ProScale

A life cycle oriented method to assess toxicological potentials of product systems

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Glossary

Allocation	Partitioning the input or output flows of a process or a product system between the product system under study and one or more other product systems [ISO 14040/44].
Article	An object which during production is given a special shape, surface or design which determines its function to a greater degree than does its chemical composition [REACH].
Benchmarking	Benchmarking could, for example, include defining an average performing product (based on data provided by stakeholders or on generic data or approximations) followed by a grading of other products according to their performance versus the benchmark [PEF guide].
Bill of materials	List of all raw materials needed to manufacture/produce a product or service and a list of all products produced.
Consumer use phase	The step of the life cycle where a consumer (in contrast to a professional worker) is using the product for its intended use or applying it into its intended application (e.g. the consumer use of wall paint consists of both its application on the wall and exposure that may occur thereafter).
Cut off criteria	Specification of the amount of material or energy flow or the level of environmental significance associated with unit processes or product system to be excluded from a study [ISO 14040/44].
Direct exposure	Exposure of humans to substances in an article during all life cycle stages of the article occurring via close contact to the process, also sometimes referred to as near-field exposure (e.g. worker during manufacturing, worker during formulation, worker/consumer during installation or use, consumer during service life, worker during end of life).
Elementary flow	Material or energy entering the system being studied that has been drawn from the environment without previous human transformation, or material or energy leaving the system being studied that is released into the environment without subsequent human transformation [ISO 14040/44].
Emission	Direct release of a pollutant to air or water as well as the indirect release by transfer to an off-site waste water treatment plant [EEA http://dataservice.eea.eu.int].
Exposure	Concentration or amount of a particular agent that reaches a target organism, system, or (sub)-population in a specific frequency for a defined duration [IPCS].

Exposure assessment	The qualitative and/or quantitative evaluation of the degree of intake likely to occur leading to adverse (health) effects resulting from human exposure to hazard [WHO].
Fate	Pattern of distribution of an agent, its derivatives, or metabolites in an organism, system, compartment, or (sub)-population of concern as a result of transport, partitioning, transformation, or degradation [IPCS].
Functional unit	Quantified performance of a product system for use as a reference unit [ISO 14040/44].
Hazard	The intrinsic properties of a substance or mixture and its potential to cause harm [CLP].
Hazard identification	The identification of known or potential health effects associated with a particular agent leading to adverse (health) effects resulting from human exposure to hazard [WHO].
Hazard characterization	The qualitative and/or quantitative evaluation of the nature of the adverse effects associated with biological, chemical, and physical agents... For chemical agents, a dose-response assessment should be performed. [WHO].
Hazard statement (H-phrase) hazards	A phrase assigned to a hazard class and category that describes the nature of the of a hazardous substance or mixture, including, where appropriate, the degree of hazard [CLP]
Impact category	Class representing environmental issues of concern to which life cycle inventory analysis results may be assigned. [ISO 14040/44].
Indirect exposure	Exposure of the general population via the environment, i.e. due to environmental emissions.
Life cycle assessment (LCA)	Compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle [ISO 14040].
Life cycle thinking	Takes into consideration all relevant environmental interactions associated with a good, service, activity, or entity from a supply chain perspective [PEF guide].
Mass flow	In ProScale, the mass flow is the amount of a substance that is needed for fulfilment of the functional unit of the product/service
Mixture	A mixture or solution composed of two or more substances [REACH].
Normalization	A step of LCA in which results are related to a reference value.
Polymer	A polymer means a substance consisting of molecules characterized by the sequence of one or more types of monomer units and comprising a simple weight majority of molecules containing at least three monomer units which are covalently bound to at least one other monomer unit or other reactant and consists of less than a simple weight majority of molecules of the same molecular weight. Such molecules must be distributed over a range of molecular weights wherein differences in the molecular weight are primarily attributable to differences in the number of monomer units. In the context of this definition a monomer unit means the reacted form of a monomer in a polymer [OECD].

Polymer of Low Concern	"Polymers of low concern are those deemed to have insignificant environmental and human health impacts. Therefore, these polymers should have reduced regulatory requirements." (OECD, 2009a). Polymers of low concern must meet the following conditions. For an average molecular weight (MW) of the polymer between 1,000~10,000 Daltons, the oligomer content is less than 10 percent at MW < 500, and less than 25 percent at MW < 1,000. Also, these polymers cannot have «an obvious content» of active functional groups. If the MW of the polymer is more than 10,000, the oligomer content must be less than two percent at MW < 500, and less than five percent at MW < 1,000. Polyesters are also considered to be of low concern.
Potency	A measure of toxic activity expressed in terms of the amount required to produce a toxic effect.
Precursor	A chemical that is transformed into another substance, as in the course of a chemical reaction, and therefore precedes that substance in the synthetic pathway.
PROCs	PROCs, short for Process Categories, are standardized use descriptors used in risk assessment, describing the tasks, application techniques or process types defined from the occupational perspective, including use and processing of articles by workers. The list of PROCs and their description is available in the ECHA Guidance on Information Requirements and Chemical Safety Assessment Chapter R.12: Use description (ECHA, 2015, pp 49-54)
Product	Any goods or service. The product can be categorized as follows; services (e.g. transport); software (e.g. computer program, dictionary); hardware (e.g. engine mechanical part); processed materials (e.g. lubricant). [ISO 14044].
Product system	Collection of unit processes with elementary and product flows, performing one or more defined functions, and which models the life cycle of a product [ISO14040/44].
Release	Emissions to air and discharges to water and soil [ISO 14040].
Risk	The probability of an adverse effect in an organism, system, or (sub)-population caused under specified circumstances by exposure to an agent [IPCS].
Risk assessment	Risk assessment is the scientific evaluation of known or potential adverse health effects resulting from human exposure to hazard [WHO].
Risk characterization	Integration of hazard identification, hazard characterization and exposure assessment into an estimation of the adverse effects likely to occur in a given population, including attendant uncertainties adverse (health) effects resulting from human exposure to hazard [WHO].
Service life	The step of the life cycle covering the period of use in service of a product after its use (see definition of Use below), e.g. the service life of a wall paint is the period during which the paint stands on the wall, exposure may occur for the building occupant.

Substance A chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition [REACH].

System boundaries A set of criteria specifying which unit processes are part of a product system [ISO 14040/44].

Toxicological potential The (human) toxicity potential (H)TP is a calculated index that reflects the potential harm of a unit of chemical based on both the inherent toxicity of a compound and its potential dose. It is used to combine exposure and toxicity information as part of the ProScale model.

Unit process The smallest element considered in the life cycle inventory analysis for which input and output data are quantified [ISO 14040/44].

Use Use of products refers to such activities as painting or installation, whether on a do-it-yourself (DIY) basis or otherwise. This does not include service life (see definition of Service life above).

List of abbreviations

BAT	Best Available Techniques
CAS	Chemical Abstracts Service
CLP	European Regulation (EC) No 1272/2008 on Classification, Labelling, Packaging
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
CSR	Chemical Safety Report
DMEL	Derived Minimal Effect Level
DNEL	Derived No Effect Level
ECF	Exposure Concentration Factor
ECHA	European CHemicals Agency
EPD	Environmental Product Declaration
ERC	Environmental Release Categories
ERR	Exposure Risk Relationship
ES	Exposure Scenarios according to REACH Article 14(4)
EU SDS	Safety Data Sheet according to REACH Annex II
EU eSDS	extended EU SDS with RMM/ES according to REACH Article 14(6)
GHS	Globally Harmonised System
HF	Hazard Factor
ISO	International Organization for Standardization
LCA	Life Cycle Assessment
LEV	Local Exhaust Ventilation
MF	Mass Flow
OEF	Organization Environmental Footprint
OEL	Occupational Exposure Limit
PEF	Product Environmental Footprint
PEFCR	Product Environmental Footprint Category Rule
PCR	Product Category Rules
PHF	Person-Hours Factor
PROC	Process Category
PSB	ProScale Building
PS	ProScale
PSU	ProScale of Unit process
PSP	ProScale of Product
REACH	EU Regulation (EC) No. 1907/2006 concerning the Registration, Evaluation, Authorisation and restriction of CHemicals
RCR	Risk Characterization Ratio
RMM	Risk Management Measures
SPER	Specific Environmental Release Categories
SVH	Substance of Very High Concern
SWED	Sector-specific Worker Exposure Description

1 | Introduction

1.1 Background and motivation

Increasingly, various stakeholders require information on human toxicity and eco-toxicity aspects of products beyond regulatory requirements for chemicals, e.g. in the framework of Life Cycle Assessment ("LCA"). Questions are raised about hazard and exposure potential from chemical constituents in products or used along their lifecycle. Although regulatory requirements are in place to ensure the safe use of chemicals in their application, the ambition to reduce the environmental impacts of products along their life cycle is often combined with an ambition to identify and reduce hazards and exposures. As there is currently no methodology available to compare hazard and exposure performance along the lifecycle and identify priorities for improvement, requirements are often based on purely hazard-based lists for priority substances without evaluating their risk in specific applications. LCA is widely used to quantify the overall environmental impact of products along the life cycle but the models for toxicity impacts are focussing on the indirect impact of chemicals emitted into the environment. This calls for a performance based indicator that can consolidate hazard and direct exposure potentials from chemicals along their life cycle, that can be applied and communicated within LCAs, Environmental Product Declarations ("EPDs") and Product Environmental Footprints ("PEFs") by (i) using life cycle thinking, (ii) using a risk-based approach for product assessments, (iii) aggregation from single product to a complete building or product solution and (iv) using existing, systematic data. REACH provides a pool of information on exposures, hazards and risks of chemicals that is not yet evaluated for this purpose.

For this reason, the ProScale Consortium was formed, with the purpose of developing a method for a hazard and exposure based scoring system for comparing chemical risks associated with products in a life cycle perspective. The ProScale partners are: BASF, Covestro, Deutsche Bauchemie, DSM, IVL Swedish Environmental Research Institute, Kingspan and Solvay. The ProScale method aims to be a science-based, transparent, pragmatic and generally applicable methodology for a toxicological exposure assessment of products in the framework of Life Cycle Assessment, and aims to: (i) assess the relevant direct exposure potential along the whole life cycle; (ii) use existing data, when available, e.g. REACH based; (iii) allow comparison in relation to technical performance; and (iv) be relevant for business-to-business and business-to-customer communication.

The idea behind ProScale was first outlined by Fritz Kalberlah (FoBIG), Eva Schmincke (Thinkstep) and Birgit Grahl (Integrahl) in a study commissioned by BASF (Kalberlah et al., 2017). It was initially focused on construction products where there is specific interest for such an indicator to be included in Environmental Product Declarations (EPD) according to EN15804+A1:2013 and building assessment schemes. The authors proposed a scoring system providing additional information for EPDs, with four combined characteristics:

- describing the inherent toxicity of a product's ingredients and constituents by a hazard score,
- considering the exposure potential of product ingredients and constituents in each specific life cycle stage by a generic weighting factor which may modify the potential health impact based on the inherent toxicity,
- applying life cycle thinking to address not only the use stage, but also the production, application and in principle end-of-life stages,

• aggregating from ingredient to product, and possibly up to complete building or system.

This initial concept, together with some suggestion of methodological elements was first presented to various stakeholders in 2015 in order to gather feedback and assess potential interest for further development. Based on the positive feedback received, BASF invited stakeholders to discuss the establishment of a consortium to further develop the method jointly into an applicable methodology that became known as ProScale. Together, the partners of the consortium defined the starting point and the goal of the method.

1.2 Stepwise development

ProScale is intended as a widely applicable method that can cover both human and eco-toxicity aspects, be applicable to any kind of products on a worldwide basis. The ProScale consortium decided to first focus on near-field human toxicity, on a limited number of applications including construction products and on application in a European context. The method can nevertheless be extended following the same principles. Figure 1 presents a stepwise development:

Tier 1 covers direct human toxicity exposure of workers or professionals to substances used in the process or contained in the product, from raw material extraction to use of the product, as well as exposure of consumers during application of DIY (Do It Yourself) products.

Tier 1 scope is completely covered by this guidance document, and relies on available data and models widely used in Europe in the context of Risk Assessment.

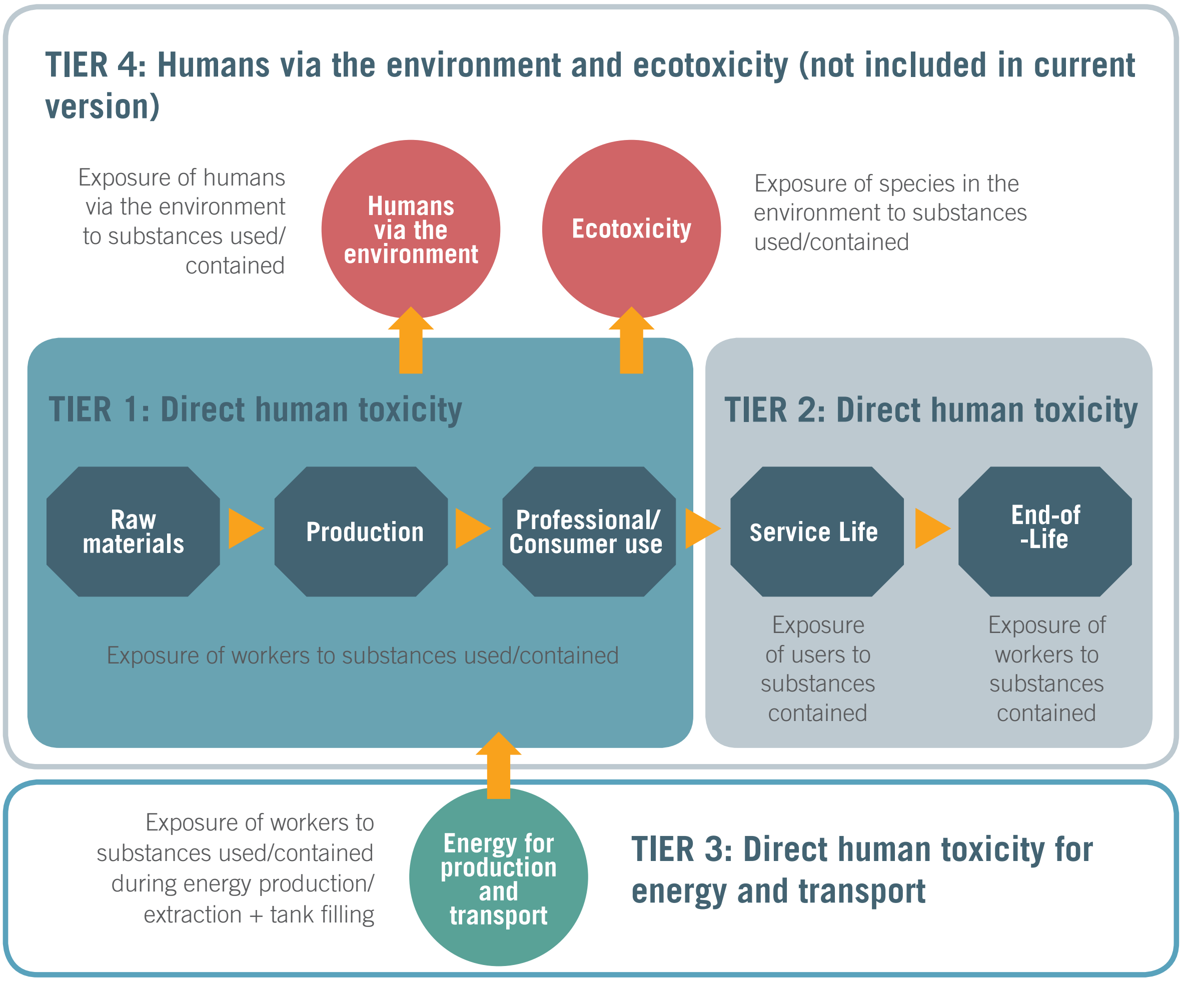
Tier 2 covers the rest of the life cycle: exposure of users (or inhabitants) to substances contained in the product during the service life of the product and the exposure of workers during the end of life.

Tier 2 follows exactly the same principle as Tier 1 but has to rely on scenario assumptions to be defined in specific Product Category Rules, as is usual in LCA/PEF/EPD. The availability of exposure models and data is lower than for Tier 1. In practice:

- The service life exposure can rely on indoor air testing data when available, or on simplified models that have a lower recognition than the models used for worker exposure.
- The end of life exposure can be approximated by applying the same models as for the production phase and using exposure conditions that are close to the end of life scenario.

Tier 3 covers the direct human exposure related to the energy production and related to transport (tank filling). These are specific unit processes for which standard values can be provided following the ProScale method.

Tier 4, which is not included in the current version of ProScale, is extending the scope to cover both exposure of humans via the environment and exposure of species in the environment to the same substances as in Tier 1, 2 and 3 (substances used or contained along the life cycle). This scope extension requires using the information from Risk Assessment in terms of eco-toxicity. The general ProScale approach can in the future be adapted to cover also Tier 4.

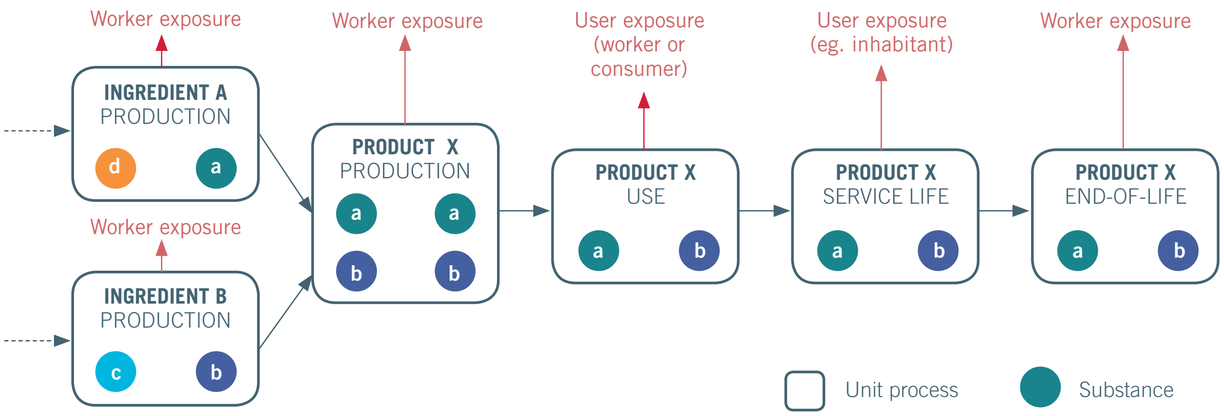


>> Figure 1 / Illustration of the stepwise development of ProScale

2 | ProScale principles

The ProScale methodology aims to assess application specific toxicological exposure potential arising from direct exposure of hazardous substances in a product along the entire lifecycle of that product. The ProScale method is based on life cycle thinking. ProScale scores can be calculated at different levels of aggregation, for example for an entire life cycle, parts of a life cycle or for a specific unit process.

