered by the exposure scenario of his supplier.

3. Extracts from the exposure scenario: scaleable variables and scaling aid

3 Application conditions	
Maximum possible quantity used	**2.46 kg / day to compensate electrolyte losses**
Local requirements	**Volume flow of receiving water: 20,000 m³/day (average low-water discharge)** **Indirect discharger with a treatment plant capacity of at least 2,000 m³/day**

4 Aid for checking whether ones own use is covered

Volume flow of receiving water (m³/day)	1,000	5,000	10,000	**20,000**	40,000	**80,000**	160,000	200,000
Maxi. quantity used/day (in kg/day)	0.12	0.6	1.23	**2.46**	4.9	9.8	19.7	24.6

4. Situation of the user related to scaleable variables

The customer runs an electroplating business in Freiburg, Germany. It applies chemicals, and uses 9 kilograms of the product daily. The company is an indirect discharger. The wastewater treatment plant has a volume flow of 2,000 m^3/day. The receiving water of the treatment plant has a volume flow (average low-water discharge (MNQ)) of 84,000 m^3/day.

5. Work steps for carrying out scaling, and results

The customer compares the quantity he uses and his receiving water volume with the values in the table. His local **receiving-water volume** lies just above the value of 80,000 m^3/day shown in the table. According to the table, in this case a quantity of 9.8 kg/day is acceptable. The customer enters a lower quantity.

It is to be expected that the customer's application as such is environmentally safe and no adverse effects in the environment occur. Adverse effects on the environment can arise, however, when several companies discharge substances into the same wastewater treatment plant or – at a local level – into the same receiving water.

6.2 Exemplary scaling for textile finishing

1. Characterization of the application and of the substance to which the exposure scenario relates.

Metal-complex dyes, among others, are used for dyeing cotton fabrics. In many cases, manufactures themselves bring their mixtures onto the market.

In this example, the registrant produces the metal-complex dye (sodium salt of a nitronaphthalene compound) and sells it as a component of its mixture Cuprasol Blue 294 to textile finishers.

The metal-complex dye does not meet the test criteria for inherently biological degradability. It has low vapour pressure (1 pascal) and is not bioaccumulative. The $PNEC_{aquatic, freshwater}$ amounts to 2 micrograms/l.

SimpleTreat modelling shows that the substance is not biologically degraded in the wastewater treatment plant, it is not adsorbed to sewage sludge and does also not volatilize in the atmosphere. It is therefore discharged more or less entirely into the receiving water.

Since the conditions of application for dyes in textile finishing strongly depend on the substrate to be coloured, process conditions and the company's local conditions, the registrant initially conducts a chemical safety assessment. Therefore he is making use of standard values for exposure-defining variables.

He wishes to provide his customers – small- and medium-sized textile finishers – with an easily applicable scaling tool. In order to prepare it he utilizes the style-sheet "*REACH_Scale_Environment_Template*".

2. Exposure-defining variables and the outcome of risk characterization by the registrant

For exposure assessment and risk characterization the registrant proceeds on the basis of the following values:

- Concentration of the metal-complex dye in the mixture: 70%
- Degree of fixation with cotton dyeing: 95%
- Effectiveness of operational partial-flow treatment (catalytic oxidation of the dye): 99%
- Emission abatement in the wastewater treatment plant: 0%
- Volume flow of the wastewater treatment plant: 20,000 m^3/day
- Volume flow of the receiving water: 180,000 m^3/day (average low-flow rate (MNQ))
- $PNEC_{aquatic,freshwater}$ 2 micrograms/l.
- Risk ratio PEC/PNEC: 0.99

The result is maximum permissible daily use of 570 kg/day of the dye mixture Cuprasol Blue 294.

Since several variables are modifiable, the registrant prepares a spreadsheet as scaling tool. It enables direct input of several parameters.

3a. Preparation of a scaling tool by the registrant using a formatting template

The registrant makes use of the formatting template "*REACH_Scale_Environment_template*" (available at: http://www.reach-info.de/dokumente/scaling/REACH_Scale_Environment_Template.xls

and http://www.umweltdaten.de/chemikalien/scaling_template_registrants.xls)

He enters the product name and his own data on exposure-defining variables in the tab sheet 4 "Input_Parameter" (see following figure).

REACH Scale F		**Environment**		**Water**	
Data input for registrants/ downstream users					
Please fill in the data relating to your product and, if necessary, a comment:				**Example**	
Name of the product	Cuprasol Blue 294			Lederplex 900	
Value	**Data**	**Unit**	**Comment**		
PNEC surface water	2	µg/liter		13	µg/liter
Volume flow of the receiving water (Remark 1)	180.000	m³/day		180.000	m³/day
Volume flow of the sewage treatment plant	20.000	m³/day		20.000	
Efficieny of the internal emission reduction	99	% decrease	*catalytic oxidation*	95	%
Reduction of substance in process (remark 2)	95	%		90	%
Emission reduced in the communal sewage treatment plant	0	%		88	%
Maximum amount used (remark 3)	570	kg/day		420	kg/day
Concentration of substance in mixture	70	%		100	%
Upper limit of the input value					
Cession of the sewage treatment plant max. (remark 4)	2000	kg		100	kg
Receiving water volume max. (remark 5)	2.000.000	m³/day		2.000.000	m³/day
Relevant substance for the calculation of the alloy	metal-complex dyes				

Remark 1: Take the mean of the low-flow water volume (MNQ) as volume of the receiving water. You can get this value from your local water authority.
Remark 2: The reduction of the substance in the process depends on several factors. There may be residual substances in the process. Cleaning operations can cause emission of he substance into wastewater. Therefore in practice often reduction of a substance in a process is lower than e.g. the degree of fixation of the substance.
Remark 3: The maximum amount used per day results in a risk characterisation ratio (PEC/PNEC) = 0,99. It is the ratio between

The formatting template then automatically produces the product-specific scaling tool in the tab sheet "4_Presettings" (see the following figure). This scaling tool later is distributed to his downstream users.

REACH Scale F	Cuprasol Blue 294	Environment Water
1. Receiving water volume (volume flow in m³/day)	1	m³/Day
Default value: 180.000 m³/day		
2. Sewage treatment plant volume (volume flow in m³/day):	1	m³/Day
Default value: 20.000 m³/day		
3. Efficiency of your "in house" emission reduction:	99,0	%
Default value: 99 % reduction catalytic oxidation		
4. Concentration of substance in mixture	70	%
Default value: 70 %		
How much kg of Cuprasol Blue 294 can you use at most under the conditions described (see 1,2,3,4,5,6)?	0 kg/day	
In case of rare applications (less then 1x/month, within 24h) a 10fold higher amount can be used	0 kg/day	
Quantity discharged into sewage treatment plant:	0,0 kg/day	
Quantity discharged into surface water:	0,0 kg/day	
If you have robust data available, you may also change also the following parameters:		
5. Usage of the substance in your application (depending e.g. on fixation)	95,0	%
Default value: 95 %		
6. Emission reduction by sewage treatment plant	0,0	%
Default value: 0 %		
Highest possible input/day at default value:	570 kg/day	

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The registrant stores his file under the name "R_Scale_Cuprasol_Blue_294". He then deletes the first, penultimate and last tab sheet in this file.

3b. Extracts from the exposure scenario: scaleable variables and scaling tools

In the exposure scenario for the dye Cuprasol Blue 294 the registrant provides the following data on scaleable variables (note: concentration of the metal-complex dye in the mixture can be modified only by the formulator and not by the user):

3 Application conditions	
Maximum possible quantity used	570 kg/day
Concentration in the product	70%
Degree of fixation	At least 95%
Partial-flow treatment (operational emission reduction)	Catalytic oxidation. Reduction of metal-complex dye concentration: at least 99%.
Local requirements	Volume flow of the receiving water : 180.000 m³ / day (average low-flow rate (MNQ)) Indirect dischargers with a wastewater treatment plant capacity of at least 20,000 m³/day (volume flow)
4 Aid for checking whether ones own use is covered	
Reference to aid on the Internet	To check your own application use the scaling tool (MODEL, non-active : http://www.cuprasol_Blau_294_scale.html)

4. Situation of the user with regard to scaleable variables

The customer uses 400 kilograms of Cuprasol Blue 294 daily. The degree of fixation is 80%. The customer is an indirect discharger. The wastewater treatment plant has a volume flow of 40,000 m^3/day. The receiving water has a volume flow of 260,000 m^3/day (MNQ).

5. Work steps for carrying out scaling, and results.

The customer compares quantity used, degree of fixation, effectiveness of oxidation and his volume flows (wastewater treatment plant and receiving water) with the values in the table.

The quantity used and receiving-water volumes indicate lower exposure. The lower degree of fixation indicates that higher exposure is to be expected. For assessment of interaction of the four factors the customer enters his values in the spreadsheet "Cuprasol_Blue_294" (see the following figure):

REACH Scale F	Cuprasol Blue 294		Environment Water
1. Receiving water volume (volume flow in m³/day)		**260.000**	**m³/Day**
Default value:	180.000 m³/day		
2. Sewage treatment plant volume (volume flow in m³/day):		**40.000**	**m³/Day**
Default value:	20.000 m³/day		
3. Efficiency of your "in house" emission reduction:		**99,0**	**%**
Default value:	99 % reduction	catalytic oxidation	
4. Concentration of substance in mixture		**70**	**%**
Default value:	70 %		
How much kg of Cuprasol Blue 294 can you use at most under the conditions described (see 1,2,3,4,5,6)?			**214 kg/day**
In case of rare applications (less then 1x/month, within 24h) a 10fold higher amount can be used			**2.137 kg/day**
Quantity discharged into sewage treatment plant:		0,4 kg/day	
Quantity discharged into surface water:		0,4 kg/day	
If you have robust data available, you may also change also the following parameters:			
5. Usage of the substance in your application (depending e.g. on fixation)		**80,0**	**%**
Default value:	95 %		
6. Emission reduction by sewage treatment plant		**0,0**	**%**
Default value:	0 %		
Highest possible input/day at default value:			**570 kg/day**

The calculation shows that the customer can use up to 214 kg per day without adverse environmental effects to be expected. The use of the textile finishers is thus not covered by the exposure scenario. In this case, a change in process management is required to achieve a reduction in effluent load through enhancement of the degree of fixation.

6.3 Exemplary scaling for leather manufacture

1. Characterization of the application and of the substance to which the exposure scenario relates.

Tanning agents are used in the manufacture of leather to preserve skins and hides. They react with skin / hide proteins, and this leads to crosslinking and enhanced preservation. One of the most important tanning agents in terms of quantity used is glutaraldehyde.