To apply ProScale to a defined functional or declared unit, the life cycle of the product has to be defined with its different unit processes. In each unit process the substances used as ingredients, produced as products and contained in the product are considered.

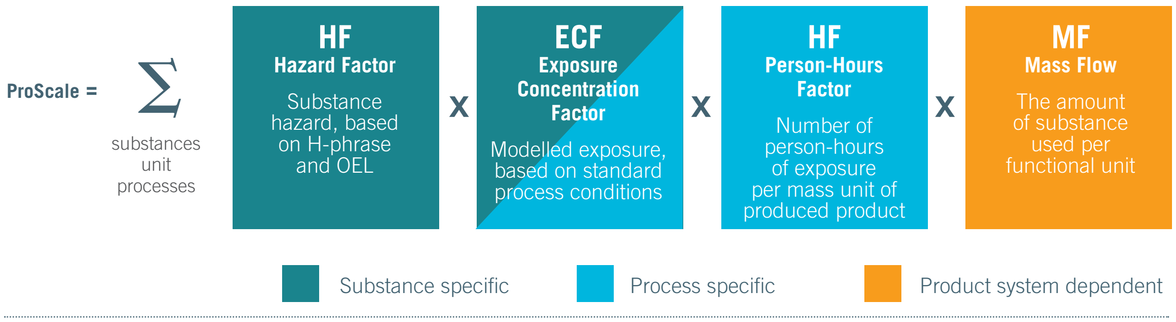


>> Figure 2 / Example of schematic product system with identified unit processes and substances.

For each substance and each unit process, ProScale combines information about the substance's toxicological properties (hazard), the specific exposure determined by the physical properties of the substance and the defined exposure conditions, the time of exposure, the population exposed and the quantity of substance used. This is done for all relevant exposure instances, all substances in all unit processes, so that eventually scores for all included exposure instances are consolidated to determine the ProScale assessment score at the required level of aggregation, see Figure 3.

The ProScale methodology is a function of the four parameters (Figure 3):

- **Hazard Factor (HF)** – Describes the hazard of a substance, reflecting health effect, severity and potency based on hazard statements (also called H-phrases) and acceptable concentration levels (e.g. OEL, DNEL).
- **Exposure Concentration Factor (ECF)** – Describes the exposure concentration of a substance based on exposure modelling using the ECETOC TRA Tier 1 exposure model.
- **Person-Hours Factor (PHF)** – Number of person-hours of exposure per mass unit of produced product or service
- **Mass Flow (MF)** – Describes the amount of a substance needed per functional unit of a product.

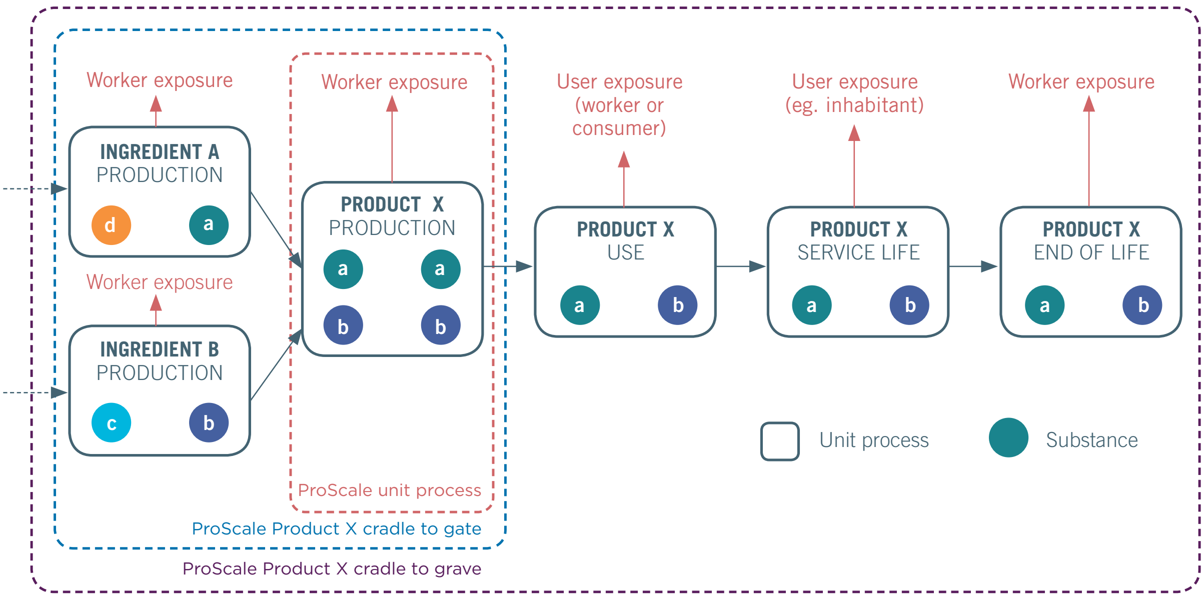


>> Figure 3 / Illustration of the ProScale methodology.

The Hazard Factor, the Exposure Concentration Factor, the Persons-Hours Factor and the Mass Flows are calculated for each substance and each unit process and then combined to establish the ProScale score.

As illustrated on Figure 4 for a simple product X:

- ProScale can be calculated for the unit process corresponding to the manufacture of the product by considering all the substances used and produced with their respective mass flows, and the exposure conditions, population and time.
- The cradle-to-gate ProScale of the product requires adding the upstream part, which corresponds to the ProScale cradle-to-gate of each ingredient. Such data could be available in a database, provided by the suppliers or specifically calculated if the process information is available.
- Establishing the cradle-to-grave ProScale of the product requires calculating and adding the downstream unit processes based on scenarios that could be defined in specific Product Category Rules.



>> Figure 4 / Different ProScale scores for part of a product system.

ProScale scores are declared separately for the different exposure routes[1] (inhalative, oral and dermal).

The general description of carrying out a ProScale assessment of a product system is thus:

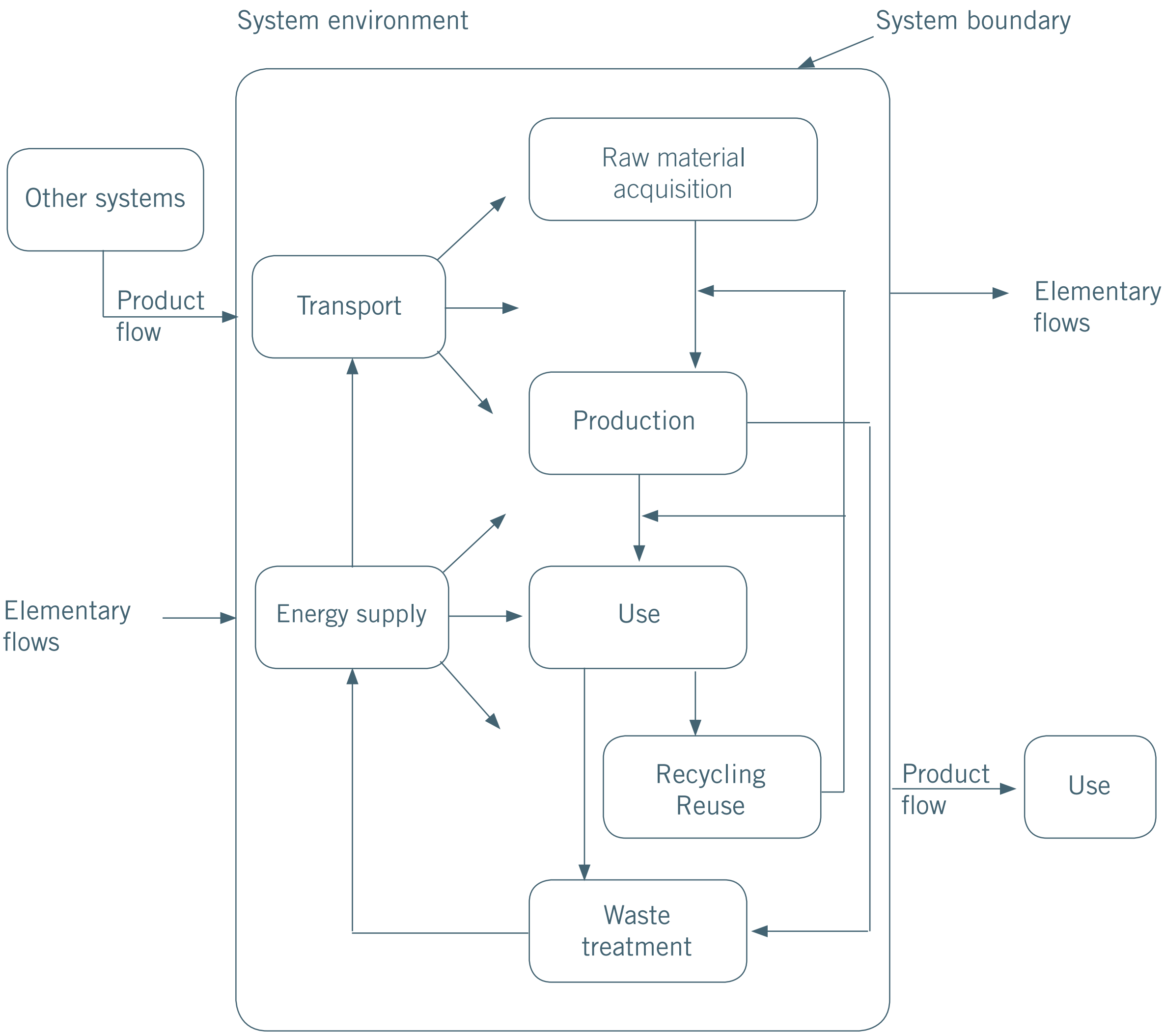
- Define the product system to be studied by identifying the unit processes and substances
- Derive and compile ProScale scores for the system's unit processes, by
  - Aggregate all unit processes of the product system with respect to their mass flow contribution to the product system
  - Developing new ProScale scores (where necessary)
- Calculate a ProScale score for all unit processes of the product system with respect to their contribution to the overall system`

The resulting ProScale score can be analysed and presented in various "dimensions", to identify the main contributing substances, process types, flowchart branches, etc., to the overall system's performance.

1 Note: ProScale scores are declared separately for the different exposure routes as no translation formula from one exposure route to another is currently included. However, an aggregated ProScale with regard to exposure routes is desirable.

3 Defining the product system

ProScale models the life cycle of a product as its product system, which performs one or more defined functions. The essential property of a product system is characterized by its function and cannot be defined solely in terms of the final products. Figure 5 shows an example of a product system.



>> Figure 5 / Example of a product system for LCA (ISO 14040:2006).

3.1 Functional unit

A product system may have a number of possible functions and the one(s) selected for a study depend(s) on the goal and scope of the study. The functional unit defines the quantification of the identified function(s) (performance characteristics) of the product. The primary purpose of a functional unit is to provide a reference to which the inputs and outputs are related. This reference is necessary to ensure comparability of the results. Comparability of results is particularly critical when different systems are being assessed, to ensure that such comparisons are made on a common basis (ISO, 2006a).

3.2 Unit processes

Product systems are subdivided into a set of unit processes which are linked to one another by flows of intermediate products and/or waste for treatment, to other product systems by product flows, and to the environment by elementary flows (see Figure 5). ISO 14040 defines a unit process as the smallest element considered in the life cycle inventory analysis for which input and output data are quantified (ISO, 2006a). Complementing the ISO definition, a unit process in the context of ProScale is a process with identified input and output and that can be described by one PROC (process category) and one Person-Hours Factor. Dividing a product system into its component unit processes facilitates identification of the inputs and outputs of the product system. In many cases, some of the inputs are used as a component of the output product, while others (ancillary inputs) are used within a unit process but are not part of the output product. A unit process also generates other outputs (elementary flows and/or products) as a result of its activities. The level of modelling detail that is required to satisfy the goal of the study determines the boundary of a unit process (ISO, 2006a).

3.3 System boundaries

The system boundaries define the unit processes to be included in the system. Ideally, the product system should be modelled in such a manner that inputs and outputs at its boundary are elementary flows. When setting the system boundary, several life cycle stages, unit processes and flows should be taken into consideration, such as; acquisition of raw materials, inputs and outputs in the main manufacturing/processing sequence, distribution/transportation, use and maintenance of products, disposal of process wastes and products and recovery of used products (including reuse, recycling and energy recovery).

ProScale can be applied to different types of product systems such as cradle-to-grave, cradle-to-gate and gate-to-gate, similar to other LCA system definitions based on ISO 14040, 14044 (ISO, 2006a; 2006b). Information on the product systems are compiled in a flow chart, identifying all unit processes in the system and how they are connected to each other in terms of mass flows from one unit process to another. For each unit process, a bill of materials shall be defined. All substances entering the unit process and leaving the unit process as products shall be considered in the bill of materials. The same cut-off rules apply regarding which substances to include as for Safety Data Sheets (SDSs). Elementary flows such as emissions of other substances into the environment shall not be included. The bill of materials should as far as possible be based on information from SDSs, where this is sufficiently reliable. Should such information be unavailable, an expert assumption to estimate the content can be made. Any such assumptions shall be reported and tested in a sensitivity analysis in accordance with LCA practice. For each unit process, one PROC and one Person-Hours Factor (PHF) shall also be defined (see section 5.1.1 and section 6 for more information).

In ProScale, all substances with H-phrases shall be included in the product system, no cut-offs. When it comes to mixtures and polymers within ProScale, the following rules apply:

- For mixtures, all substances that have to be mentioned in the SDS of the mixture shall be considered in the unit process where the mixture is used. If only ranges are given, the upper interval of the declared concentration shall be used.
- For polymers sold as mixtures (e.g. with plasticizers and solvents included), all individual substances shall be considered. If the polymeric content has no H-phrase or is considered a polymer of low concern (PLC), its hazard factor will be equal to zero.
- For chemical products that are reactive (often polymeric), the composition is changing during the process. For these products, only the composition when entering the process and the composition when leaving the process is considered.

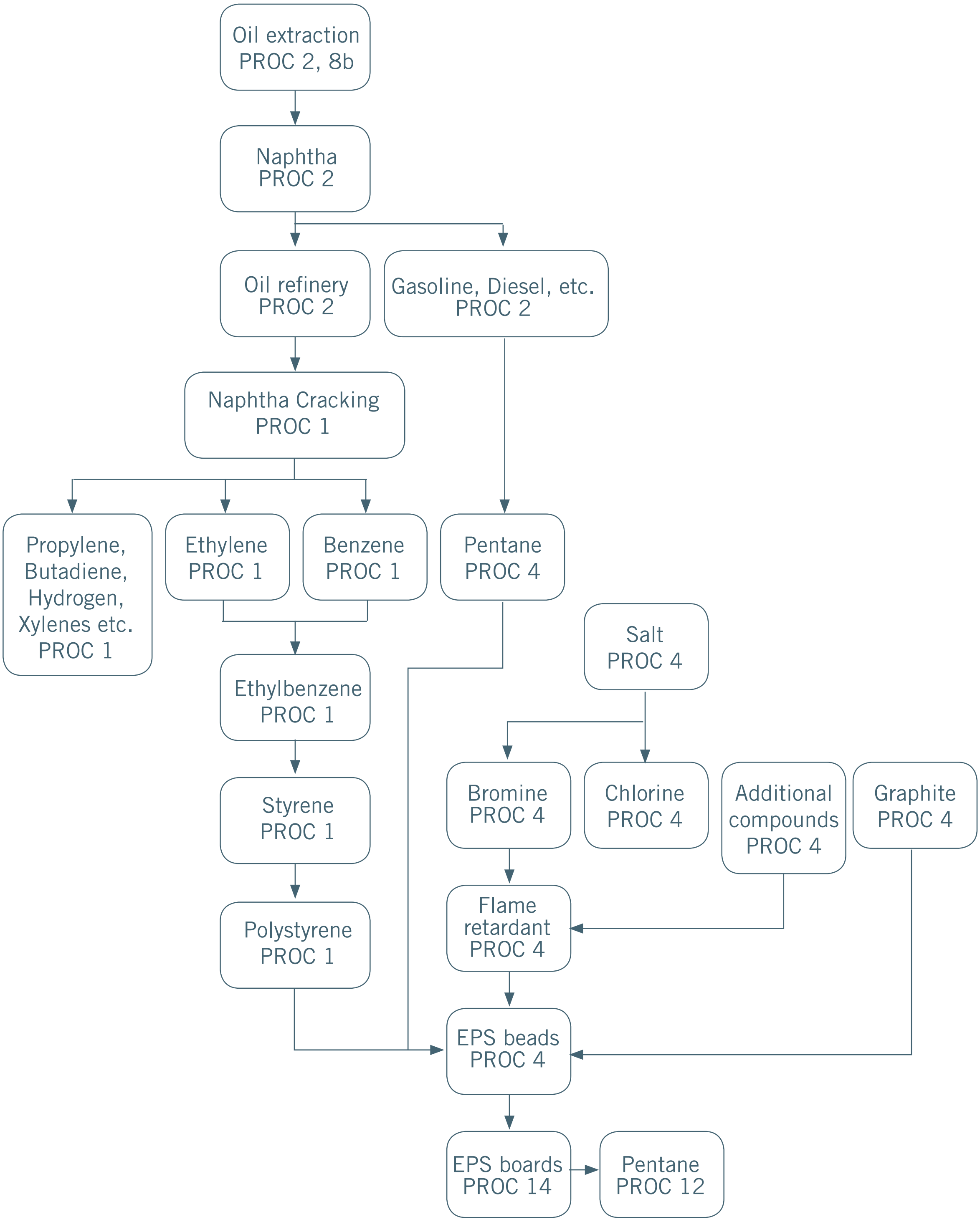
3.4 Allocation

In the case that a unit process has multiple outputs in ProScale, there is a need to allocate the ProScale score of that process between the different outputs. ISO defines allocation as the partitioning of the input or output flows of a process or a product system between the product system under study and one or more other product systems (ISO, 2006a). Thus, by allocating the ProScale score to the different outputs, the ProScale score of the unit process is partitioned between the different outputs so that the ProScale score is lower when only considering one or some of the outputs compared to all outputs.

In ProScale, it is recommended to use the same allocation method as in the data sets used for the calculations of the LCA.

3.5 Example – Defining the product system

Here, the production of expanded polystyrene (EPS) insulating boards is used as an example of how to define the product system. When defining the product system, the practitioner should start by determining the functional unit and what life cycle stages to include in the study, i.e. cradle-to-grave, cradle-to-gate or gate-to-gate. In the EPS insulating board example, the functional unit is one kg of EPS insulating board, and the product system covers cradle-to-gate. Figure 6 shows a flow chart with relevant unit processes within the product system of the EPS insulating board, all inputs and outputs to and from the unit processes, and the PROC for each unit process.