In tanning processes a large proportion of glutaraldehyde is consumed through reaction with skins and hides. In the tannery, moreover, process water from tanning generally combines with alkaline wastewater from the preliminary process step of unhairing that contains high concentrations of protein. A large proportion of the residual quantity of glutaraldehyde from the tanning process reacts with this protein.

Glutaraldehyde is readily biodegradable, has low vapour pressure (10 pascals at 20°C) and is not bioaccumulative. The $PNEC_{aquatic,freshwater}$ amounts to 1.25 micrograms/l.

SimpleTreat modelling shows that the substance is to a large extent degraded in the wastewater treatment plant. Merely 12% of the substance quantity discharged into the treatment plant reaches the receiving water.

2. Exposure-defining variables and the outcome of risk characterization by the registrant.

The registrant manufactures glutaraldehyde for different applications. His customers are generally not users of chemicals, but rather formulators. Part of this glutaraldehyde is sold to manufacturers of tanning agents. For exposure assessment and risk characterization the registrant proceeds on the basis of the following values:

- Concentration of glutaraldehyde in the mixture: 100% (the concentration of glutaraldehyde in the ready-to-use mixture varies greatly depending on the formulator. The registrant assumes that glutaraldehyde is applied as a pure substance. The actual concentration in the product is allowed for by the customer).
- Degree of fixation in the tanning process: 90%
- Effectiveness of operational partial-flow treatment (together with wastewater from the unhairing vessel): 95%
- Emission abatement in the wastewater treatment plant: 88%[12]
- Volume flow of the wastewater treatment plant: 20,000 m^3/day
- Volume flow of the receiving water: 180,000 m^3/day (average low-flow rate)
- $PNEC_{aquatic,freshwater}$: 1.25 micrograms/l.
- Risk ratio PEC/PNEC: 0.99

The result is a maximum permissible quantity of glutaraldehyde to be used of 417 kg/day.

[12] Such abatement can be effected through mechanical processes, degradation, adsorption to effluent sludge and volatilization of the substance in the atmosphere.

Concentrations of glutaraldehyde in tanning agents can vary greatly depending on the formulator. In tanneries, moreover, the degree of fixation, the effectiveness of operational partial-flow treatment and the volume flow of the receiving water can differ substantially from the assumptions of the registrant.

Since several exposure-defining variables are modifiable, the registrant uses a spreadsheet as scaling tool that has been prepared by manufacturers of leather auxiliaries at the industry association level. It enables direct input of several parameters.

3. Extracts from the exposure scenario: scaleable variables and scaling tool

3 Application conditions	
Maximum possible quantity used	417 kg/day
Concentration in the product	100%
Degree of fixation	At least 90%
Partial-flow treatment (operational emission reduction)	Combination of process wastewater with wastewater from the unhairing vessel. Glutaraldehyde reduction: at least 95%.
Local requirements	Volume flow of the receiving water: 180,000 m^3 / day (average low-flow rate (MNQ)) Indirect discharger with volume flow in a wastewater treatment plant of at least 20,000 m^3/day
4 Tool for checking whether ones own application is covered	
Reference to the aid on the Internet	To facilitate examination of your application use the scaling tool (MODEL, non-active: http://www.leder.abwasser.scale.html)

Calculation of the maximum allowable daily usage rate under REACH for a tanning agent in leather processing

product for leather processing			glutaraldehyd		
Please fill in substance specific information from the safety data sheet or from the relvant exposure scenario of your distributor:			Please fill in your site and process specific information:		
concentration of substance in mixture	100,00	%	efficiency of your site specific emission abatement system	95,00	%
			daily waste water flow at your site	20.000	m^3/day
efficiency of emission abatement in municipal waste water treatment plant:	88,00	%	average daily low-flow rate of receiving water, where the sewage is dumped into (direct or indirect discharge)	180.000	m^3/day
$PNEC_{aquatic}$ for most sensitive organism in freshwater	1,25	µg/l	Reduction of substance in process	90,00	%

For a chemical employed regularly your company is allowed to use the following amount of the leather processing agent every day without adverse effects in the environment to be expected.	**417**	**kg/day**
In case of rare applications (less than 1x/month, within 24h) your company is allowed to use a higher amount of the substance without adverse effects in the aquatic environment to be expected.	**4167**	**kg/day**

4. Situation of the user with regard to scaleable variables

The customer is a formulator that uses glutaraldehyde as raw material for production of the tanning agent Gerberol 70S, which is a mixture. As far as environmental exposure is concerned, glutaraldehyde is the main ingredient of the mixture.

The concentration of glutaraldehyde in Gerberol 70S is 50%. The formulator states in his exposure scenario the maximum daily quantity of Gerberol 70S that can be applied by its customers.

In the case of degree of fixation, operational partial-flow treatment and receiving-water volume he adopts the assumptions of the registrant.

5. Work steps for carrying out scaling, and results

The formulator enters 50% in the spreadsheet for concentration in the product. Since the other parameters remain unchanged, there arises for Gerberol 70S a maximum possible quantity to be used of 834 kg/day.

He communicates this quantity and the accompanying values of other exposure-defining variables to the tanner in the safety data sheet for Gerberol 70S. In order that the tanner can examine company-specific values, the formulator also makes the spreadsheet available to the tanner, with the value "50% for concentration of glutaraldehyde in Gerberol 70S.

7 Literature on the topic of scaling

Extensive guidelines have been published by the European Chemicals Agency (ECHA) on the conduct of chemical safety assessment and on the obligations of downstream users. In these guidance documents the topic of "scaling" is dealt with a number of times.

- ECHA Guidance for Downstream Users describes initially in Section 5.2.5 the basics of scaling, as well as the conditions under which scaling is not possible. (http://echa.europa.eu/documents/10162/17226/du_en.pdf)
- Section 5.3 of ECHA Guidance for Downstream Users contains a flow chart, in which the individual steps are explained that a downstream user should undertake to examine whether his applications are covered by the exposure scenario. In annotation "i" the scaling procedure is then described in detail.
- ECHA Guidance on Information Requirements and Chemical Safety Assessment addresses, in Chapter R.16, Section 16.3.5, environment-related scaling, and provides further information. (http://echa.europa.eu/documents/10162/17224/information_requirements_r16_en.pdf)
- The most detailed presentation on the topic is found – rather unexpectedly – in Part G of ECHA Guidance on Information Requirements and Chemical Safety Assessment, concerning guidance on preparation of extensions to the safety data sheet (SDS). Here, in Annex G-1, scaling methods are presented and examples given. (http://echa.europa.eu/documents/10162/17224/information_requirements_part_g_en.pdf)

8 Annex

8.1 Supplementary information on scaling

Under REACH scaling provides a highly important opportunity to ensure that improvements in environmental protection are achieved at the scene of the event, with the user. Scaling requires basic knowledge of exposure assessment on the part of the user. Scaling has first to be considered and prepared by the registrant in the conduct of chemical safety assessments and preparation of exposure scenarios, in order that the downstream user can also carry out scaling.

Scaling tools have been developed at the European level for more than two years. During this period certain manufacturers have been working on scaling tools. The tools are characterized by a highly varied complexity. At present, there is no officially agreed recommendation for action that, on the basis of examination of existing concepts, provide users with the required support for scaling.

8.1.1 Background: REACH and scaling

The topic of scaling is addressed in the REACH Regulation in connection with the obligations of downstream users. Among their main obligations is examination of whether their application conditions are covered by the exposure scenarios prepared by their suppliers. Should this not be the case, the user is required to carry out a chemical safety assessment and to prepare chemical safety reports himself.

The possibilities for action on the part of the downstream user, who receives an extended safety data sheet with the exposure scenario, are summarized in the following figure. Scaling has an important function in the process of examining whether the user's application is covered by the exposure scenario.

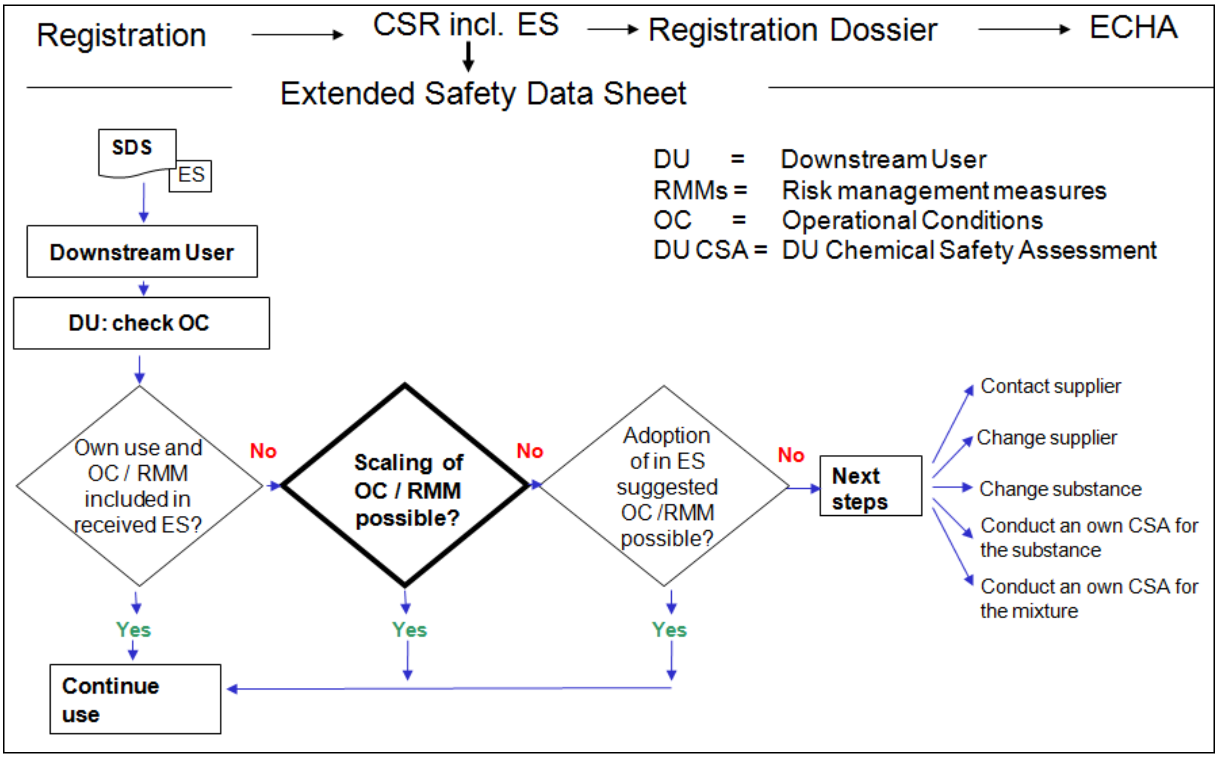

Figure 5: Downstream users and examination of their application conditions

The figure shows the tasks and possibilities for action of downstream users, following receipt of an extended safety data sheet (source: authors' own presentation).