>> Figure 6 Product system for the production of EPS insulation board from cradle-to-gate.

4 | Hazard Factor

The Hazard Factor (HF) describes the hazard of a substance in ProScale, reflecting health effect severity and potency. The Hazard Factor of a substance shall be established separately for each exposure route (dermal, inhalation, oral), resulting in hazard factors which may be different for each of the three routes. As a consequence, the ProScale score is also obtained separately for each route. In further developments of ProScale it may be decided to combine the ProScale score for the three routes into one ProScale score once an approach to translation is developed. It is also possible to exclude one or more routes, e.g. the oral route for professional and industrial applications.

The HF is based on two input data; the substance hazard statement (H-phrase) and the Occupational Exposure Limits (OEL) or Derived No-Effect Level (DNEL) when OELs are not available.

H-phrases are widely available and acceptable statements that express the health hazard of a substance. The Globally Harmonised System (GHS) is an internationally agreed-upon system, created by the United Nations. It is a common and coherent approach to defining and classifying hazards, and communicating information on labels and safety data sheets. Target audiences include workers, consumers, transport workers, and emergency responders. A more detailed justification for choosing H-phrases to express the health hazard of a substance is given in Annex 1. In ProScale, H-phrases are grouped in 5 hazard classes, see Table 1. The H-phrase with the highest class defines the class of the corresponding exposure route and each class receives a maximum and a minimum hazard factor. Grouping H-phrases is a method to collect substances that need the same level of control to protect against health risks arising from hazardous substances used in the workplace.

An Occupational Exposure Limit (OEL) is an upper limit of the acceptable concentration of a hazardous substance in workplace air for a particular material or class of materials. OELs were chosen by the ProScale team as the indicator for potency in preference to other health exposure limits (DNEL, DMEL etc.) for the following reasons: 1) as the OELs are revised and established by authorities and 2) as the OELs are used both in the EU and other regions such as the US. By using OELs rather than DNEL/DMEL, ProScale will therefore receive a higher degree of robustness as a method. However, OELs are not available for all relevant substances. If OELs are not available, it is possible to use DNELs instead. A more detailed justification for choosing OEL as the currently preferred indicator for potency of a substance is given in Annex 1.

In ProScale, OELs reflect the potency of a substance, which allows establishing distinctions between substances with low effect thresholds and with high effect thresholds; the lower the threshold, the higher the potency. The ProScale HF is chosen accordingly, so the lower the threshold the higher the ProScale Hazard Factor. Substances with high OEL receive the default Hazard Factor for the corresponding hazard class. Substances with low OEL or no OEL at all (conservative assumptions), receive a higher Hazard Factor. The inhalation OEL is used as a proxy for all exposure routes and all groups of exposed persons (e.g. consumers). Exposure limit values (similar to OEL) for other exposure routes and other groups of persons have very limited availability, which is why the OEL for inhalation is considered as a valid proxy for potency in general.

A transformation to a numeric factor is based on a combination of the H-phrase class and the OEL (see 4.2) in order to get a dimensionless number that can be multiplied with the other ProScale factors (Exposure Concentration Factor and Person-Hours Factor).

For mixtures, each identified substance shall be considered with its individual H-phrase, and not the H-phrase of the mixture. In most cases testing data for mixtures are not available, and starting from substances and combining these data will give all ProScale users the same starting point. Substance without H-phrase but with an identified OEL or DNEL belong to hazard class A but have a maximum Hazard Factor of 1. Substances without both H-phrase and OEL/DNEL have a Hazard Factor of zero.

Hierarchies of valid data sources for H-phrases and OELs are established to ensure that different values are not chosen for the same substance, see Section 4.3.

The grouping of H-phrases into hazard classes, the OEL correction and the numeric transformation are incorporated in the ProScale Excel template, so that ProScale users only need to introduce the CAS-number, or possibly the H-phrase and the OEL, into the template to calculate Hazard Factors. The template also calculates Exposure Concentration Factors and ProScale scores.

4.1 Grouping of H-phrases into hazard classes

H-phrases are grouped in five so-called ProScale hazard classes A-E (Table 1) where class A corresponds to the lowest hazard and class E corresponds to the highest hazard. The ProScale hazard class of a substance is established separately for each exposure route; dermal, inhalation and oral. The H-phrase that corresponds to the highest class determines the class for that exposure route. Some H-phrases are not specific to one exposure route, and are therefore considered for all routes, which is the case for CMR substances. E.g. for CMR, category 1, substances will end up in class E for all exposure routes. EU specific H-phrases are included in the ProScale hazard classes, but are used for the EU only. Other GHS systems may also have specific H-phrases (e.g. Australia which is using AUH070 and AUH071). Explanations to the H-phrases can be found in Annex 2.

The severity and reversibility of effects were discussed in several meetings and a web-conference including experts from several companies, and the grouping in Table 1 is the result of that work. Other H-phrase grouping models were studied in the development process: IFA, COSHH, EMKG, Solvay system S-OEB to inform the ProScale approach.

Some CMR substances with respective H phrases (H340, H350, H360, H362) have an officially recognized safe dose. It means it is recognized and accepted that an exposure to these substances below a defined threshold will not have a CMR effect. The hazard score for such substances are divided by 3. A substance is considered to have an officially recognized safe dose when an OEL is given in one of the official registers mentioned in chapter 4.3.2. (OEL).

Table 1 Grouping of H-phrases into hazard classes in ProScale.

ProScale hazard class	H-phrases according to GHS/CLP, grouped by exposure route
E - "CMR" **10 000 – 100 000** (highest hazard)	All routes : H340, H350, H360, H362*
D – "Fatal" 1000 – 10 000	Dermal: H310 Inhalation: H330, H334, EUH032 Oral: H300 All routes: H341, H351, H361, H372
C – "Toxic" **100 – 1 000**	Dermal: H311, H314, H317, H318, EUH070 Inhalation: H331, EUH029, EUH031, EUH071 Oral: H301, H304 All routes: H370, H373
B – "Harmful" **10 - 100**	Dermal: H312, H315, H319, Inhalation: H332, H335 Oral: H302 All routes: H371
A – "Maybe harmful" **1 - 10** (lowest hazard)	Dermal: H313, H316, H320, EUH066 Inhalation: H333, H336 Oral: H303, H305

** For CMR substances with officially recognized safe dose the derived hazard score is reduced by a factor of 3*

4.2 Numeric transformation and calculation of the Hazard Factor

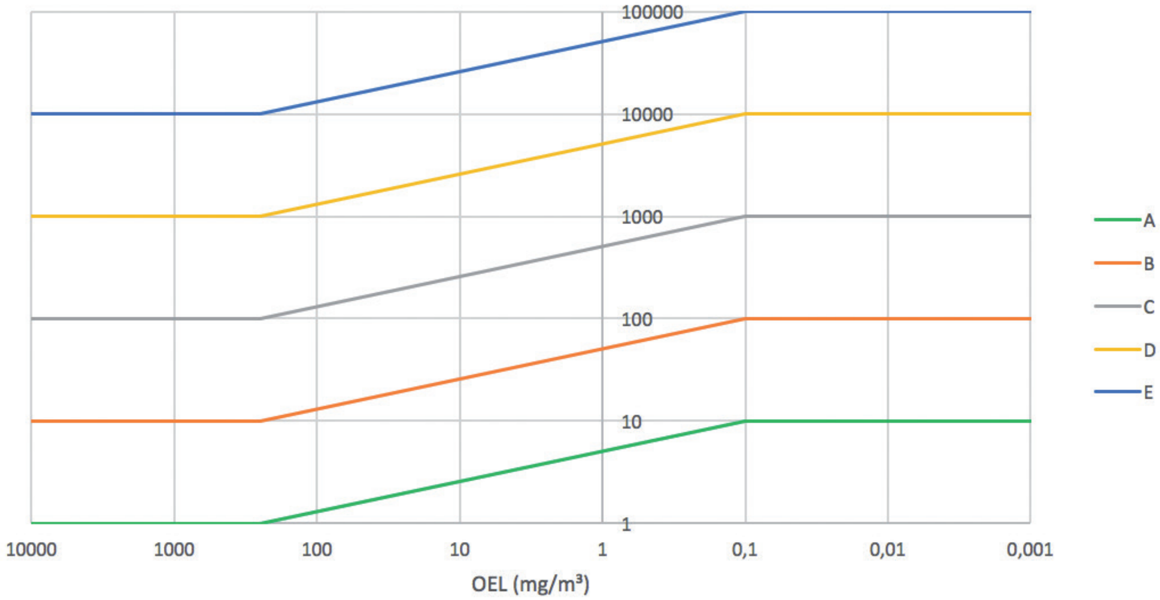
OEL variations within each class have been analysed based on a set of 229 substances and the conclusions were used as a basis for the decisions described below. A calculation function (Figure 7) for the hazard factor has been established with following principles:

- A factor of 10 between minimum and maximum within each class.
- When the OEL is above 250 mg/m³, the ProScale Hazard Factor is the minimum of the class. This OEL corresponds to the percentile 90 of the analysed data set[2].
- When the OEL is below 0.1 mg/m³, the ProScale Hazard Factor is the maximum of the class. This OEL corresponds to the percentile 10 of the analysed data set[3].

2 The analysed data set covers 229 substances. The data set was reviewed in a study by Sheffers et al. (2016) and was assessed as being representative for Solvay, i.e. a chemical company with a quite diverse portfolio.

3 The analysed data set covers 229 substances. The data set was reviewed in a study by Sheffers et al. (2016) and was assessed as being representative for Solvay, i.e. a chemical company with a quite diverse portfolio.

- Between these two OEL values, the ProScale Hazard Factor is following a log-linear transformation as described in Figure 7 (logarithmic scale).
- When the OEL is unknown, the ProScale Hazard Factor is always the maximum of the class, in order not to underestimate the hazard of the substance.
- For CMR substances with officially recognized safe dose the derived hazard score is divided by 3.



>> Figure 7 Hazard Factor function.

4.3 Hierarchy for data sources

The hierarchies for selecting H-phrases and OELs were based on expert judgements within the ProScale consortium and are set out in descending order within Sections 4.3.1 and 4.3.2.

4.3.1 H-phrases

1. **Disseminated information from the REACH dossiers available via ECHA website.**
   These values have to integrate the harmonized CLP classification but may include additional health hazards based on more recent data. See Annex 3 for instructions on how to find H-phrases on the ECHA webpage.
2. **Harmonized CLP classification (CLP Annex VI).**
   These values are harmonized and validated

3. **Notified CLP classification from ECHA website considering the 1st row (joint entry or entry with the most notifications).**
   Notification may not always include H-phrases from harmonized classification and REACH dossier, and is therefore ranked lower in the hierarchy. See Annex 4 for instructions on how to find notified CLP classifications on the ECHA webpage.
4. **SDS from the supplier.**
   SDS from supplier may not always include H-phrase from harmonized classification and REACH dossier and is therefore ranked lower in the hierarchy.

4.3.2 OEL

For OELs, the ideal data source would be a consolidated database of several OEL data sources (German, Dutch, European, American) and possibly DNEL with a selection of the most relevant ones. The Consortium will continue to investigate whether such database exists. Until then, the temporary solution is to use the following data hierarchy:

1. **German OEL TRGS900**
   Most easily available. Available OEL automatically provided in the ProScale Excel template
   http://www.baua.de/de/Themen-von-A-Z/Gefahrstoffe/TRGS/TRGS-900.htm nnn=true
2. **TLV value**
   (OEL-values from American Conference of Governmental Industrial Hygienists) from Hazmap
   https://hazmap.nlm.nih.gov
3. **European OEL**
   Established by the Scientific Committee on Occupational Exposure Limits (SCOEL).
   More info on the SCOEL:http://ec.europa.eu/social/main.jsp?catId=148&intPageId=684&langId=en
   List of OELs: https://circabc.europa.eu/faces/jsp/extension/wai/navigation/container.jsp
4. **Dutch OEL**
   http://www.ser.nl/nl/themas/arbeidsomstandigheden/grenswaarden
5. **DNEL from REACH dossier**
   DNELs for long term inhalation exposure of workers shall be considered favourably only if these are based on an inhalation study. See Annex 5 for instructions on how to find DNELs on the ECHA webpage.

If none of the above is established, the OEL/DNEL is not considered and the Hazard Factor will default to the maximum of the class.

The ProScale Excel template automatically provides the German OEL TRGS900 values. So far, it has not been possible to extract the full list from the other OEL sources or DNELs from REACH dossiers.

5 | Exposure Concentration Factor

The Exposure Concentration Factor (ECF) in ProScale describes the potential concentration that a person is exposed to during a specific process or activity. It does not reflect the real exposure and cannot be the basis for a risk assessment but rather is a conservative factor allowing discriminating between different exposure scenarios. Exposure can occur along the entire life cycle of a product, thereby exposing different groups of people. Workers can be exposed during production, use and end-of-life of a product, while consumers can be exposed during use (e.g. do-it-yourself) and service life. Exposure Concentration Factors are derived for each unit process identified within the studied product system.

The Exposure Concentration Factor in ProScale is based on exposure modelling. Modelling was chosen as the preferred approach to estimate potential exposure concentrations in ProScale as it yields transparent and reproducible results. The ECETOC Targeted Risk Assessment (TRA) Tier 1 approach (ECETOC, 2009; 2012; 2014a) is used to estimate potential exposure concentrations for all life cycle stages except service life, as this stage is not included in the Tier 1 approach. The model was chosen as it is: 1) easy to use, 2) requires a small amount of input information, 3) is a preferred approach for evaluating consumer and worker health risks in REACH (ECHA, 2016 a; b) and 4) yields a conservative estimate.

To obtain the Exposure Concentration Factor, the modelled potential exposure concentration is transformed into a dimensionless factor via a route-specific transformation function. A high value means high exposure potential while a low value means low exposure potential.

The ECETOC TRA Tier 1 algorithms and the numeric transformation have been incorporated in the ProScale Excel template, so that ProScale users only need to use the template to calculate Exposure Concentration Factors. The template also calculates Hazard Factors and ProScale scores.

5.1 Worker exposure – Production and Use

The ECETOC TRA Tier 1 approach estimates worker exposure via the inhalation and dermal exposure routes. Oral exposure of workers is not included in ECETOC TRA and not considered relevant by ProScale (in normal conditions, workers are not swallowing substances). It is therefore not included.

Within ECETOC TRA Tier 1, worker exposure via inhalation is modelled as a function of the following input parameters:

- PROC – standardized process categories defined in REACH
- Use – industrial/professional
- Physical state – solid/volatile
- Risk Management Measures (RMM) – yes/no (LEV, PPE, RP)

- Fugacity (likelihood to become airborne) – negligible/low/medium/high
  Requires information on vapour pressure for volatiles and dustiness for solids
- Concentration based exposure modifier

Within ECETOC TRA Tier 1, dermal exposure of workers is modelled as a function of the following input parameters:

- PROC – standardized process categories defined in REACH.
- Use – industrial/professional.

In order to estimate the exposure concentration for workers, the above mentioned input parameters need to be specified for each unit process and substance. The sections below describe the input parameters in more detail.

5.1.1 PROCs

PROCs, short for Process Categories, are standardized use descriptors used in risk assessment, describing the tasks, application techniques or process types defined from the occupational perspective, including use and processing of articles by workers. The list of PROCs and their description is available in Annex 6 (ECHA, 2015, pp 49-54).

PROCs need to be assigned to each unit process in the studied product system in order to estimate exposure concentrations for each process. When assigning PROCs to each unit process, use the following stepwise method:

1. For each unit process in your product system, identify the relevant PROC, i.e. the one representing your process conditions, from the ECHA list of PROCs (ECHA, 2015).

2. If it is not clear which PROCs are correct, check if a use-map is published for the relevant sector, either on the ECHA webpage[4] or on the webpages of trade organisations. If not, generic exposure conditions for a sector can be found in the Sector-specific Workers Exposure Descriptions (SWED).

3. If there is no SWED, check the SDS, eSDS or the exposure scenario (ES) of the supplier or ask the plant manager for information on PROCs.

4. If it is still uncertain which PROC should be used, select PROCs based on expert judgement of your exposure conditions. As a guidance:
   - Chemicals manufacturing is covered by PROCs 1 to 4.
     Choose PROC 4 if you are unsure of which to choose.

4 / http://echa.europa.eu/csr-es-roadmap/use-maps

- Transfer to and from the process steps should be considered when it is not covered in the PROC, i.e. for all process that are not continuous.
  Transfer processes are covered by PROCs 8a, 8b and 9.
  Choose PROC 8a if you are unsure of which to choose.

5.1.2 Use

There are two categories of use that can be chosen when estimating worker exposure:

- Industrial – used at industrial site
- Professional – used in the public domain by a professional user

Industrial use is default for all manufacturing and formulation phases and professional use is default for the use phase (except DIY products, see section 5.2).

For the same substance and PROC, industrial use will result in lower exposure than professional use.

5.1.3 Physical state

Specify the physical state of each substance. The options are[5]:

- Solid
- Liquid (considered as volatile)

When solids are dissolved into a liquid, their fugacity is not determined by their solid form. The physical state “liquid” shall therefore be considered and a vapour pressure of 0.000001 kPa shall be used. This corresponds to a negligible fugacity (see 5.1.5)

5.1.4 Risk management measures

When estimating worker exposure with ECETOC TRA, it is possible to account for available risk management measures (RMMs), such as local exhaust ventilation (LEV), respiratory protection equipment (RPE) and gloves (PPE).

Unambiguous rules need to be in place to keep the use and choice of RMMs transparent and reproducible[6]. To achieve this, a strict definition of the RMMs which shall be used within the ProScale

5 / Note: ECETOC TRA does not cover aerosols. A rule how to handle aerosols will be developed.

6 / Whether RMMs should be considered should not be decided by the single assessor individually. The decision shall be taken based on the rules for a certain activity and should be documented in a central document like e.g. Product Category Rule (PCR), Product Environmental Footprint Category Rule (PEFCR) or a similar document.

worker exposure estimation is necessary. Following these requirements, in ProScale, RMMs shall only be considered when there is a legal requirement to have RMMs in a specific region/industry sector/ process or when Sector-specific Worker Exposure Descriptions (SWEDs) from the relevant industry sector are available.

Legal requirement is in place when e.g. RMMs are required for a specific use scenario in one of the following cases:

- The EU eSDS and EU SDS requires RMM (e.g. personal protective equipment or LEV
- Region specific legal or professional association require RMM

If RMM are only recommended then they should not be applied within ProScale worker exposure estimation. For example if the P-phrase within an SDS or MSDS recommends wearing gloves during the use of a product, this RMM should not be used within the ProScale worker exposure estimation. The justification for not using the RMM in that case is that it may not be required in the use defined by a PROC within the ProScale calculation. E.g. when a hazardous substance is handled under PROC 1 there is no need for the worker to wear gloves even if this is recommended by the P-phrase in the SDS. In addition, RMMs shall not be considered for consumer use of products.