We should like to accentuate at this point that the possibility of scaling can only be utilized when qualitative deviations from the exposure scenario do not exist, and when support for scaling is provided in the exposure scenario.

If the use of the downstream user is not covered by the exposure scenario he can adapt his processes to the conditions laid down in the exposure scenario (as indicated in the final rhombus – "Implementation of RMMs /OC in the ES" – in Figure 5). For instance, he applies additional precipitation measures, as described in the exposure scenario, in order to reduce the residual content of a substance in process wastewater.

Should he not follow this course, he has a number of options that are indicated as "further steps" in Figure 5.

- He can inform the responsible supplier of his application and request that the supplier prepare an exposure scenario that corresponds to his application conditions.
- He can conduct his own chemical safety assessment for his application and, where necessary, inform his customers accordingly.
- He can switch to another supplier that covers his application in an extended safety data sheet.

These steps generally all involve considerable effort. The carrying out of a chemical safety assessment is likely to impose an excessive demand on the majority of downstream users, even when they have to concern themselves "merely" with their own application. It is at least questionable whether in this case of formal fulfilment of requirements a satisfactory level of protection is actually achieved.

Against this background it is important, not only for economic stakeholders, but also – in our opinion – for official monitoring and control, that as many applications as possible are covered by exposure scenarios of a high quality.

Even within specific industries, applications of one and the same substance in different companies can vary widely. It can be expected from neither the manufacturer of a substance nor from the formulator that brings the mixture with the particular substance onto the market, that he be familiar with all details of applications and application conditions, and able to examine them with respect to the occurring emission situation.

In his exposure scenarios the manufacturer or formulator can therefore communicate safe operational conditions merely on the basis of standard assumptions for identified applications. In the case of downstream users, other operational conditions and other risk-management measures will exist in individual cases.

The topic of scaling is therefore highly important.

Under REACH, scaling (which literally means: adaptation or alignment) is understood to mean that the downstream user adapts the exposure assessment provided in the exposure scenario to his own application conditions. This in turn means that he modifies key aspects or parameters of exposure assessment, insofar as he inputs the values that are present in the company (for instance, the daily quantity used). By means of simple calculations he can check whether the expected exposure under his specific operational conditions is safe or not.

Despite deviations in individual exposure-defining variables, the use of the downstream user is then covered by the exposure scenario of his supplier. Through specification of scaling tools the supplier then has the opportunity to broaden the range of application conditions that are covered by his exposure scenario.

Existing scaling tools differ considerably in terms of their complexity. It can be a matter of simple linear correlations: "If half the quantity of substance is used, exposure duration can be twice as long". It can also be necessary to make use of electronic assessment tools.

Scaling is only possible when the supplier specifies relevant scaling rules or scaling tools in his exposure scenario. By this means it is shown that the applicability and limits of scaling have been assessed and are documented in the chemical safety report by the supplier for identified applications. When the registrant specifies assessment tools, he should also identify the related input variables that he has applied for exposure assessment and risk characterization.

8.2 Exposure assessment tools and the ScIDeEx scaling tool

8.2.1 ECETOC TRA, Version 2

ECETOC TRA ("targeted risk assessment") is an tool for assessment of exposure, which has been developed by the ECETOC research group. The tool is regarded as preferred model of stage 1 for assessment of exposure at workplaces (ECHA Guidance on Information Requirements and Chemical Safety Assessment, Part D, Section 5.3).

The completely revised version of ECETOC TRA (ECETOC TRA Version 2010, http://www.ecetoc.org/tra) enables assessment of environmental exposure, consumer exposure as well as inhalative and dermal exposure at workplaces.

ECETOC TRA is available only in an English-language version, and comprises individual Microsoft Excel® files for the areas of workplace and consumers. In addition, an integrated tool has been developed that, apart from exposure assessment for workers and consumers, also comprises environmental exposure assessment. User manuals are available for all three constituent parts.

Compared with the preceding, Internet-based version, ECETOC TRA Version 2010 is now a Microsoft Excel®-based tool, and it includes numerous changes that are described in detail in the accompanying Technical Report.

Many of the changes realized in the new version aim at enhanced integration into the process of exposure assessment pursuant to REACH (for instance, introduction of PROCs (process categories)). ECETOC TRA is now more a tool of exposure assessment than – as before – a targeted risk assessment (TRA) tool. After the input of PNECs or analogue values it is still possible, however, to calculate risk values. Further details of the background to the changes and the scope of the new version are to be found in the Technical Report.

The basis for environmental exposure assessments in ECETOC TRA is provided by EUSES in the form of the TGD Excel spreadsheet. With this, release estimates, PEC calculations as well as conclusive risk characterization (that is, the forming of risk ratios) can be conducted.[13]

In ECETOC TRA, environmental exposure assessments are part of the so-called integrated tool. For assessment of worker exposure, ECETOC TRA has modules, additional to the integrated tool, which can be used independent of each other. Environmental exposure assessment can only be undertaken in the integrated tool.