5.1.5 Fugacity

The fugacity describes the likelihood of a substance to become airborne. When the fugacity is higher, the modelled exposure will be higher.

In ECETOC TRA, the fugacity of volatile liquids is classified into four different categories based on the vapour pressure of the substance/mixture according to the criteria in Table 2. The vapour pressure shall be assessed at ambient temperature of 25°C. The physical state of solids dissolved into a liquid shall be considered as “liquid”, and a vapour pressure of 0.000001 kPa shall be used, which corresponds to a negligible fugacity.

Recommended data sources for vapour pressure of substances/mixtures are:

1. REACH dossier
2. SDS
3. The vapour pressure of organic substances determined via the following tool: EpiSuite which is used in official QSAR calculations: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface

Table 2 Fugacity of volatile liquids, table extracted from ECETOC TRA (ECETOC, 2016)

Vapour pressure at 25°C (kPa)	Fugacity
< 0.00001	Negligible (below VP cut-off)
0.00001 to < 0.5	Low
0.5 to 10	Medium
> 10	High

For solid substances, ECETOC TRA classifies the fugacity into four different categories based on the criteria in Table 3.

For solid substances dispersed into a liquid, the following rules apply:

- For exposure scenarios where aerosols are formed (PROC 11, PROC 7), the same rule applies as for solids, i.e. the fugacity of the substance is classified into four different classes based on the criteria in Table 3.
- For exposure scenarios where no aerosols are formed, the exposure concentration shall be considered as zero.

Solid substances dissolved in a liquid shall be considered as liquids with a negligible fugacity, see Table 2.

Table 3 Fugacity of solids, table extracted from ECETOC TRA (ECETOC, 2016)

General description	Relative dustiness potential	Typical materials	TRA Selection Value
Not dusty	1	Plastic granules[a], pelleted fertilisers	Low
Slightly dusty	10 - 100 times dustier	Dry garden peat, sugar, salt	
Dusty	100 - 1,000 times dustier	Talc, graphite	Medium
Very/extremely dusty	More than 1,000 times dustier	Cement dust, milled powders, plaster, flour, lyophilised powders, (process fumes[b])	High

a) Exposures to materials where a substance is contained and bound in a matrix (e.g. pigment within plastic, filler within paint) should also be included in this category. Although the real exposure is actually determined by a combination of physical form and the bioavailability of the substance within the matrix, because the bioavailability is very low under such circumstances, then this will result in a low exposure potential.

b) Process fumes (e.g. rubber, welding, soldering) behave like gases and would be considered within this category if exposures to such complex mixtures are considered in any risk assessment.

5.1.6 Concentration based exposure modifier

The concentration of a substance in a mixture is an important exposure determinant when it comes to inhalation and dermal exposure (ECETOC, 2012). For these two routes of exposure, the following exposure modifying factors apply to substances in preparations.

Table 4 Concentration based exposure modifier for inhalation and dermal exposure (ECETOC, 2012)

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

5.2 Consumer exposure – Use

The ECETOC TRA Tier 1 approach estimates consumer exposure during the consumer use phase (e.g. from DIY installation) via the exposure routes inhalation, dermal and oral. However, ECETOC TRA does not cover consumer exposure during the service life.

Within ECETOC TRA Tier 1, consumer exposure during the consumer use phase is modelled as a function of the following input parameters (same for all exposure routes):

- Fugacity
- Product category and subcategory

In order to estimate the exposure concentration for consumers, the above mentioned input parameters need to be specified for each unit process and substance. The sections below describe the input parameters in more detail.

5.2.1 Fugacity

When estimating consumer exposure with ECETOC TRA, the fugacity is described by the vapour pressure for each substance/mixture, here stated in kPa. Recommended data sources for vapour pressure of substances/mixtures are presented in section 5.1.5. Exposure modifying factors apply to substances in preparations.

5.2.2 Product category and subcategory

ECETOC TRA has a number of predefined product categories and subcategories. There are currently 13 different product categories covering 46 different subcategories, see Annex 7. For these predefined product categories and sub categories, default information on use and exposure conditions have been compiled which make it possible to estimate consumer exposure during use. ECETOC TRA also allows the user to define own product categories with specific use and exposure conditions. However, in ProScale it is recommended to use the predefined product categories when estimating consumer exposure concentrations. If a product category of interest is not addressed by one of the predefined product categories, one shall check if it is possible to approximate the products and its use conditions by one of the predefined product categories. More information on the underlying default information used to estimate consumer exposure can be found in the TRA user guide (ECETOC, 2014 a, b).

5.3 Consumer exposure – Service life

Consumer exposure during service life is estimated differently than exposure during production and use of products, as ECETOC TRA Tier 1 does not include exposure during service life. The inhalation exposure for service life is instead a function of the released amount of a substance and the ventilated air volume according to Equation 5.1 below.

$$\text{Exposure (service life)} = \frac{\text{Released amount [kg])}}{\text{Ventilated air volume}} = \frac{\text{SER[kg / (m}^2\text{h)]} \times \text{Area}_{\text{product}}\ [\text{m}^2] \times \text{Time[h]}}{V_{\text{room}}\ [\text{m}^3] \times \alpha[\text{h}^{-1}] \times \text{Time[h]}} \qquad \textit{(Eq. 5.1)}$$

The released amount of a substance during a given time can be estimated by multiplying the SER (Specific area Emission Rate) (kg/m^{2}h) with the surface area of the product used in the reference room and the given time (hr). SERs can be derived either by measurements using emission chambers or by modelling. There are existing emission models that estimate releases during service life, such as the emission model used by OECD in their Emission Scenario Document on Plastic Additives[7]. As these models have not been validated

7 / http://www.oecd-ilibrary.org/docserver/download/9714291e pdf?expires=1499347493&id=id&accname=guest&checksum=4AE18CC7E85666F 20053F4A7090079BE for use within ProScale, there is no recommendation on what model to use.

The ventilated air volume can be estimated using the volume and the air exchange rate (α) of the reference room multiplied by the given time. According to the standard EN 16516 Construction products: "Assessment of release of dangerous substances - Determination of emissions into indoor air", the volume of the reference room is 30 m^3 and the air exchange rate in the reference room is 0.5 per hour. To achieve the ECF, the exposure as derived above is modified according to Section 5.5.

5.4 Worker exposure – End-of-life

The end-of-life phase of a product's life can often be the least specified within the lifecycle. Unless there is a particular regulatory requirement governing the management of a product at end-of-life, the choice of end-of-life management can be any one of the following:

- Re-use
- Reclaim
- Recycle
- Disposal – Incineration
- Disposal – Landfill

In terms of the ProScale approach, the default assumption for a particular product group may well be already established under the Product Category Rules (PCR) associated with the Environmental Product Declaration, so it is beholding on the ProScale practitioner to investigate the relevant product group and make justified choices for the end of life scenario. It is not the purpose of this Guidance to provide further direction on scenario selection.

However, what is self-evident is that virtually all of the options above will require an intervention (i.e. a decommissioning step). In many cases, this may involve the dismantling of an assembly. Where design has taken end-of-life management into account, the dismantling may be achievable without the de-construction of the component parts. However, in many cases, the decommissioning step may result in compromising the integrity of these parts and additional exposure to chemicals contained therein (e.g. the de-manufacturing of refrigerators).

One of the requirements, therefore, is to understand which substances might be present at this decommissioning (end of service life) stage. For products being assessed by ProScale, the bill of materials should be clear. However, there may be changes in composition occurring during the service life which also need to be considered. Occasionally, this may involve further chemical reaction, in which case the new substances need to be identified. However, more typically, there is likely to be a loss of chemical content during the service life, resulting in a lower chemical content at end-of-life. This can typically be determined by sampling such products at the end of their service life, but where this is not possible, adopting the bill of materials at the beginning of the service life is viewed as a conservative default approach. For the specific case of volatile materials used in the production phase, we can assume at first approximation that they are completely disappeared at the end-of-life of a product during the demolition. Nevertheless, when a volatile material is clearly identified during the decommissioning or demolition phases (e.g. as retained blowing agents in insulation materials), it must be included in the analysis of the end-of-life.

Once the potential for chemical exposure is established for workers in the decommissioning phase, the likely health impacts can be considered. This will need to consider the processes involved in dismantling assemblies and separating the component parts. Often, one of the most significant considerations, especially in the demolition of buildings, is the generation of dust. The health impacts of these physical sources can be as great, or greater, than the chemical hazards faced. Much depends on the method used to dismantle the relevant assemblies. Such processes can be characterised using ECETOC TRA as described below.

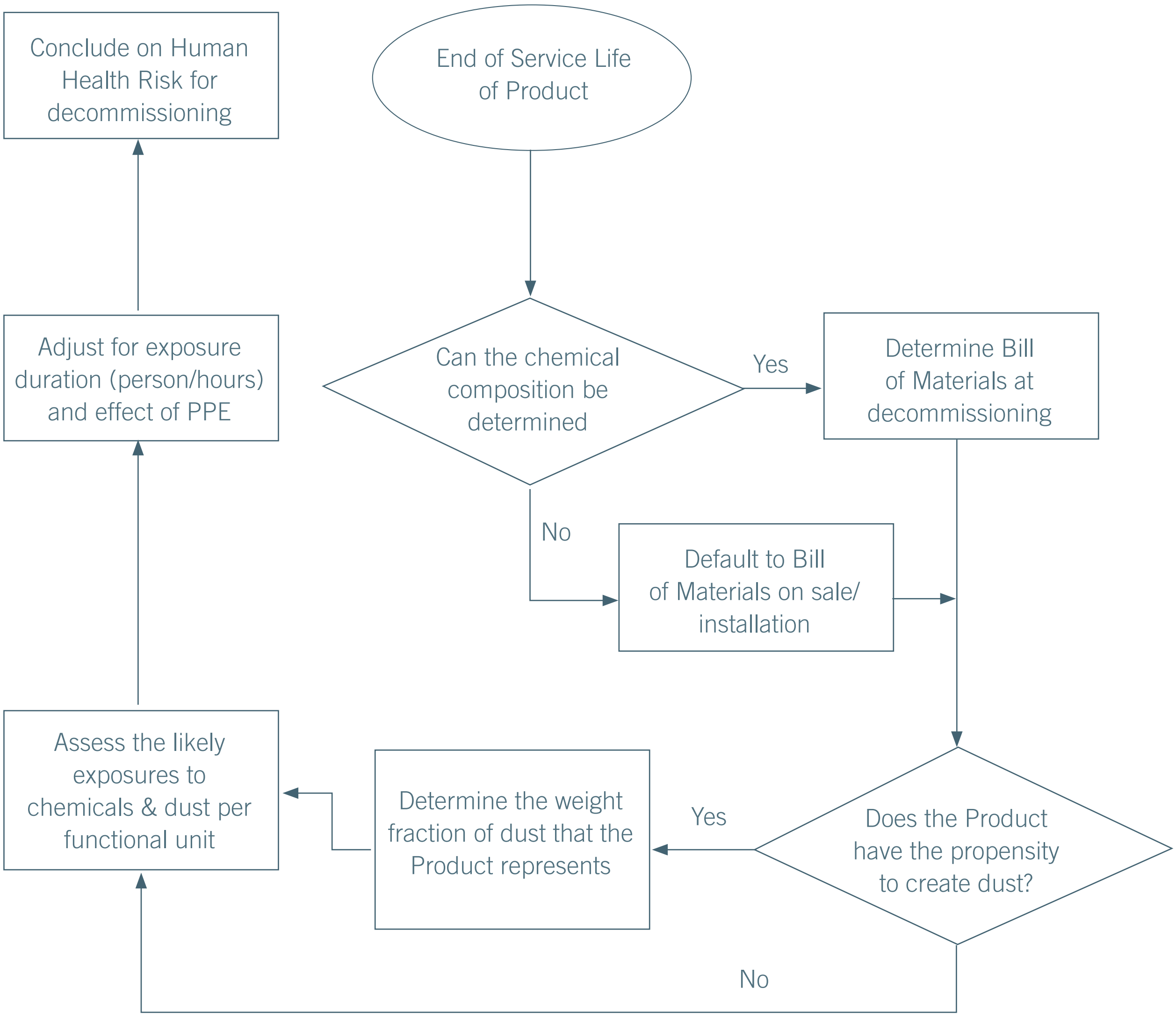
Worker exposure during end-of-life is estimated using the ECETOC TRA Tier 1 approach. This is the same approach as for exposure of workers during production and installation, and a complete description of all the input parameters and how to estimate exposure concentrations is given in section 5.1 above. However, there are no PROCs assigned specifically for end-of-life processes. Table 5 lists PROCs that can be used as proxies for exposure conditions during different end-of-life processes in ProScale[8].

Table 5 End-of-life processes and corresponding PROCs

End-of-life process	PROC
Dismantling	PROC 19/PROC 21
Sorting (manual)	PROC 19/PROC 21
Sorting (automatic)	PROC 24
Shredding	PROC 24
Transfer and transport	PROC 8a / PROC 8b

It should be noted that the focus here is on the decommissioning/dismantling step, not the final choice of end-of-life management, which is likely to be more relevant to long-term environmental impacts and therefore out-of-scope of this current Guidance.

8/ Note: Work is currently ongoing in the ProScale consortium to see if there are other methods available to estimate worker exposure during end-of-life.



In conclusion, the decision-making process can be summarised as follows:

The treatment of dust exposure is a particularly challenging area for assessment, bearing in mind the number of potential contributors. With particle or fibre size being critical components, it is recognised that contributions calculated through simple weight fraction is a default position and that expert judgement should be brought to bear wherever possible to assess the risk and the value of personal protective equipment (PPE).

Second life of a product

For the re-use, reclaim and recycle processes, there is a methodological choice for the sharing of the ProScale impact between the first and second life of the product. The practitioner should document his choice for the end-of-life allocation in a pragmatic way. As an example, in the building sector, the demolition of a product or a building is part of the first life of the building. If the demolition residues need to be sorted, crushed, transported for a further re-use or recycling, these last phases of transformation should be attributed to the second life of the product in the new application. The demolition residues are considered as a waste, and so do not contribute to the environmental burden or inherited ProScale burden of the second life under normal circumstances.

In some cases, if the sampling for chemical content in the demolition residues shows “warning” results, it is recommended to include these chemicals in the new ProScale assessment.

5.5 Numeric transformation and calculation of the Exposure Concentration Factor

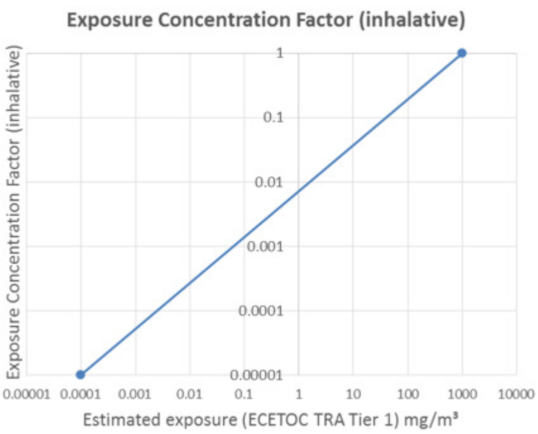
To obtain the Exposure Concentration Factor, the modelled exposure concentration is transformed into a dimensionless factor via a logarithmic transformation function which is route specific. The transformation also gives the Exposure Concentration Factor the same weight as the Hazard Factor. The Exposure Concentration Factor ranges from 10-5 to 1, where a low value means low exposure potential while a high value means high exposure potential.

The logarithmic transformation function is route specific and is based on the range of the modelled exposure for each exposure route, see Table 6. The ranges for inhalation and dermal exposure come from the minimum and maximum values from the ECETOC TRA exposure tool for workers, since the worker exposures were the starting point in ProScale. However, the ECETOC TRA exposure tool for workers does not estimate oral exposure. We then looked at the consumer exposure via the ECETOC TRA exposure for consumers. The consumer tool gives estimates for inhalation, dermal and oral exposure. However, the ranges of exposure for consumers are very large, so it was decided to keep the ranges for inhalation and dermal from the exposure range for workers. For oral exposure, the range is instead based on the minimum and maximum values for oral exposure for consumers, to counter the fact that the worker exposure tool gives no estimate of oral exposure.

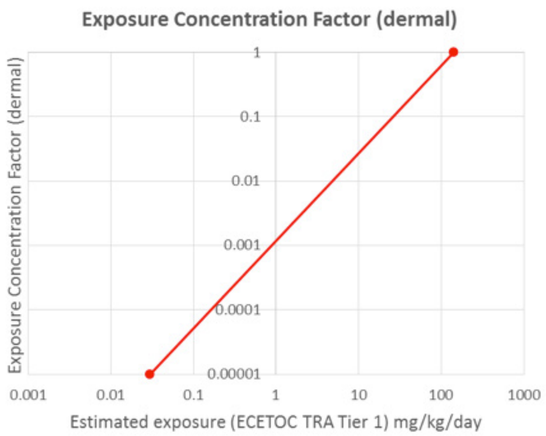
The transformation from modelled exposure to Exposure Concentration Factors is visualised in Figure 8 to Figure 10 below. The transformation functions are incorporated into the ProScale template.

Table 6 Range of modelled exposure for each exposure route

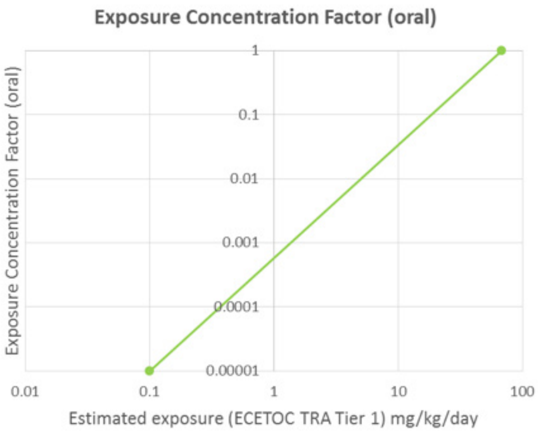
Route of exposure	Exposure concentration	
	Lowest value	**Highest value**
Inhalative (worker exposure)	0.0001 mg/m³	1000 mg/m³
Dermal (worker exposure)	0.03 mg/kg/day	141.43 mg/kg/day
Oral (consumer exposure	0.1 mg/kg/day	67.5 mg/kg/day



>> Figure 8 Transformation of inhalative exposure



>> Figure 9 Transformation of dermal exposure



>> Figure 10 Transformation of oral exposure

6 | Person-Hours Factor

The Exposure Concentration Factor in ProScale is not related to the throughput of the unit process at stake. In order to allow a meaningful aggregation along the life cycle, a Person-Hours Factor (PHF) has been introduced. The PHF connects the Exposure Concentration Factor to the throughput of a unit process, thus transforming the potential exposure concentration to a dose so that the ProScale score can be related to the functional unit.

6.1 Person-Hours Factor – Production and Use

The Person-Hours Factor for production and use of products is an estimate of manpower work needed per kg (or ton) of output of a process. The equations below show how PHFs are calculated for the production and use of products.

$$\text{PHF (production processes) [hr/kg]} = \frac{\text{Annual hours worked [hr / year]}}{\text{Annual production volume [kg / year]}} \quad \textit{(Eq.6.1)}$$

$$\text{PHF (use) [hr/kg]} = \frac{\text{Exposure duration [hr]}}{\text{Amount of product used [kg]}} \quad \textit{(Eq.6.2)}$$

For production processes, the PHF is calculated as a function of annual hours worked and annual production volume. The annual hours worked is in itself a function of the number of full time equivalents for an industrial sector or specific process, multiplied by the number of hours that each full time employee work during a year. This is then related to the annual production volume of that industrial sector or specific process.

Use of products here refers to processes such as painting or installation of a product. The PHF is calculated based on the exposure duration and the amount of product that is used. The exposure duration is in itself a function of how long the product is used and how many people that is exposed during that time.

An example of how to calculate PHFs for production processes is given in section 6.4

6.2 Person-Hours Factor – Service life

PHFs for service life can be derived for products in indoor environments. At this stage, it is not possible to estimate the toxicological potential for products during service life outdoors as PHFs are missing. To calculate PHFs for service life indoors, use Equation 6.3 below.

$$\frac{\text{Population density indoor } \frac{\text{people}}{\text{m}^2} \times \text{Area}_{\text{(reference room)}} \ [\text{m}^2] \times \text{Lifetime of product [hr]}}{\text{Mass of product per reference room [kg]}} \qquad \textit{(Eq.6.3)}$$

The average population density within the EU has been estimated to 0.02 people per m^2 based on a population of 510 million people (Eurostat, 2016) and an indoor area of 25 billion m^2 (EC, 2016) within the EU. The area of the reference room is 12 m^2 according to the standard EN 16516 Construction products: “Assessment of release of dangerous substances - Determination of emissions into indoor air”. An example of how to calculate PHF for service life is given in section 6.4.

For service life, no default values have been derived, as it depends so much on the specific conditions of how the product is used.

6.3 Default Person-Hours Factors

Default Person-Hours Factors have been derived for a number of industrial sectors and processes. These default values have been derived based on information on full time equivalents and throughput per industry sector in a single EU country or the entire EU depending on which information that was available. This information has been obtained from BREF documents, industry associations and environmental reports. Thus, the default Person-Hours Factors represents the manufacturing conditions in EU. Each default PHF is based on data from a number of different manufacturing processes and countries/regions, where the highest value obtained was chosen as the default PHF. The default PHFs have been divided into four different categories; manufacturing processes, filling of different containers, waste management and professional and consumer use. The default Person-Hours Factors are presented in Table 7. If the process of the default PHF covers more than one unit process, and these unit processes are physically separated, the Person-Hours Factor can be divided by the number of unit processes. If the unit processes are not physically divided, the default Person-Hours Factor should be used for each unit process.

In ProScale, the default Person-Hours Factors shall be considered as the primary data source for Person-Hours Factors. If the PHF for a specific process is missing, approximate values for the PHF for that process shall be checked, if it is possible, with one of the existing default Person-Hours Factors. If not, own Person-Hours Factors can be derived using the equations above.

When calculating new Person-Hours Factors, it is recommended to use figures for entire industry sectors rather than using information relating to a single company, so that the PHF represents an industry average. Recommended data sources for information about manpower work and output of a process are:

BREF documents/BAT documents
Industry associations
Company environmental reports

Table 7 Default Person-Hours Factors for different types of processes

Process	Person-Hours Factor (hr/kg)
Manufacturing processes	
Organic commodity chemicals manufacturing, large to medium size chemical plant	1E-03
Organic commodity chemicals manufacturing, small to medium size chemical plant	3E-03
Oil and fuel handling, depot	1E-03
Inorganic chemicals manufacturing, large to medium size chemical plant	6E-03
Fine/specialty chemicals manufacturing, small to medium size chemical plant	1E-03
Plastics manufacturing	3E-03
Plastics processing	1E-03
Mixing and blending batch processes, such as paint manufacturing	2E-02
Oil extraction	4E-04
Portland cement and limestone manufacturing	8E-04
Steel manufacturing	2E-03
Non-ferrous metal manufacturing	2E-02
Transportation by tank ship, tank truck and train	4E-04
Filling	
Filling of an oil tanker	4E-07
Filling, low viscous materials (<100 mPa*s) - drum, can, IBC, tank etc.	4E-06
Filling, middle viscous materials (100-1000 mPa*s) - drum, can, IBC, tank etc.	8E-06
Filling, high viscous materials (>1000 mPa*s) - drum, can, IBC, tank etc.	1E-04
Use (professional and consumer)	
Painting, professional use	2E-01
Painting, consumer use	4E-01
Removing paint from brush with solvent based paint removal - professional or consumer use	2
Service life (consumer)	
No default values derived	
Waste management	
Waste incineration	3E-04

6.4 Examples – Calculating Person-Hours Factors

6.4.1 PHF for a production process

Here, mineral oil refining is used as an example of how to calculate Person-Hours Factors for production processes. According to the Reference Document on Best Available Techniques (BAT) for Mineral Oil and Gas Refineries (IPPC, 2003), the mineral oil refinery sector in EU, Switzerland and Norway has approximately 55000 direct employees and processes around 700 million tonnes oil per year. Here, it is assumed that these employees are full time employees and that a full time employee works approximately 2000 hours per year. Using the figures above and Equation 6.1, a Person-Hours Factor of 1.6×10-4 is obtained for mineral oil refining in the EU. The mineral oil refinery is one of the data sets that have been used to derive the PHF for organic commodity chemicals manufacturing, large to medium size chemical plant (Table 7).

$$\text{PHF (Mineral oil refining) [hr/kg]} = \frac{\text{Annual hours worked [hr / year]}}{\text{Annual production volume [kg / year]}} = \frac{(55\,000 \times 2\,000)}{7 \times 10^{11}} \approx 1.6 \text{ x } 10^{-4}$$

6.4.2 PHF for professional or consumer use

Here, painting of indoor walls is used as an example of how to calculate PHFs for use of products. In this example, it has been assumed that a professional painter works for one hour, during which he paints 15 m^2. For each m^2, approximately 0.3 kg paint is used. Using these figures and Equation 6.2, a Person-Hours Factor of 880 is obtained for

$$\text{PHF (painting) [hr/kg]} = \frac{\text{Exposure duration [hr]}}{\text{Amount of product used}} = \frac{1}{15 \times 0.3} \approx 0.2$$

6.4.3 PHF for service life

The service life of PVC flooring in the reference room is used as an example of how to calculate PHF for service life of products indoor. As mentioned in section 6.2 above, the population density for the EU is approximately 0.02 people per m^2 for indoor environments and the area of the standard room is 12 m^2. It has been assumed that the lifetime of PVC flooring is 10 years which corresponds to approximately

88 000 hours, and that the weight of PVC flooring is approximately 2 kg/m^2 which corresponds to 24 kg of product in the reference room. Using these figures and Equation 6.3, a Person-Hours Factor of 900 is obtained for the service life of PVC flooring in the reference room.

PHF (service life,PVC flooring) [hr/kg]

$$= \frac{\text{Population density indoor } \frac{\text{people}}{\text{m}^2} \times \text{Area}_{\text{(reference room)}} \ [\text{m}^2] \times \text{Lifetime of product [hr]}}{\text{Mass of product per reference room [kg]}}$$

$$= \frac{0.02 \times 12 \times 88\,000}{24} \approx 900$$

7 | Mass Flow

The Mass Flow (MF) in ProScale is included to take into consideration the amount of a substance that is needed for fulfilment of the functional unit of the product/service. When calculating ProScale scores, it is necessary to derive a MF for each substance and unit process.

The MF is derived by looking at the functional unit of the product of study and its bill of materials. The method needs to consider which substances/materials are used in the product and in what amount.

The MFs are calculated by multiplying the mass of the functional unit with the mass fraction of the substance used or produced in a unit process. When multiple unit processes are used, the mass fraction of the inputs need to be multiplied with the mass fractions of the downstream unit processes.

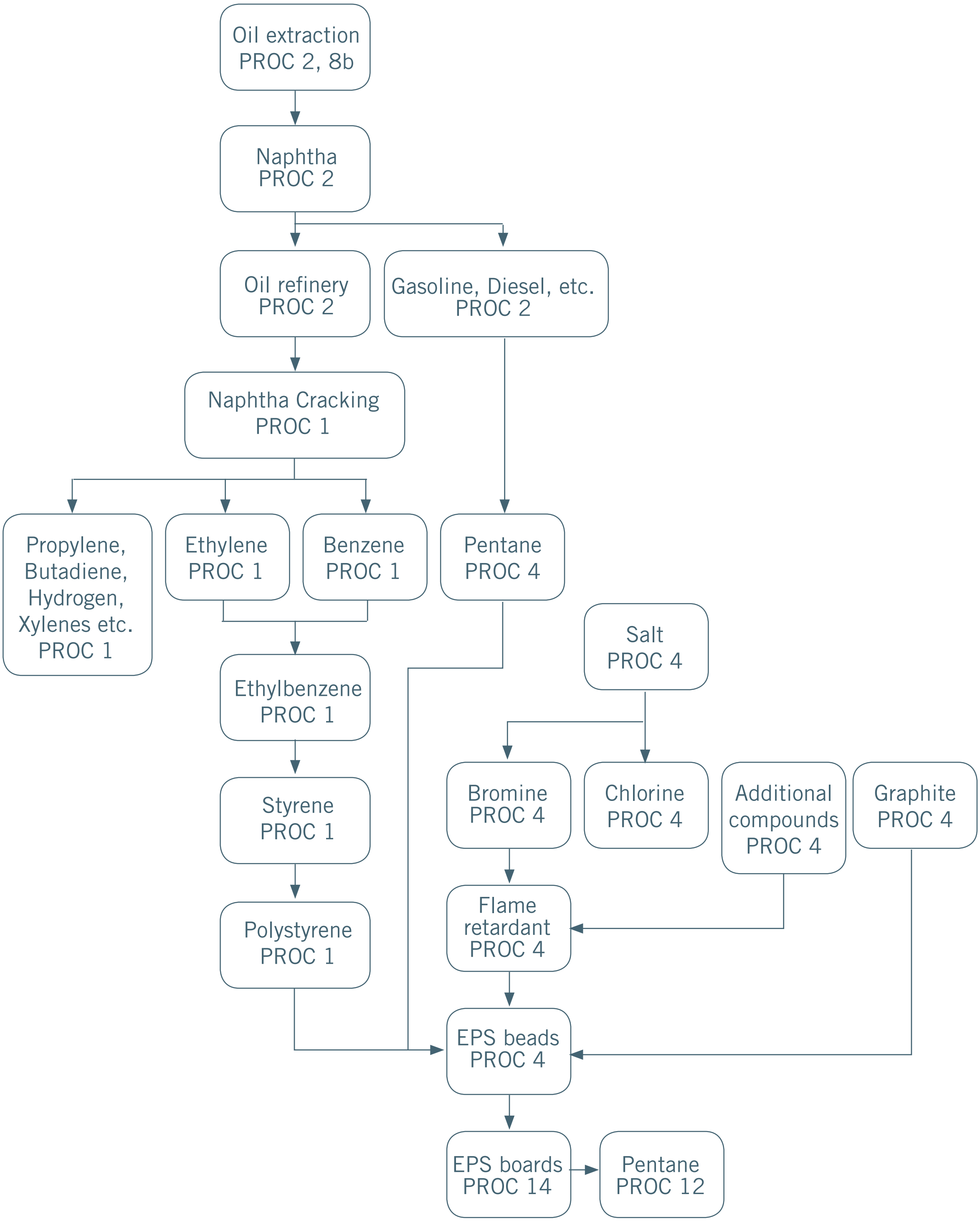
When considering the MFs of all inputs and outputs of a unit process, mass balance shall be obtained for each unit process, i.e. the sum of all input shall be equal to the sum of all outputs for each unit process. If mass balance in not obtained, an input or output might be missing or there is an error in the calculation.

In the case of purchased products the MF can be derived from the mass fractions listed in the relevant SDS of the supplier. In the case of ranges the highest fractions of the relevant components have to be used in the ProScale calculations.

7.1 Example – Calculating Mass Flows

Here, the production of EPS insulating boards will be used to show how to calculate mass flows. This example will calculate mass flows for all inputs and outputs of the four unit processes ethylbenzene production, styrene production, polymerisation EPS and production EPD board. These four unit processes and their inputs and outputs are visualised in the flow chart in Figure 11. The mass fraction of all inputs and outputs for the four unit processes of the example is presented in Table 8. The functional unit for the system is 1 kg EPS board.

The MFs are calculated by multiplying the mass of the functional unit with the mass fraction of the substance used or produced in a unit process. When multiple unit processes are used, the mass fraction of the inputs need to be multiplied with the mass fractions of the downstream unit processes, see calculation examples below for



>> Figure 11 Product system of the EPS insulating board production.

Table 8 Inputs and outputs of four unit processes in the EPS insulating board production

Unit process	Mass fractions - Inputs	Mass fractions - Outputs
Ethylbenzene production	Benzene, 70%	Ethylbenzene, 100%
	Ethylene, 30%	
Styrene production	Ethylbenzene, 102%	Styrene, 100%
		Hydrogen, 2%
Polymerisation EPS	Styrene, 90%	EPS beads, 100%
	Pentane, 5%	
	HBCD, 1%	
	Graphite, 4%	
Production EPS board	EPS beads, 100%	EPS board, 100%

Mass Flows – ethylbenzene production:

MF (benzene,ethylbenzene prod.)=(1×0.9×1.02×0.7)×1=0.64 kg per functional unit

MF (ethylene,ethylbenzene prod.)=(1×0.9×1.02×0.3)×1=0.28 kg per functional unit

MF (ethylbenzene,ethylbenzene prod.)=(1×0.9×1.02×1)×1=0.92 kg per functional unit

Mass Flows – styrene production:

MF (ethylbenzene,ethylbenzene prod.)=(1×0.9×1.02)×1=0.92 kg per functional unit

MF (styrene,ethylbenzene prod.)=(1×0.9×1)×1=0.9 kg per functional unit

MF (hydrogen,ethylbenzene prod.)=(1×0.9×0.02)×1=0.02 kg per functional unit

Mass Flows – polymerisation EPS:

MF (styrene,polymerisation EPS)=(1×0.9)×1=0.9 kg per functional unit

MF (pentane,polymerisation EPS)=(1×0.05)×1=0.05 kg per functional unit

MF (HBCD,polymerisation EPS)=(1×0.01)×1=0.01 kg per functional unit

MF (graphite,polymerisation EPS)=(1×0.04)×1=0.04 kg per functional unit

MF (EPS beads,polymerisation EPS)=(1)×1=1 kg per functional unit

Mass Flows – production of EPS boards:

MF (EPS beads,prod.EPS boards)=(1)×1=1 kg per functional unit

MF (EPS board,prod.EPS boards)=1 kg=functional unit

8 | Calculating ProScale scores

ProScale scores can be calculated on two different levels of aggregation:

- ProScale of Unit process (PSU) – assesses the toxicological potential of all substances in one unit process
- ProScale of Product (PSP) – assesses the toxicological potential of all substances in all unit processes of a product

A PSP can also be defined for a cradle-to-gate system, so that a compound can have a PSP cradle-to-gate score, which includes all upstream processes.

The ProScale scores are route specific, thus a separate score is obtained for each exposure route[9].

The ProScale functions have been incorporated in the ProScale template, so that ProScale users only need to fill in the necessary input information to obtain ProScale scores.

8.1 ProScale of Unit process (PSU)

ProScale of Unit process describes the toxicological potential of all substances « i » in one unit process « u ». A separate PSU is calculated for each exposure route « route ».

$$PSU_{u,\,route} = \sum_i HF_{i,\,route} \times ECF_{i,\,u,\,route} \times MF_{i,u} \times PHF_u \qquad \text{(Eq. 8.1)}$$

If a unit process has multiple outputs, the PSU shall be allocated to the different outputs. By allocating the PSU to the different outputs, the PSU is partitioned between the different outputs so that the PSU is lower when only considering one or some of the outputs compared to all outputs. In ProScale, mass allocation is the chosen default method for allocation, giving all outputs the same PSU per kg output.

8.2 ProScale of Product (PSP)

ProScale of Product describes the toxicological potential of all substances « i » in all unit processes of a product « u ». A separate PSP is calculated for each exposure route « route ».

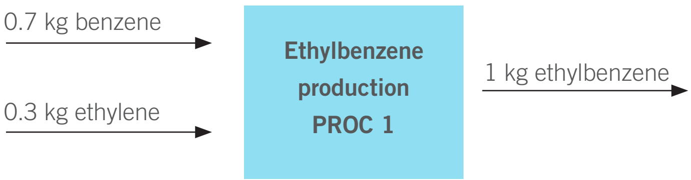
$$PSP_{route} = \sum_u PSU_{u,\,route}$$

$$= \sum_u \sum_i (HF_{i,\,route} \times ECF_{i,\,u,\,route} \times MF_{i,u} \times PHF_u) \qquad \text{(Eq.8.2)}$$

9 / Note: At the moment, it is not possible to aggregate the ProScale scores for different exposure routes to obtain a single ProScale score.

8.3 Example – Calculating PSU

Here, the production of ethylbenzene is used as an example of how to calculate ProScale of Unit process (PSU). Here, the functional unit is 1 kg of ethylbenzene. Benzene and ethylene are reacted in an acid-catalysed reaction to produce ethylbenzene (Figure 12). Approximately 0.7 kg benzene and 0.3 kg ethylene is needed to produce 1 kg of ethylbenzene.



>> Figure 12 Unit process for production of ethylbenzene

All inputs necessary to calculate Hazard Factors and Exposure Concentration Factors for all three substances are presented in Table 9. These values have been obtained by following the instructions in Sections 4 and 5.