[13] The TGD Excel spreadsheet has been revised by ECETOC in co-operation with Radboud University Nijmegen. The revised version of ECETOC TRA has been available since the autumn of 2009. The former version of the TGD Excel spreadsheet is no longer up to date.

The new version of ECETOC TRA (Version 2) utilizes the same input variables as EUSES. It already contains newly-developed environmental release categories (ERCs) of REACH Gudidance Document R.16. There is also the possibility to work with specific environmental release (spERCs) which were developed by several industry associations. ECETOC TRA leads to the same result variables as EUSES.

The environment-related part of ECETOC TRA comprises two modules: estimation of release and calculation of predicted environmental concentration (PEC). The module for estimation of release initially uses environmental release categories corresponding to the TGD Excel spreadsheet. It offers four alternatives to ERCs: specific environmental release categories, default values from the A and B tables of the earlier Technical Guidance Document on risk assessment of existing and new substances (http://ecb.jrc.ec.europa.eu/tgd/), data from OECD Emission Scenario Documents and measured, company-specific emission data.

For further information please visit: http://www.ecetoc.org/tra (registration is required). There you can download the ECETOCTRA-Tool (MS Excel® spreadsheet) and instructions. Print version: ECETOC 2004, ECETOC 2009TR.

8.2.2 ES-Modifier

Objectives and scope of the ES-Modifier

The ES-Modifier was developed by Danish and Dutch consultancy companies on the initiative of the Confederation of Danish Industry (DI), and with the support of the Danish Environmental Protection Agency (Danish EPA). DI is the proprietor of the ES-Modifier. The software (Prototype 3.0, May 2010) is freely available at: http://es-modifier.dhigroup.com/, and is presently Excel-based (as of March 2011). A final version is planned that will no longer be Excel-base and is intended to be directly deployable in the ECHA chemical safety and report tool CHESAR.

The aim is to provide downstream users with a tool, with which they can examine and, where applicable, modify the exposure scenarios (ES) that they receive from their suppliers. According to the definition applied in the ES-Modifier, the downstream user works within the application conditions of the exposure scenario for a particular substance (pure substance or in a mixture), when all risk characterization ratios (RCRs) are smaller than 1; that is, when exposure is less than the corresponding, effect-related DNEL or PNEC.

According to information from the developer, the ES-Modifier is aimed at the target group of downstream users with little experience in risk assessment, but with basic knowledge of chemistry and toxicology. Formulators that receive several exposure scenarios for the substances that are intended to be used in mixtures can apply the ES-Modifier to examine such exposure scenarios and to adapt them for their own use and that of their customers.

The ES-Modifier handles not only human exposure (exposure of workers and consumers), but also environmental exposure, and works in the main with information that can be taken from the REACH-conform safety data sheets of suppliers.

Description of the ES-Modifier

The ES-Modifier is Excel-based and comprises the following exposure assessment models:

- For occupational exposure ECETOC TRA (all exposure pathways), Stoffen Manager and EMKG-EXPO-TOOL[14] (only for inhalative exposure) as well as RiskOfDerm (only for dermal exposure[15]).
- For consumer exposure ECETOC TRA and EUSES (all exposure pathways).
- For environmental exposure EUSES.[16]

It requires at different stages input information:

- Selection of life-cycle stages (manufacture, formulation and processing). For end-use and service life, the group of users has to be selected; that is, industrial, professional or consumer.
- Description of use by means of "descriptors", in accordance with ECHA Guidance on Information Requirements and Chemical Safety Assessment, 2010, Chapter R.12), with the four descriptors: sector of use (SU), product category (PC), article category (AC) and environmental release categories (ERC).
- Intrinsic substance properties: physicochemical properties (for example, log Pow, vapour pressure and water solubility), regional PEC aquatic, regional PEC soil and hazard data (DNEL and PNEC)
- When used as a component of a mixture: composition of the mixture.

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[14] EMKG ("Einfaches Maßnahmenkonzept Gefahrstoffe"); in English: Easy-to-use workplace control scheme for hazardous substances. The EMKG-EXPO-TOOL has been developed by the German Federal Institute for Occupational Safety and Health (BAuA) and is freely available at: (http://www.reach-helpdesk.de/en/Exposure/Exposure.html?__nnn=true).

[15] RiskofDerm is an exposure assessment tool for skin exposure. It has been developed by the Dutch institution TNO and is freely available at: (http://www.eurofins.com/product-testing-services/services/research–development/projects-on-skin-exposure-and-protection/riskofderm—skin-exposure-and-risk-assessment.aspx)

[16] Introductions into important exposure assessment tools are provided in Part IV of the REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains: (https://www.vci.de/Themen/Chemikaliensicherheit/REACH/Seiten/REACH-Praxisfuehrer.aspx#).

- Additional input data can be required depending on the exposure assessment model used.

Risk characterization ratios (RCRs)for human exposure via inhalative and dermal pathways (RCR) and for all environmental compartments (water, air, soil, sewage treatment plant) are displayed graphically as bars, which change from green to red when RCR exceeds the value of 1. The latest version of the ES-Modifier (Prototype 3.0, May 2010) also contains a module for preparation of an exposure scenario.

Evaluation

The ES-Modifier incorporates all current exposure assessment models. It allows modification of all relevant input variables and thus recalculation of risk ratios of individual substances in a mixture. The user can determine the parameters that are decisive for the outcome of risk characterization. That enables the downstream user to adapt model parameters to his particular application. He can also compare the results of different exposure assessment models.