Table 9 Inputs for calculation of Hazard Factor and Exposure Concentration Factor for ethylbenzene production in ProScale

Input parameters	Benzene	Ethylene	Ethylbenzene
CAS	71-43-2	74-85-1	100-41-4
H-phrases	H225 H350 (O,D,I) H340 (O,D,I) H372 (O,D,I) H304 (O) H319 (D) H315 (D)	H220 H336 (I)	H225 H332 (I) H373 (O,D,I) H304 (O)
OEL	3.25	247	88
Physical state (Fluid/Solid)	Fluid	Fluid	Fluid
Vapour pressure (kPa)	10	8100	0.952
PROC	1		
Use (Industrial/Professional)	Industrial		
RMM (Yes/No)	No		

By inserting the data in Table 9 in the ProScale template, both Hazard Factors and Exposure Concentration Factors are obtained. The Person-Hours Factor was selected from the list of default Person-Hours Factors (Table 7, Organic commodity chemicals manufacturing, large to medium size chemical plant) and the Mass Flows were obtained from Figure 12.

Table 10 ProScale parameters for Ethylbenzene production

ProScale		Benzene	Ethylene	Ethylbenzene
Hazard Factor	**Inhalative**	1.20E+04	3.35E-01	4.53E+01
	Dermal	1.20E+04	0	4.53E+01
	Oral	1.20E+04	0	4.53E+01
Exposure Concentration Factor	**Inhalative**	2.68E-04	2.68E-04	2.68E-04
	Dermal	1.20E-05	1.20E-05	1.20E-05
	Oral (consumer only)	-	-	-
Person-Hours Factor		1E-03		
PROC		1		
Mass Flow		0.7	0.3	1

PSU for both inhalation and dermal exposure were calculated based on Equation 8.1 and the data in Table 10, see calculations below.

PSU(ethylbenzene prod., inhalative) $= \sum_i HF_{i,\, route} \times ECF_{i,\, u,\, route} \times MF_{i,u} \times PHF_u$

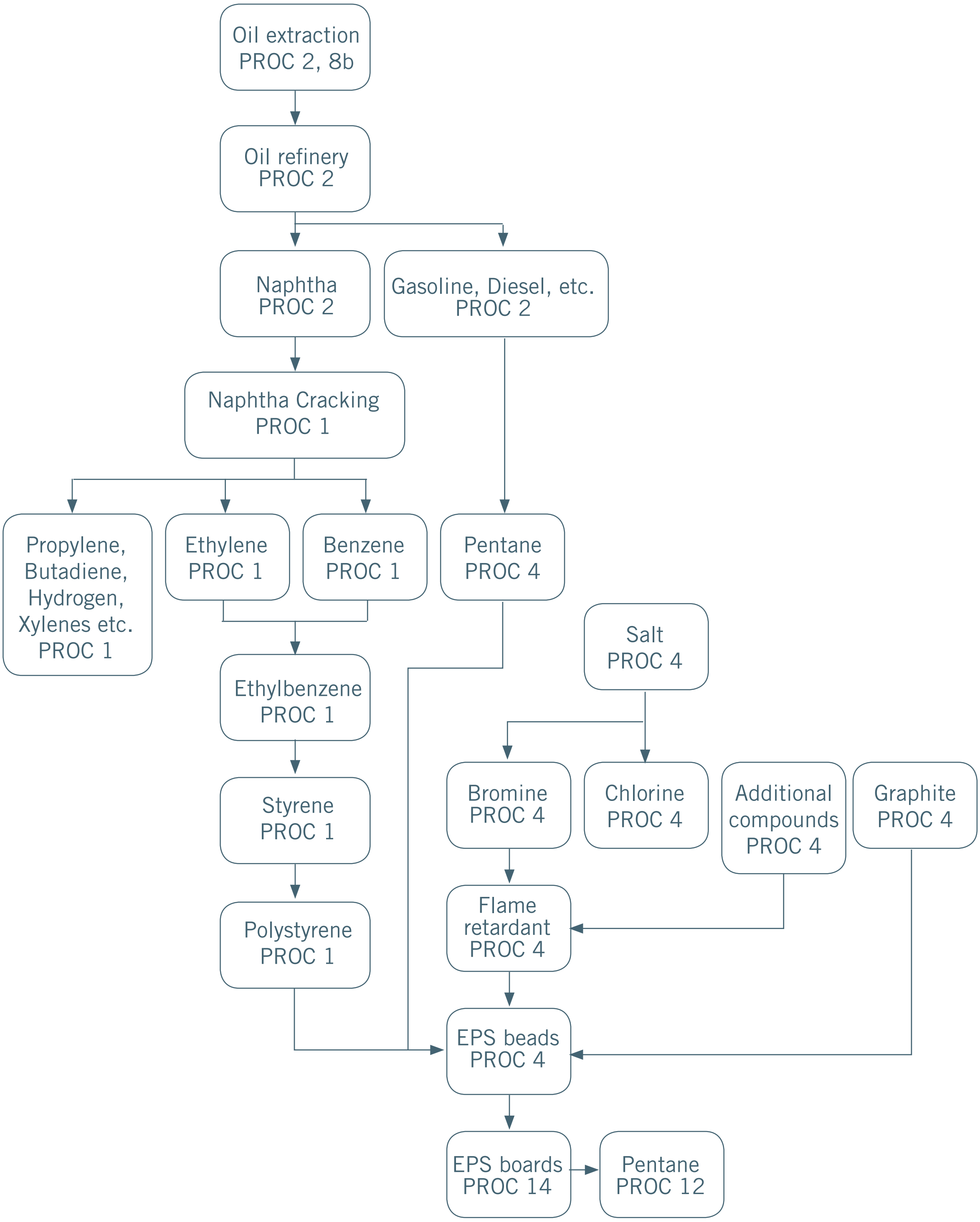
$$=((1.20 \times 10^4 \times 2.68 \times 10^{-4} \times 0.7) + (3.35 \times 10^{-1} \times 2.68 \times 10^{-4} \times 0.3) + (4.53 \times 10^1 \times 2.68 \times 10^{-4} \times 1)) \times 1 \times 10^{-3} = \mathbf{2.26 \times 10^{-3}}$$

PSU(ethylbenzene prod., dermal)$= = \sum_i HF_{i,\, route} \times ECF_{i,\, u,\, route} \times MF_{i,u} \times PHF_u$

$$=((1.20 \times 10^4 \times 1.20 \times 10^{-5} \times 0.7) + (4.53 \times 10^1 \times 1.20 \times 10^{-5} \times 1) \times 1 \times 10^{-3}) = 1.01 \times 10^{-4}$$

8.4 Example – Calculating PSP

The example for insulation boards aggregates all PSU information from cradle-to-gate together when the final insulation boards are produced. It considers the petrochemical steps as well as the blowing agent production, the flame-retardant production and the production of graphite as additional compound in the grey EPS (Polystyrene) board. The subsequent usage of PROCs, H-phrases, concentration factor calculation and Person Hours Factor linked with the mass flows needed along the



>> Figure 13 System boundaries and life cycle steps to produce grey EPS insulation boards without the use-phase and end of life.

whole supply chain are calculated and can be aggregated to a final figure. The pre-chain factors need to be added consequently along the whole life cycle as shown in Table 11.

Figure 13 shows the cradle-to-gate system boundaries for EPS insulation boards.

The results can be shown in different ways. One option is to show all the product contributions linked with the pre-chain, another option is to list the results product by product. Table 11 shows all summarized ProScale factors including the pre-chain. Polystyrene is the most significant material due to the high input to the boards. It is followed by the pentane impact and the flame retardant.

Table 11 ProScale PSP in toxicity points of the insulation materials test case

	Polystyrene	Pentane	Graphite	Flame retardant	Neopor beads	Pentane (board prod)
Inhalation	1,56E-01	9,16E-03	0	1,61E-03	0	9,59E-03
Dermal	1,54E-03	7,91E-05	0	6,37E-06	0	7,91E-05
Oral	0	0	0	0	0	0

Table 12 shows, which materials along the life cycle have the highest impact. That is oil production, followed by the Naphtha input and the Benzene. Polystyrene as material has no direct impact, because it does not have an H-phrase as a material.

Table 12 ProScale PSP in toxicity points of the materials used along the whole life cycle

	Oil	Naphtha	Ethylene	Benzene	Ethyl-benzene	Styrene	Poly-styrene
Inhalation	8,03E-03	3,50E-03	7,49E-08	7,44E-03	3,76E-05	3,71E-04	0
Dermal	3,59E-04	1,56E-04	0	3,33E-04	1,68E-06	1,66E-05	0
Oral	0	0	0	0	0	0	0

9 | Using the ProScale template

The described ProScale methodology is incorporated into an Excel template to facilitate the application to entire life cycles. The Excel template consists of several sheets, which are color-coded as follows:

ProScale template	H-Phrase-Database	EF-Inhalation	PHF-Industrial processes

RED	main sheet for user inputs ("THE" ProScale template)
BLUE	sheets containing data and calculations for the Hazard Factor (HF)
ORANGE	sheets containing data and calculations for the Exposure Concentration Factor (ECF)
PURPLE	sheet containing a Person-Hours Factor (PHF) database for selected industrial processes

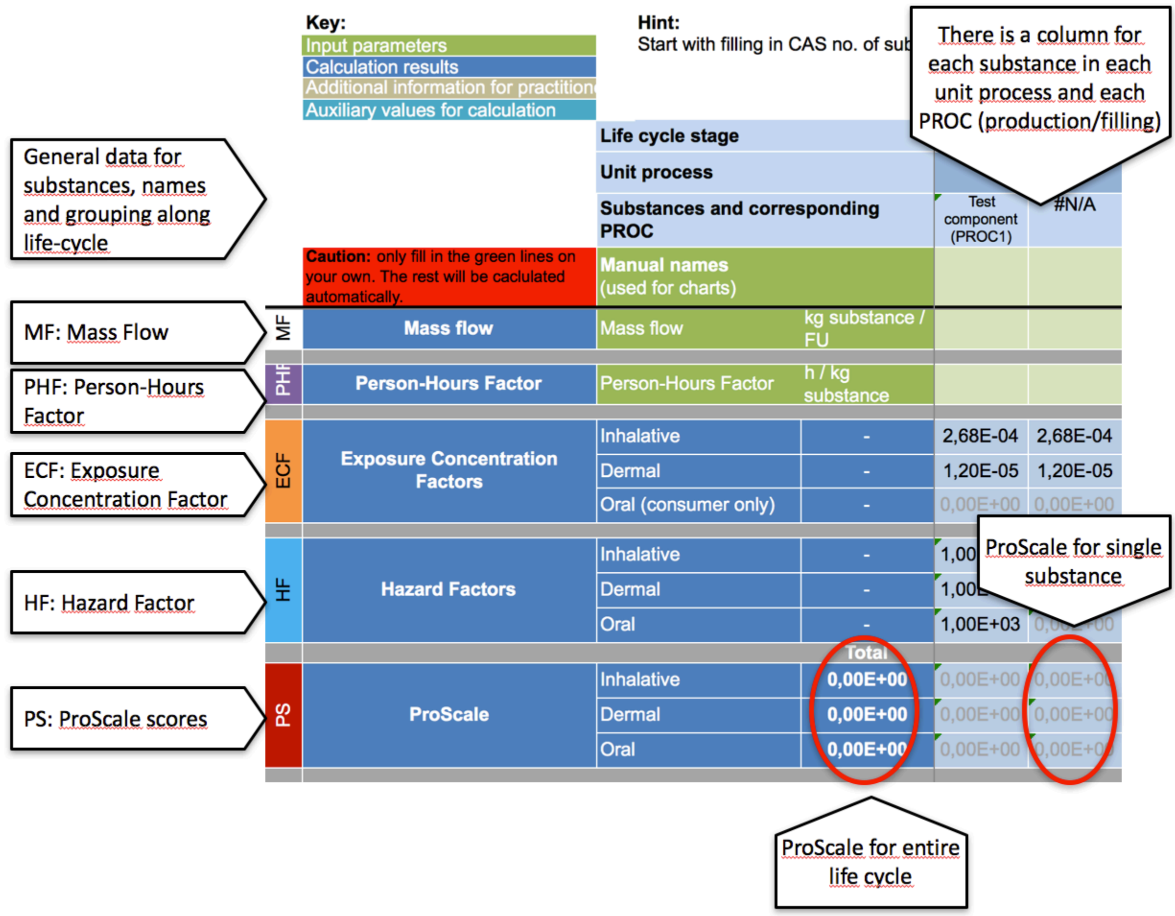
In most cases, it is sufficient to work with the main sheet "ProScale template". In case some substance data are not covered by the included database, manual entries can be made in the sheets "H-Phrase-Database" and "OEL-Database".

9.1 Sheet "ProScale template"

The sheet "ProScale template" is divided into six sections:

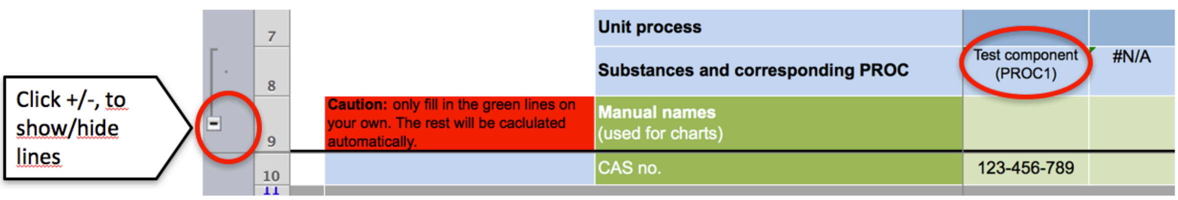
1. General data for substances, names and grouping along life-cycle
2. Mass Flow (MF)
3. Person-Hours Factor (PHF)
4. Exposure Concentration Factor (ECF)
5. Hazard Factor (HF)
6. ProScale scores (PS)

For each substance in each unit process and each PROC (e.g. production or filling PROC), a column has to be filled with the user inputs in sections 1-5 to be able to calculate the ProScale scores (section 6) for each substance and the entire life-cycle.



>> Figure 14 Overview of sheet "ProScale template" (some columns are hidden here for simplicity).

As a starting point, it is recommended to enter the life cycle stages and unit processes as well as the manual names of the substances from a process flow chart (see section 3.3). Then, CAS numbers should be entered for each substance. The template automatically fills in some data (e.g. H-phrases and OEL) if corresponding data exist in the included database. To check whether the substance is in the H-Phrase-Database, look for a substance name entry in line 8 (show line 8 by clicking plus sign).

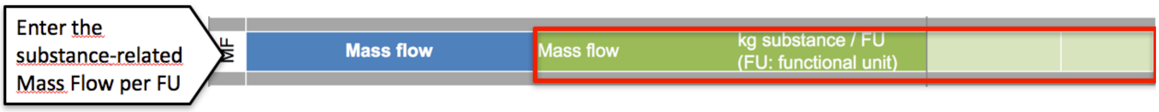


>> Figure 15 Check if substance/CAS no. is in H-Phrase-Database.

If no substance name is generated in line 8, please add your substance and corresponding H-phrases manually in sheet "H-Phrase-Database" (see section 9.2). Please note that substances are not "found" if a substance is listed with more than one CAS no. in the H-Phrase-Database. A workaround for now is to simply add a row in the sheet "H-Phrase-Database" with a single CAS-number and the corresponding H-phrases, just as for a new substance.

9.1.1 Entering Mass flows

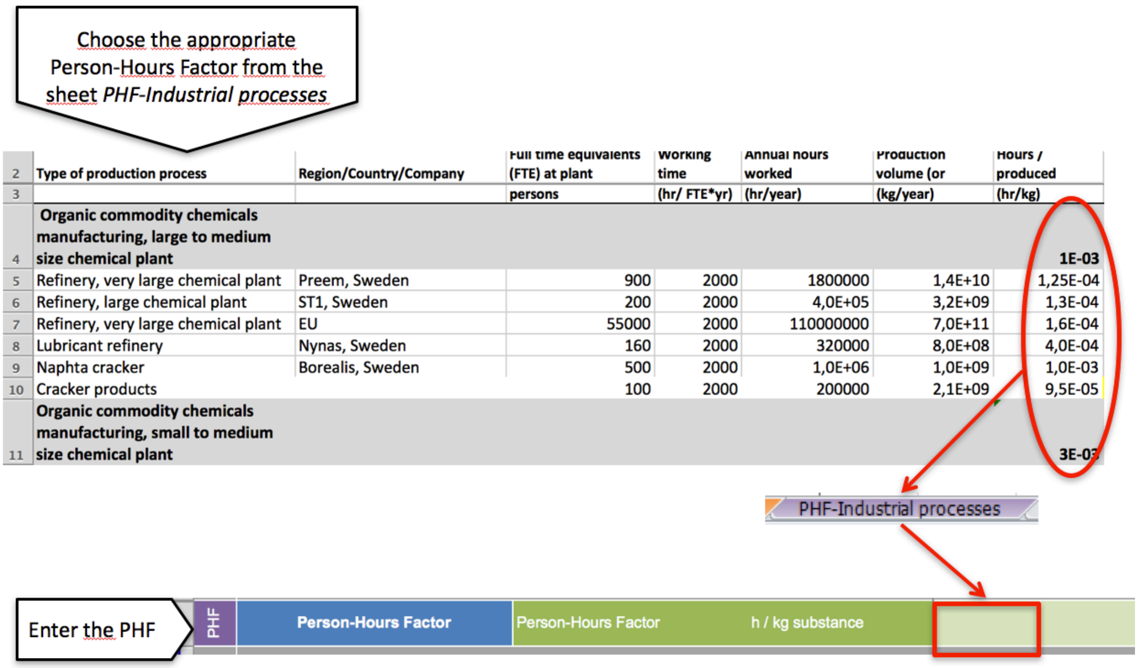
The mass flow for each substance is manually entered in line 14.



>> Figure 16 Enter Mass flows for each substance as amount in kg related to the functional unit.

9.1.2 Entering Person-Hours Factors

The Person-Hours Factors are equal for all substances of a unit process. For the substances of a unit process, choose a Person-Hours Factor, which is appropriate for the corresponding unit process, from the sheet "PHF-Industrial processes".



	Type of production process	Region/Country/Company	Full time equivalents (FTE) at plant persons	Working time (hr/ FTE*yr)	Annual hours worked (hr/year)	Production volume (or (kg/year)	Hours / produced (hr/kg)
2							
3							
4	**Organic commodity chemicals manufacturing, large to medium size chemical plant**						**1E-03**
5	Refinery, very large chemical plant	Preem, Sweden	900	2000	1800000	1,4E+10	1,25E-04
6	Refinery, large chemical plant	ST1, Sweden	200	2000	4,0E+05	3,2E+09	1,3E-04
7	Refinery, very large chemical plant	EU	55000	2000	110000000	7,0E+11	1,6E-04
8	Lubricant refinery	Nynas, Sweden	160	2000	320000	8,0E+08	4,0E-04
9	Naphta cracker	Borealis, Sweden	500	2000	1,0E+06	1,0E+09	1,0E-03
10	Cracker products		100	2000	200000	2,1E+09	9,5E-05
11	**Organic commodity chemicals manufacturing, small to medium size chemical plant**						**3E-03**

>> Figure 17 Enter an appropriate Person-Hours Factor from the sheet "PHF-Industrial processes".

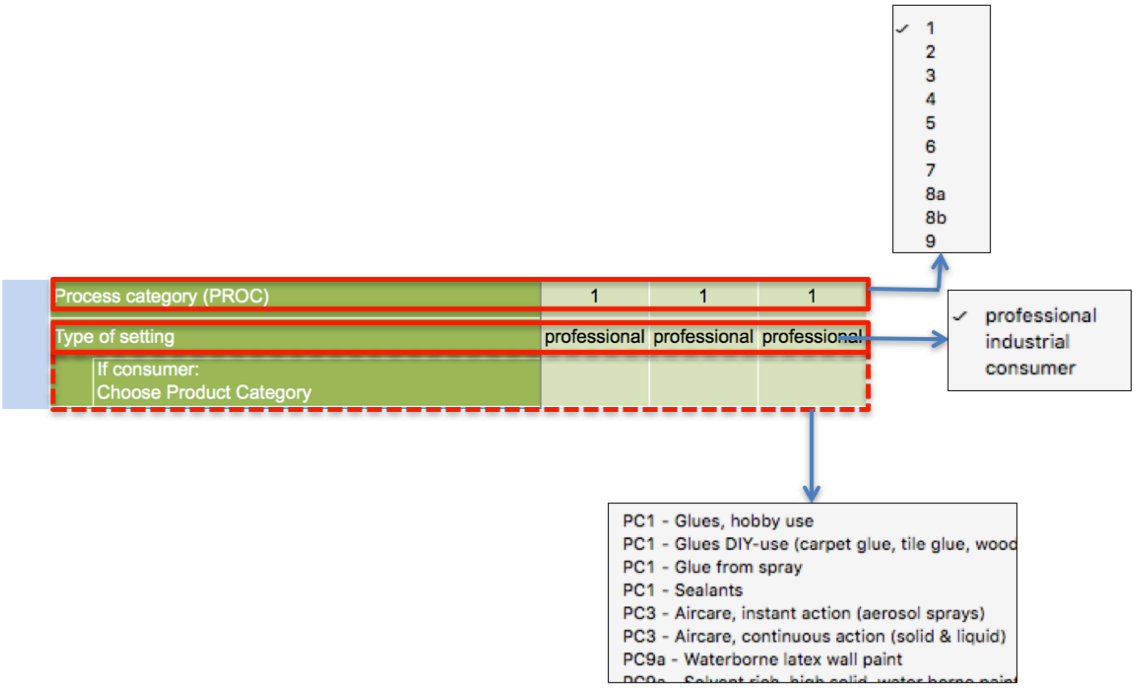
9.1.3 Entering data for Exposure Concentration Factors

Several data have to be entered to be able to calculate the Exposure Concentration Factors (ECF), as illustrated by the green lines in Figure 18.

23	ECF		Process category (PROC)		1	1	1
25			Type of setting		professional	professional	professional
26			If consumer: Choose Product Category				
29			State of substance	fluid (gas & liquid) or solid?	fluid	fluid	fluid
32			If fluid or consumer: Vapour pressure	kPa			
33			If solid: Dustiness of a solid		n/a	n/a	n/a
39		Inhalative exposure	Local Exhaust Ventilation (LEV)		No	No	No
44			Respiratory protection (RP)		No	No	No
45			Final Inhalative Exposure	ppm (volatiles) mg/m³ (solids)	1,00E-02	1,00E-02	1,00E-02
48		Dermal Exposure	Consider LEV for dermal exposure		no	no	no
53			Dermal Personal Protective Equipment (PPE)		No	No	No
54			Final Dermal Exposure	mg/(kg$_{BW}$*day)	3,43E-02	3,43E-02	3,43E-02
55		Oral Exposure	Final Oral Exposure	mg/(kg$_{BW}$*day)			
56		Exposure Concentration Factors	Inhalative	-	2,68E-04	2,68E-04	2,68E-04
57			Dermal	-	1,20E-05	1,20E-05	1,20E-05
58			Oral (consumer only)	-	0,00E+00	0,00E+00	0,00E+00

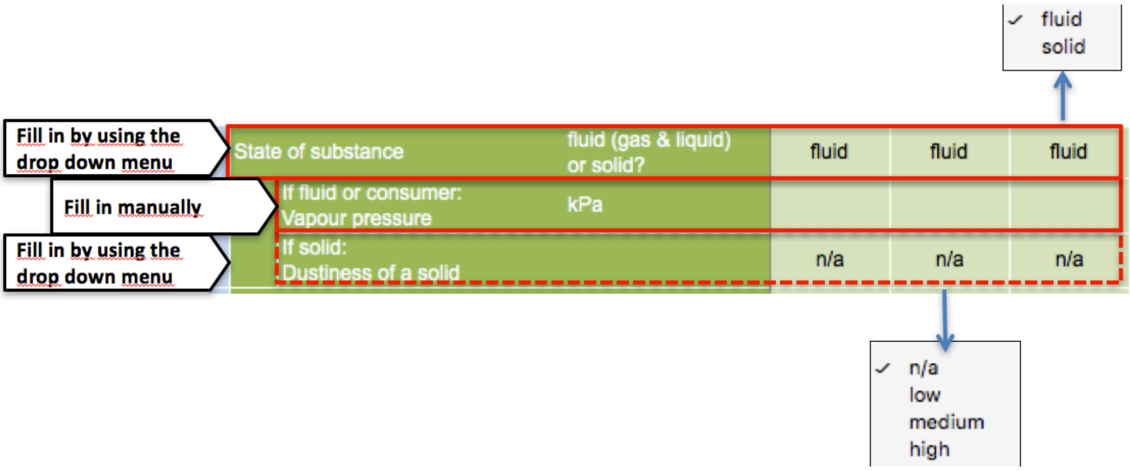
>> Figure 18 Overview of data inputs and outputs for the Exposure Concentration Factors (ECF).

First, enter a Process category (PROC) in line 23 by choosing from the drop-down menu. A description of PROCs can be found in line 21 (show by clicking plus sign on left of line 23) as well as in the (hidden) sheet “PROCs_Aux”. Also choose a type of setting from the drop-down menu in line 25. For “consumer”, please also choose a Consumer Product Category from the drop-down menu in line 26.



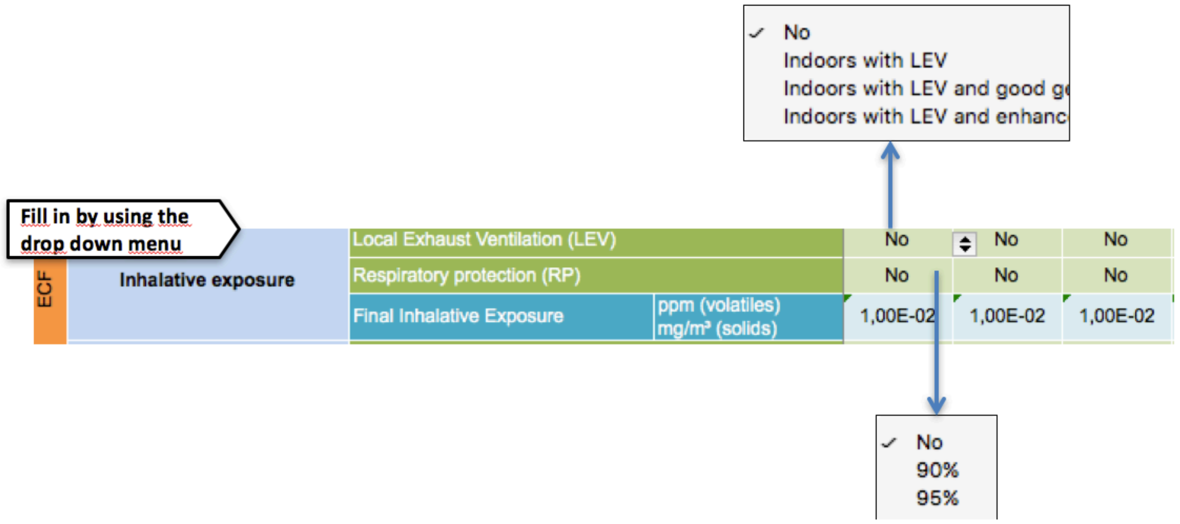
>> Figure 19 Drop-down menus for PROC, type of setting and product category for consumers.

To be able to calculate the inhalation exposure, please fill in data regarding the state of substance, the vapour pressure or the dustiness of a solid (see Figure 20).

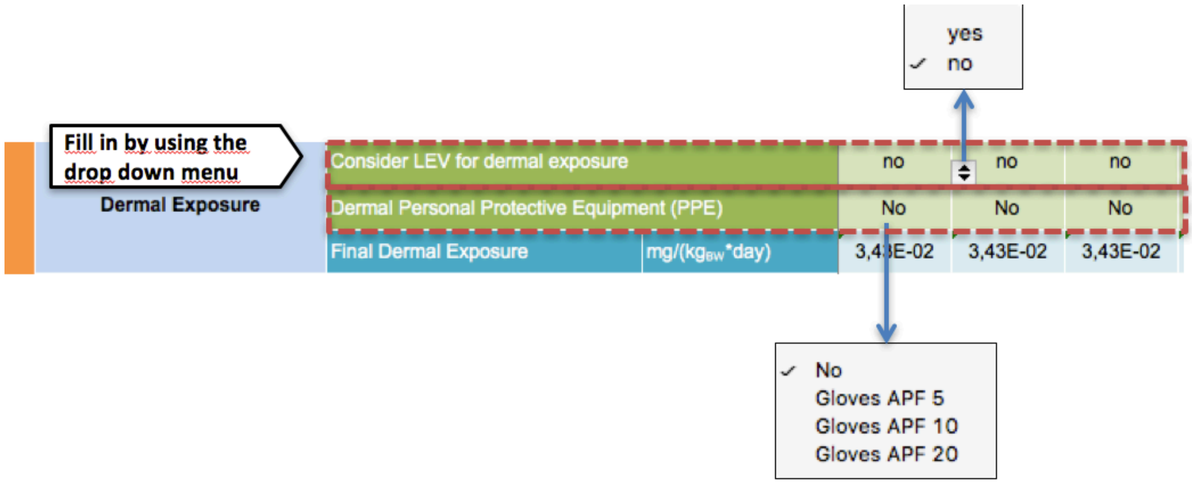


>> Figure 20 Substance data input for calculation of inhalation exposure.

If Risk Management Measures are in place (see section 5.1.4), choose from the drop-down menus for local exhaust ventilation (LEV) and respiratory protection (RP) for inhalation exposure (see Figure 21) and for LEV and personal protective equipment (PPE) for dermal exposure (see Figure 22).



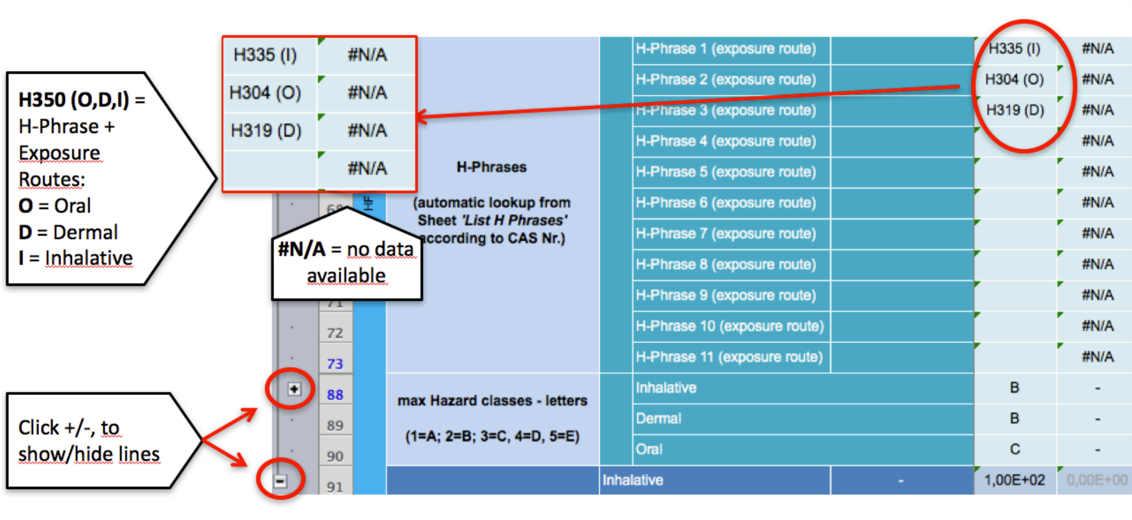
>> Figure 21 Drop-down menus for risk management measures for inhalation exposures.



>> Figure 22 Drop-down menus for risk management measures for dermal exposures.

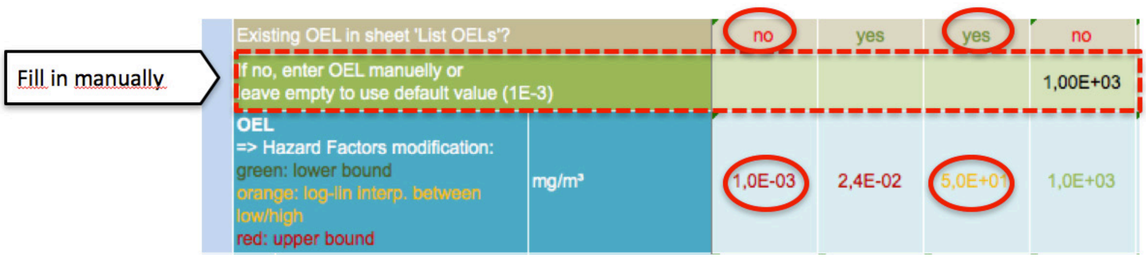
9.1.4 Entering and checking data for Hazard Factors

For Hazard Factor calculation, please check if H-Phrase-Database lists the right H-phrases. To do so, show the H-phrases in the database by clicking the plus signs next to line 91. If “#NV” is shown, no data are found in the H-Phrase-Database. For hazardous substances, please add substance and H-phrases manually (see section 9.2).



>> Figure 23 Check H-phrases as listed in the H-Phrase-Database.

The Hazard Factor (HF) is adapted for substances with a low occupational exposure limit (OEL). The OEL is automatically entered from the OEL-Database if the corresponding CAS no. is listed there. Line 60 shows whether an OEL exists for the substances (yes/no). For no, you can enter an OEL manually in line 61. For yes, you can overwrite the database value by entering a value in line 61. Whether the database or manual OEL value changes the HF is visualized in line 62: green values correspond to the lower bound of the corresponding Hazard Class and red values to the upper bound. Values in-between are indicated in orange.



>> Figure 24 Check OEL as listed in the OEL-Database and change/enter OEL manually.

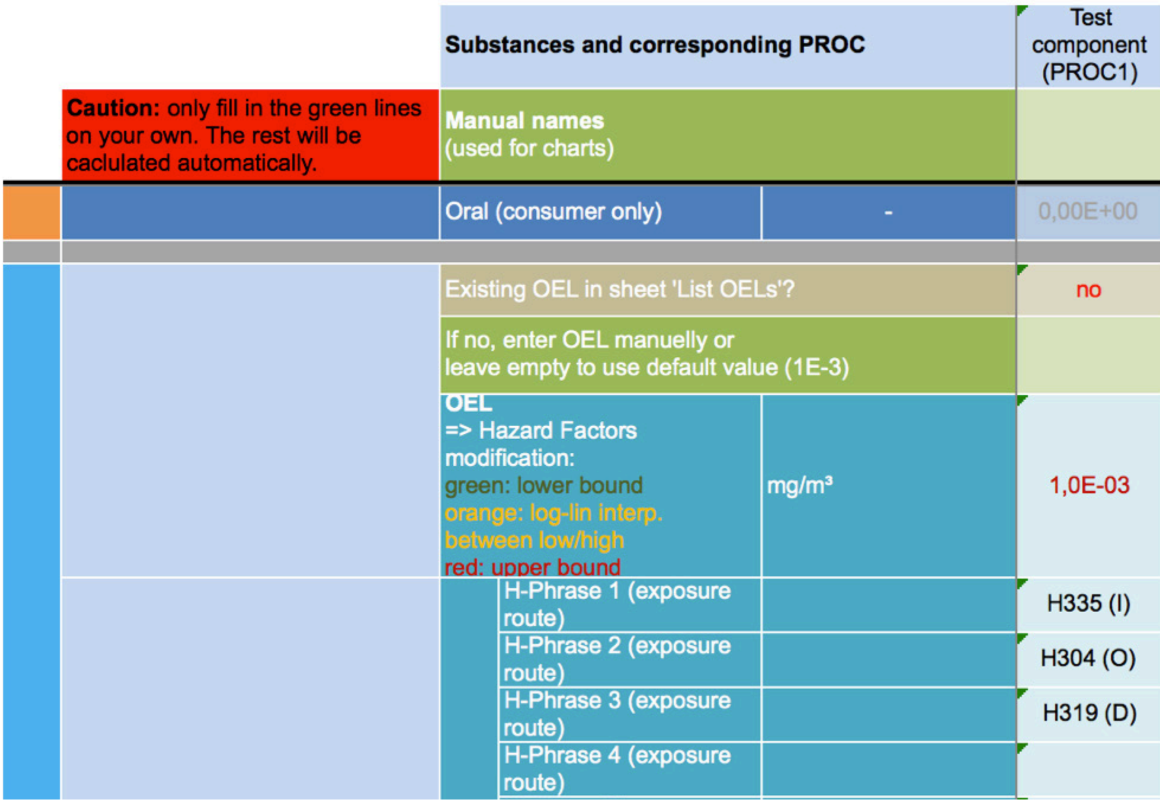
9.2 Sheet “H-Phrase-Database”

The ProScale Excel template (Version 1.4) automatically provides an unofficial excel table containing the substances with harmonised classification and labelling up until the Seventh Adaptation to Technical Progress, i.e. Commission Regulation (EU) No 2015/1221 amending, for the purposes of its adaptation to technical and scientific progress, Regulation (EC) No 1272/2008 of the European Parliament and of the Council on classification, labelling and packaging of substances and mixtures (the CLP Regulation). Therefore, the template so far does not cover the suggested hierarchy of H-Phrase sources.

If substances necessary for a ProScale calculation are not available in the list it is possible to enter additional substances manually. To add an additional substance the sheet “H-Phrase-Database” must be opened. The additional substance should be inserted in the last not used column. An International Chemical Classification, the CAS number and up to eleven H-Phrases must be entered.

Figure 25 Substances can be added to the H-Phrase-Database by manually entering data in the sheet “H-Phrase-Database”. Up to 11 H-phrases can be entered.