Since practically all assessment details can be modified, the user of the ES-Modifier tool requires support in deciding both on the form of modification of the exposure scenario and the model that scaling represents within the framework of the existing exposure scenario, as well as on what is to be regarded as the new exposure scenario. Support for description of the limits and possibilities of the tool should also be made available.

Application of the ES-Modifier requires basic knowledge of exposure assessment and the exposure assessment model it incorporates. Experienced product safety experts of companies that manufacture mixtures on an industrial scale are therefore one target group among users.

The required input data can largely be taken from the REACH-conform safety data sheet. Manual input of all relevant information concerning all substances in a mixture can require a great deal of time.

8.2.3 Emission assessment modules from the Matrix Project of the Federal Environment Agency

The Federal Environment Agency commissioned in 2006, within the framework of an R & D project, the development of two industry-specific, environment-related emission estimation tools ("Matrix Project"[17]).

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[17] R & D Project FKZ 204 67 456, Branch- and product-related emission estimation tool for manufacturers, importers, and downstream users within the REACH system. Developed by Ökopol GmbH, Öko-Institut e.V. and ChemieDaten GmbH. Final Report 2006. http://www.umweltbundesamt.de/uba-info-medien/dateien/3017.htm

The methodology applied in the estimations is in line with European Technical Guidance Documents on Risk Assessment of Existing and New Substances.[18] Industry-specific data on process conditions have been taken from OECD emission scenario documents for the respective industry.

The calculation modules have been developed as flexible, Java-based Internet applications. They have been available on the Internet since 2006 and are freely available at www.emissiontool.com.

Calculation is conducted in the modules on a user-friendly interface according to equations that are also used in the EUSES emission estimation tool. The procedure thus corresponds to the guidance documents, which have been published by ECHA on environmental exposure assessment and risk assessment.

The modules concern plastic additives and photochemicals, and cover the entire life of the chemicals (manufacture, formulation, application, use and disposal).

The exposure estimation modules consider only the environmental compartment surface water (freshwater). The elements of the Use Descriptor system could not yet be considered, since at the time of preparation of the modules this system had not been developed.

Further information on the Matrix Project is to be found at: http://www.emissiontool.com/tool/ (see the following figure).

[18] EU Technical Guidance Document on Risk Assessment ("Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment of New Notified Substances, Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances and Directive 98/8/EC of the European Parliament and of the Council concerning the Placing of Biocidal Products on the Market", 2003).

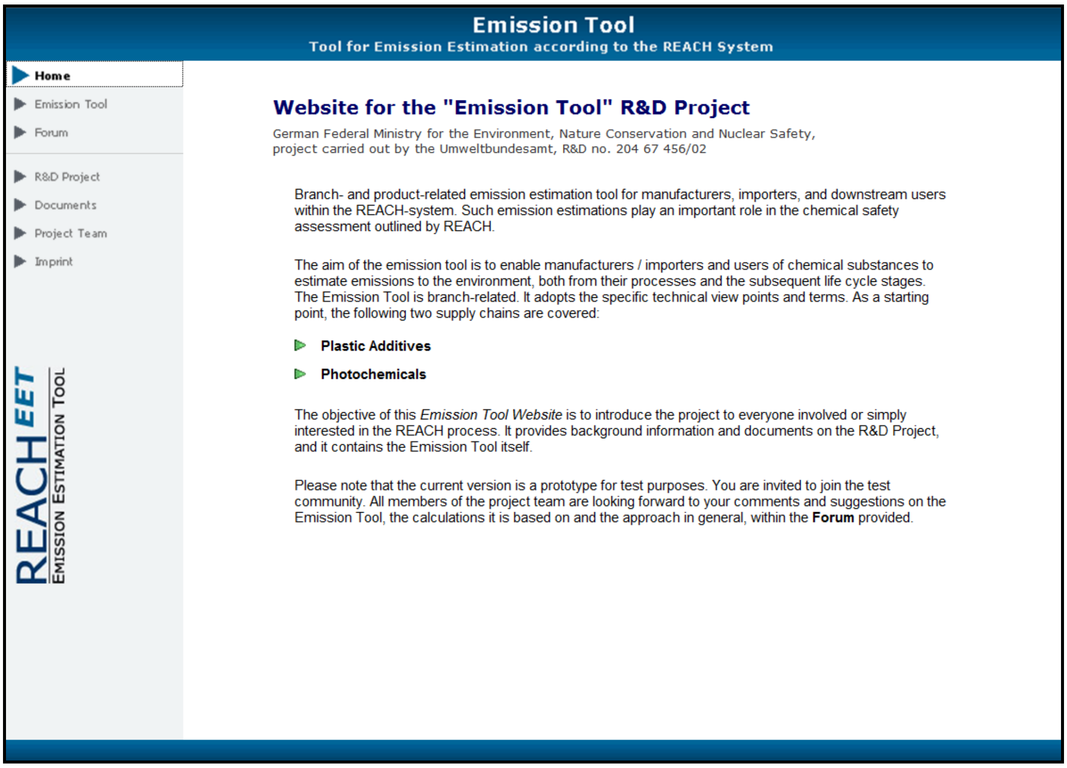

Figure 6: Homepage of the emission estimation tool from the Matrix Project

8.2.4 ScIDeEx

In the exposure assessment tool ECETOC TRA, Version 2 (see Section 8.2.1) several exposure-modifying factors (EMFs) can be modified by the user. This functionality enables the scaling of exposure-defining variables. The RiskOfDerm model offers, too, a certain degree of flexibility that can be utilized by downstream users for scaling.

The ScIDEEx tool presented here concerns exposure of workers and has no bearing on environmental exposure.

Despite emphasis of ScIDeEx on industrial safety, it is presented here because the basic principle of ScIDeEx is also of interest for the development and further development of environment-related scaling tools. The starting point is an already existing tool for exposure assessment, for which a suitable, supplementary scaling tool is being developed. This supplementary tool is less complex and demands less experience and knowledge than the exposure assessment tool.

Applied to the problem of environmental exposure that could mean, for instance, that specific assessment tools exist for the exposure assessment of metals, which go beyond standard application of EUSES. They can be used as the starting point for deduction of a scaling tool for metals with emphasis on environmental exposure.

The ScIDeEx tool provides helpful suggestions for such deduction.

The use of ECETOC TRA and RiskOfDerm requires a certain degree of experience. Supplementary aids have been developed, with which scaling becomes a simple task for downstream users. The ScIDeEx tool (scaling of inhalative and dermal exposure) has been developed by the chemicals concern Merck AG, in order that scaling of the exposure of workers can be undertaken on the basis of ECETOC TRA 2. ScIDeEx supports scaling of inhalative and dermal exposure by downstream users.

The following figure displays exemplarily the structure of the tool (provisional status).

		TRA 2.0 Exposure values		Exposure Modifying Conditions						Scaled Exposure values		Risk Characterisation Ratios (RCR)			
Process Category	Description of Process Category	Inhalative Exposure [ppm] DOA > 4 h; no Ventilation; pure Substance	Dermal Exposure [mg / kg bw / day]; DOA > 4 h; no Ventilation; pure Substance	Duration of activity	Substance used in a preparation? If yes select concentration range (w/w)	Ventilation	Effectiveness of respiratory protective equipment (RPE) [%]	Effectiveness of Ventilation for Inhalative Exposure [%]	Effectiveness of Ventilation for Dermal Exposure [%]	Inhalative exposure [ppm]	Dermal Exposure [mg / kg bw day]	Inhalative Exposure	Dermal Exposure	Total Exposure (inhalative + dermal)	Select PROCs (activities) which may be performed by one worker within an 8 h workshift
PROC1	1 - Use in closed process, no likelihood of exposure	0.1	0.34	> 4 h	no	none	no RPE	0	0	0.1	0.34	0.01	0.03	0.04	no
PROC2	2 - Use in closed, continuous process with occasional controlled exposure	50	1.37	> 4 h	no	none	no RPE	0	0	50	1.37	2.50	0.12	2.62	no
PROC3	3 - Use in closed batch process (synthesis or formulation)	100	0.34	> 4 h	no	none	no RPE	0	0	100	0.34	5.00	0.03	5.03	no
PROC4	4 - Use in batch and other process (synthesis) where opportunity for exposure arises	250	6.86	> 4 h	no	none	no RPE	0	0	250	6.86	12.50	0.62	13.12	no
PROC5	5 -Mixing or blending in batch processes (multistage and/or significant contact)	500	13.71	> 4 h	no	none	no RPE	0	0	500	13.71	25.00	1.25	26.25	no
	DNEL(inhal) [ppm for volatiles] ; [mg/m3 for solids]		20									Risk Characterisation Ratio Total Exposure (Aggregated Uses)			0.00
	DNEL(dermal) [mg/kg bw/day]		11												

An Excel-based tool based on ECETOC TRA, Version 2. The values in the spreadsheet are in each case substance-specific.

Figure 7: The scaling tool SclDeEx (scaling of inhalative and dermal exposure).

The downstream user can adapt three exposure-modifying factors to his situation:

- duration of the activity,
- concentration of the substance in the mixture, and
- type of ventilation.

These variables have a linear influence on the level of exposure. This means that the original exposure values that, with a conservative approach, assume high exposure are simply multiplied by a fixed factor. The following table shows exemplary exposure-modifying factors depending on duration of the activity.

Table 19: Dependence of exposure level on duration of the activity (DOA).

Duration of the activity DOA)	Exposure-modifying factor (EMF)
> 4 h	No change (Factor = 1)
1–4 h	0.6
15 mins.–1 h	0.2
< 15 mins.	0.1

ScIDeEX also enables total exposure to be calculated, when several activities are carried out by the same employee. In such a case, the exposure values of individual process categories are added to provide a value for total exposure. Any combination of process categories can be calculated in the tool.

Suppliers can provide a link in their exposure scenarios to a Website in which the ScIDeEx tool for a specific substance is available.

Figure 7 displays a possible substance-specific version of the ScIDeEx for downstream users. By contrast, stakeholders who themselves prepare exposure scenarios require a generic version, from which substance-specific versions can be deduced. Such generic versions will have the following features:

- all process categories (PROCs) are covered,
- non-applicable PROCs are simply removed through deletion of the corresponding lines,
- the user can insert data into ECETOC TRA, Version 2 that represent a conservative estimation of exposure, and
- the user copies the formatting template and stores it as a substance-specific version.

This substance-specific version can then be made available to downstream users.

8.3 Practical Guide to Scaling

The Practical Guide to Scaling is available at:

www.reach-info.de/dokumente/scaling/reach_scaling_practical_guide.pdf