The inserted substance can then be used in the “ProScale template” like any other substance. To check whether the substance has been properly integrated into the H-Phrase-Database, look for a substance name entry in line 8 of the “ProScale template” sheet.



>> Figure 26 Screenshot of sheet “ProScale template” visualizing an inserted substance

9.3 Sheet “OEL-Database”

The ProScale Excel template automatically provides the German OEL TRGS900 values. This is a temporary solution following the preliminary hierarchy of OEL/DNEL sources. If no OEL for a given substance is available in the database the following sources can be used and an OEL can manually be entered as described:

1. German OEL TRGS900 (implemented into the template)
2. TLV value
3. European OEL
4. Dutch OEL
5. DNEL from REACH dossier

	A	B	C
1 2	CAS-Nr.	Substance name	OELs (mg/m$^{3)}$
3	75-07-0	Acetaldehyd	9,10E+01
4	67-64-1	Aceton	1,20E+03
5	75-05-8	Acetonitril	3,40E+01
6	107-02-8	Acrylaldehyd	2,00E-01
7	79-10-7	Acrylsäure	3,00E+01
8	309-00-2	Aldrin (ISO)	2,50E-01
9		Alveolengängige Fraktion	1,25E+00
10		Einatembare Fraktion	1,00E+01
11	107-18-6	Allylalkohol	4,80E+00
12	35554-44-0	1-(2-(Allyloxy)-2-(2,4-dichlorphenyl)ethyl)-1H-imidazol ((Imazalil)	2,00E+00
13	2179-59-1	Allylpropyldisulfid	1,20E+01
14	64-18-6	Ameisensäure	9,50E+00
15	141-43-5	2-Amino-ethanol	5,10E+00

>> Figure 27 Screenshot of sheet “OEL-Database”.

10 | References

ECETOC (2009). Addendum to ECETOC Targeted Risk Assessment Report No. 93 - Technical Report No. 107, December 2009. [Online]. Available: http://www.ecetoc.org/technical-reports.

ECETOC (2012) ECETOC TRA version 3: Background and Rationale for the Improvements. Technical Report No. 114. July 2012. [Online]. Available: http://www.ecetoc.org/tra.

ECETOC (2014a) Addendum to TR114: Technical Basis for the TRA v3.1 - Technical Report No. 124. June 2014. [Online]. Available: http://www.ecetoc.org/technical-reports.

ECETOC (2014b). Targeted Risk Assessment: User Guide for the integrated tool TRAM, Version 3 update to version 3.1. June 2014. [Online]. Available: http://www.ecetoc.org/tra.

ECETOC (2014c). Targeted Risk Assessment: Addendum to the User Guide for the Standalone Consumer Tool – Version 3.1. June 2014. [Online]. Available: http://www.ecetoc.org/tra.

ECETOC (2016). Targeted Risk Assessment (TRA) – Targeted Risk Assessment Tool TRA v3.1. Available: http://www.ecetoc.org/tools/targeted-risk-assessment-tra/ [2016-10-10].

ECHA (2015) Guidance on Information Requirements and Chemical Safety Assessment Chapter R.12: Use description (Version 3.0, December 2015). European Chemicals Agency, Helsinki, Finland.

ECHA (2016a). Guidance on information requirements and chemical safety assessment, Chapter R15: Consumer Exposure Estimation (Version 3.0, July 2016). European Chemicals Agency, Helsinki, Finland.

ECHA (2016b). Guidance on Information Requirements and Chemical Safety Assessment Chapter R.14: Occupational exposure assessment (Version 3.0, August 2016). European Chemicals Agency, Helsinki, Finland.

Kalberlah, F., Schmincke, E., Saling, P., de Hults, Q. (2017).Performance indicator for potential health impact Analysis within LCA framework and for Environmental Product Declaration (EPD), Int J LCA, 2017, submitted.

International Organization for Standardization (ISO) (2006a). ISO 14040:2006 Environmental management – Life cycle assessment – Principles and framework. Geneva, Switzerland.

International Organization for Standardization (ISO) (2006b). ISO 14044:2006 Environmental management – Life cycle assessment – Requirements and guidelines. Geneva, Switzerland.

OECD 2009a. DATA ANALYSIS OF THE IDENTIFICATION OF CORRELATIONS BETWEEN POLYMER CHARACTERISTICS AND POTENTIAL FOR HEALTH OR ECOTOXICOLOGICAL CONCERN, ENV/JM/MONO(2009)1, http://www.oecd.org/chemicalsafety/risk-assessment/42081261.pdf

Sheffers , T., Doornaert, B., Berne, N., van Breukelen, B., Leplay, A., van Miert, E. (2016). On the Strength and Validity of Hazard Banding. Ann Occup Hyg. 2016 Nov; 60(9): 1049–1061.

11 | Annexes

Annex 1: Assessment of input data for hazard factor

	H-phrase	OEL	DNEL
Information	Reflects health effect severity	Reflects health effect potency	Reflects health effect potency
Quality	+++ High acceptability, harmonized system. Allows to discriminate SVHC, which is important for the public and stakeholders. Some difference between suppliers but not with CLP Annex VI (harmonized classification) and REACH dossiers.	++ High quality and acceptability as they are established by independent expert groups. May however be a bit less up to date than DNELs. Differences between countries	+ Lower acceptability as more dependent of the supplier of the data. Differences between suppliers.
Availability	+++ Harmonized classification and REACH dossiers are easily available worldwide for all marketed products. Some substance may however be unclassified but however relevant.	+ OEL are easily available but not covering all relevant substances.	++ More DNELs available than OEL.
Regional consideration	+++ Recognized outside of EU US EPA is also considering an approach based on H-phrase and OEL.	++ OEL are used in other regions (US…) but established in different ways. US EPA is also considering an approach based on H-phrase and OEL.	- DNEL are only related to REACH (EU)

Conclusion	It is proposed to use a combination of H-phrase and OEL for the ProScale Hazard Factor. The H-phrase is used to reflect the health effect severity and the OEL as a modifier to reflect the potency. For the H-phrases, following hierarchy is proposed: 1. Disseminated information from the REACH dossiers available via ECHA website: these values have to integrate the harmonized CLP classification but may include additional health hazard based on more recent data. 2. Harmonized CLP classification (CLP Annex VI): these values are harmonized and validated 3. Notified CLP classification from ECHA website considering the 1st row (joint entry or entry with the most notifications). Notification may not always include H-phrase from harmonized classification and REACH dossier and is therefore ranked lower in the hierarchy. 4. SDS from the supplier. SDS from supplier may not always include H-phrase from harmonized classification and REACH dossier and is therefore ranked lower in the hierarchy (equivalent to notified CLP classification). For the OEL, following approaches are proposed: - Ideal solution: a consolidated database of several OEL data sources (German, Dutch, European, American) and possibly DNEL with a selection of the most relevant one. It will be investigated whether such database exists - Temporary solution: 1. German OEL: most easily available. Automatically provided in our excel tool. Following other sources can additionally be used: 2. TLV value 3. European OEL 4. Dutch OEL 5. DNEL as a possibility

Annex 2: Hazard Statements (H-phrases)

Hazard Statement Code	Hazard Statement
H300	Fatal if swallowed
H301	Toxic if swallowed
H302	Harmful if swallowed
H303	May be harmful if swallowed
H304	May be fatal if swallowed and enters airways
H305	May be harmful if swallowed and enters airways
H310	Fatal in contact with skin
H311	Toxic in contact with skin
H312	Harmful in contact with skin
H313	May be harmful in contact with skin
H314	Causes severe skin burns and eye damage
H315	Causes skin irritation
H316	Causes mild skin irritation
H317	May cause an allergic skin reaction
H318	Causes serious eye damage
H319	Causes serious eye irritation
H320	Causes eye irritation
H330	Fatal if inhaled
H331	Toxic if inhaled
H332	Harmful if inhaled
H333	May be harmful if inhaled
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled
H335	May cause respiratory irritation
H336	May cause drowsiness or dizziness
H340	May cause genetic defects
H341	Suspected of causing genetic defects
H350	May cause cancer
H351	Suspected of causing cancer
H360	May damage fertility or the unborn child
H361	Suspected of damaging fertility or the unborn child
H361d	Suspected of damaging the unborn child
H362	May cause harm to breast-fed children
H370	Causes damage to organs
H371	May cause damage to organs
H372	Causes damage to organs through prolonged or repeated exposure
H373	May cause damage to organs through prolonged or repeated exposure
EUH032	Contact with acids liberates very toxic gas (inhalation)
EUH029	Contact with water liberates toxic gas (inhalation)
EUH031	Contact with acids liberates toxic gas (inhalation)
EUH066	Repeated exposure may cause skin dryness or cracking (dermal)
EUH070	Toxic by eye contact (dermal)
EUH071	Corrosive to the respiratory tract (inhalation)

Annex 3 : Product and article categories and subcategories

Code	Name	Explanations and examples
PROC1	Chemical production or refinery in closed process without likelihood of exposure or processes with equivalent containment conditions.	Describes the general nature of processes taking place in sectors where the manufacture of substances or production of mixtures takes place or processes with closed process conditions as applied in chemical industry. The closed transfers inherent to the process including closed sampling are included. Open transfers to charge/discharge the system are not included.
PROC2	Chemical production or refinery in closed continuous process with occasional controlled exposure or processes with equivalent containment conditions	Describes the general nature of processes taking place in sectors where the manufacture of substances or production of mixtures takes place (continuous processes that involve limited manual interventions), or processes with equivalent closed process conditions as applied in chemical industry. The closed transfers inherent to the process including closed sampling are included. Open transfers to charge/discharge the system are not included.
PROC3	Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment condition	Describes the general nature of processes taking place in sectors where the manufacture of substances or production of mixtures takes place (batch processes that involve limited manual interventions) or processes with closed process conditions as applied in chemical industry. The closed transfers inherent to the process including closed sampling are included. Open transfers to charge/discharge are not included.
PROC4	Chemical production where opportunity for exposure arises	Describes the general nature of processes taking place in sectors where the manufacture of substances or production of mixtures takes place (processes where the nature of the design does not exclude exposure). The closed transfers inherent to the process including closed sampling are included. Open transfers to charge/discharge the system are not included.

Code	Name	Explanations and examples
PROC5	Mixing or blending in batch processes	Covers mixing or blending of solid or liquid materials in the context of manufacturing or formulating sectors, as well as upon end use. Charging/discharging of the blending vessel and sampling are considered separate activities and are not included in this PROC.
PROC6	Calendering operations	Processing of large surfaces at elevated temperature e.g. calendering of textile, rubber or paper
PROC7	Industrial spraying	Air dispersive techniques i.e. dispersion into air (= atomization) by e.g. pressurized air, hydraulic pressure or centrifugation, applicable for liquids and powders. Spraying for surface coating, adhesives, polishes/cleaners, air care products, blasting. The reference to 'industrial' means that workers involved have received specific task training, follow operating procedures and act under supervision. Where engineering controls are in place, they are also operated by trained personnel and regularly maintained according to procedures. It is not meant that the activity can only take place at industrial sites.
PROC8a	Transfer of substance or mixture (charging and discharging) at non-dedicated facilities	Covers general transferring operations of large quantities of chemicals from/to vessels, containers, installations or machinery without dedicated engineering controls in place for reducing exposure. Transfer includes loading, filling, dumping, bagging and weighing.
PROC8b	Transfer of substance or mixture (charging and discharging) at dedicated facilities	Covers general transferring operations from/to vessels or containers with provision of dedicated engineering controls in place for reducing exposure: it addresses operations where material transfers are undertaken at locations that are specifically designed and operated for the transfer of larger quantities (tens of kilos and higher) of chemicals and where the exposure is primarily related to the un-coupling/coupling activity rather than the transfer itself. Such situations include tanker loading bays and drum filling. Transfer includes loading, filling, dumping, bagging.

Code	Name	Explanations and examples
PROC9	Transfer of substance or mixture into small containers (dedicated filling line, including weighing)	Filling lines specifically designed to both capture vapour and aerosol emissions and minimise spillage. This PROC can also be used to cover sampling operations.
PROC10	Roller application or brushing	This includes application of paints, coatings, removers, adhesives or cleaning agents to surfaces with potential exposure arising from splashes. This PROC can also be assigned to tasks such as cleaning of surfaces using long-handle tools.
PROC11	Non industrial spraying	Air dispersive techniques i.e. dispersion into air (= atomization) by e.g. pressurized air, hydraulic pressure or centrifugation, applicable for liquids and powders. Includes spraying of substances/mixtures for surface coating, adhesives, polishes/cleaners, air care products, blasting. The reference to 'non-industrial' is to differentiate where conditions mentioned in PROC7 cannot be met. It is not meant that the activity can only take place at non-industrial sites.
PROC12	Use of blowing agents in manufacture of foam	Use of substances to facilitate the process of production of foams by forming gas bubbles in a liquid mixture. It can be either a continuous or a batch process.
PROC13	Treatment of articles by dipping and pouring	Treatment of articles by dipping, pouring, immersing, soaking, washing out or washing in substances; Includes handling of treated objects (e.g. from/to treatment basin, after drying, plating). The service life of the article after the treatment needs to be reported separately.
PROC14	Tabletting, compression, extrusion, pelletisation, granulation	This covers processing of mixtures and/or substances into a defined shape for further use.
PROC15	Use as laboratory reagent	Use of substances at small scale in laboratories (less than or equal to 1 l or 1 kg present at workplace). Larger operations in laboratories and R+D installations should be treated as industrial processes. This includes the use in quality control processes.

Code	Name	Explanations and examples
PROC16	Use of fuels	Covers the use of (solid and liquid) fuel (including additives), including transfers via the closed system, where limited exposure to the product in its unburned form is expected. Assignment of PROC 8 or PROC 9 not needed in this case. The exposure to exhaust gases is not covered.
PROC17	Lubrication at high energy conditions in metal working operations	Covers metal working processes where the lubricants are exposed to high temperature and friction e.g. metal rolling/ forming processes, drilling and grinding, etc. Transfers for refilling or discharging from/to reservoirs are not covered.
PROC18	General greasing / lubrication at high kinetic energy conditions	Use of lubricant or greasing agents in high kinetic energy conditions, including manual application. It does not refer to any filling operation.
PROC19	Manual activities involving hand contact	Addresses tasks, where exposure of hands and forearms can be expected; no dedicated tools or specific exposure controls other than PPE can be put in place. Examples are manual mixing of cement and plasters in construction works or mixing of hair dyes and bleaches.
PROC20	Use of functional fluids in small devices	Includes the filling and emptying of systems containing functional fluids (including transfers via the closed system) e.g. heat and pressure transfer fluids; takes place on routine basis Example: charging and discharging of motor and engine oils, brake fluids, home appliances. Assignment of PROCs 8-9 not needed in this case.
PROC21	Low energy manipulation and handling of substances bound in/ on materials or articles	Cover activities such as manual cutting, cold rolling or assembly/disassembly of material/article. It can also be used for handling/transfer of massive (metal) objects.
PROC22	Manufacturing and processing of minerals and/or metals at substantially elevated temperature	Describes the general nature of processes taking place at smelters, furnaces, refineries, ovens, excluding casting, tapping and drossing operations. When the temperature has decreased , the handling of the cool material can be covered by PROC21 or PROC26.

PROC23	Open processing and transfer operations at substantially elevated temperature	Describes certain processes taking place at smelters, furnaces and ovens: casting, tapping and drossing operations. Covers also hot dip galvanising raking of melted solids in paving and water granulation. When the temperature has decreased, the handling of the cold material can be covered by PROC21 or PROC26.
PROC24	High (mechanical) energy work-up of substances bound in /on materials and/or articles	Substantial thermal or kinetic energy applied to substance by e.g. hot rolling/forming, grinding, mechanical cutting, drilling or sanding, stripping.
PROC25	Other hot work operations with metals	Welding, soldering, gouging, brazing, flame cutting.
PROC26	Handling of solid inorganic substances at ambient temperature	Transfer and handling of ores, concentrates, metals and other inorganic substances in solid (but not massive) potentially dusty form. Assignment of PROC8a, PROC8b or PROC9 not needed in this case. The handling of massive objects should be addressed with PROC21.
PROC27a	Production of metal powders (hot processes)	Production of metal powders by hot metallurgical processes (atomisation, dry dispersion).
PROC27b	Production of metal powders (wet processes)	Production of metal powders by wet metallurgical processes (electrolysis, wet dispersion).
PROC28	Manual maintenance (cleaning and repair) of machinery	Covers maintenance activities for uses where the maintenance is not already included in any of the other process categories. The category covers for example: • activities when closed systems are opened and potentially entered for cleaning • generally dedicated/separate cleaning tasks conducted on a shift or less frequent basis (e.g. between individual production batches) • removal of splashes around the machinery removal of filters or material from filters • cleaning of floors that are not directly around the machinery, but still need cleaning for instance because of dust deposition when handling a dusty product

Annex 4: Product and article categories and subcategories

Product/article category	Product/article sub-category
PC1:Adhesives, sealants	Glues, hobby use
	Glues DIY-use (carpet glue, tile glue, wood parquet glue)
	Glue from spray
	Sealants
PC3:Air care products	Aircare, instant action (aerosol sprays)
	Aircare, continuous action (solid & liquid)
PC9a: Coatings, paints, thinners, removers	Waterborne latex wall paint
	Solvent rich, high solid, water borne paint
	Aerosol spray can
	Removers (paint-, glue-, wall paper-, sealant-remover)
PC9b: Fillers, putties, plasters, modelling clay	Fillers and putty
	Plasters and floor equalizers
	Modelling clay
PC9c: Finger paints	Finger paints
PC12: Fertilizers	Lawn and garden preparations
PC13: Fuels	Liquids
PC24: Lubricants, greases, and release products	Liquids
	Pastes
	Sprays
PC31:Polishes and wax blends	Polishes, wax / cream (floor, furniture, shoes)
	Polishes, spray (furniture, shoes)
PC35:Washing and cleaning products (including solvent based products)	Laundry and dish washing products
	Cleaners, liquids (all-purpose cleaners, sanitary products, floor cleaners, glass cleaners, carpet cleaners, metal cleaners)
	Cleaners, trigger sprays (all-purpose cleaners, sanitary products, glass cleaners)
AC5:Fabrics, textiles and apparel	Clothing (all kind of materials), towel
	Bedding, mattress
	Toys (cuddly toy)
	Car seat, chair, flooring

Product/article category	Product/article sub-category
AC6: Leather articles	Purse, wallet, covering steering wheel (car)
	Footwear (shoes, boots)
	Furniture (sofa)
AC8: Paper articles	Diapers
	Sanitary towels
	Tissues, paper towels, wet tissues, toilet paper
	Printed paper (papers, magazines, books)
AC10: Rubber articles	Rubber handles, tyres
	Flooring
	Footwear (shoes, boots)
	Rubber toys

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